University of Venda
Creating Future Leaders

UNIVERSITY OF VENDA,
THOHOYANDOU, LIMPOPO PROVINCE,
SOUTH AFRICA

University of Venda

SCHOOL OF MATHEMATICAL AND NATURAL SCIENCES

DEPARTMENT OF CHEMISTRY

COMPUTATIONAL STUDIES OF SULFONYLUREAS MOLECULES

BY

VUKEYA THEMBANI SILAS,

STUDENT NUMBER: 11628584

This thesis is submitted in fulfilment of the requirements for the degree of Master's in chemistry.

SUPERVISOR: PROF. LILIANA MAMMINO
Department of Chemistry, University of Venda,
Thohoyandou, South Africa

CO-SUPERVISOR: Dr. CATERINA GHIO
Institute for Physico-Chemical Processes,
Molecular Modelling Lab, Pisa, Italy

April 2021

Declaration

I, Thembani Silas Vukeya hereby declare that this thesis for the award of a Master's degree in Chemistry, submitted by me, has never previously been submitted for a higher degree or diploma at this or any other University. And that to the best of my knowledge and belief, the thesis contains no material previously published or written by another person except where due reference is made in the thesis itself.

Signature: …………………………… Date: 20 July 2021

Acknowledgements

I would like to acknowledge the following for the help and support they provided:

- Professor L. Mammino (supervisor)
- Dr. Caterina Ghio (Co-supervisor)
- Mrs. M.K. Vukeya (Mother)
- My family
- Ms. N. Tshilande
- Dr S.S. Mnyakeni Moleele (HOD of chemistry department)
- Mr. D.O. Sipoyo
- My friends
- Sasol-NRF foundation for funding.
- Centre for High Performance Computing (CHPC) for allowing me access to utilize their platform to perform calculations

Abstract

Computational studies are very important for biologically active molecules and for the development of new drugs, because the biological activities depend on their molecular structures and properties. This work presents the results of a conformational study of selected sulfonylureas molecules in *vacuo*. Sulfonylureas are a class of synthetic organic compounds containing a thiourea group (sulfonyl and urea groups bonded together) attached to a benzene ring, a substituent (R) on the thiourea, and another substituent (R′) linked to the benzene ring by a two– or three–carbon atom chain attached to an oxygen atom which is directly attached to the benzene ring in para position with respect to the thiourea group. The interest in this class of compounds is that some compounds are used in the treatment of type 2 diabetes. Molecules with different R and R′ substituents have been considered. Full-optimization calculations were performed in *vacuo* using Density Functional Theory (DFT) and Hartree Fock (HF) methods. Attention was given to the identification of stable conformers of each of the molecules considered (obtainable by rotation of relevant bonds) and of the conformers' stabilizing factors. The molecular properties considered include the relative energies of the conformers, the parameters of the intramolecular hydrogen bonds (IHBs), the dipole moments, the HOMO–LUMO energy gaps, and the vibrational frequencies of relevant bonds (in particular, the N–H bonds, because the N–H groups may be IHB donors).

The results indicate that the number and type of IHBs are the major stabilizing factors. A maximum of three simultaneous IHBs are possible in the thiourea group. This includes the presence of bifurcated IHBs (bifurcation on the hydrogen atom of the donor), which are present in most of the stable conformers. The vibrational frequencies of the N–H bonds show changes occurring when these bonds form IHBs. The changes showed a rare phenomenon, that is, a blue shift (frequency increase) for certain IHBs, and also a much more common phenomenon (red shift. i.e., frequency decrease) for other IHBs. The geometry of the thiourea moiety, the nature of R and R′, the orientation and the length of the chain between the benzene ring and R′ also show some influence on the calculated molecular properties.

Acronyms

ATP: Adenosine triphosphate

CHPC: Centre for High Performance Computing

DFT: Density Functional Theory

DME: Diabetic macular edema

GGA: Generalized gradient approximation

GTOs: Gaussian type orbitals

HF: Hartree-Fock

HOMO: Highest Occupied Molecular Orbital

IHB: Intramolecular Hydrogen Bond

KATP: ATP-dependent K^+

LCAO: Linear Combination of Atomic Orbitals

LDA: Local Density Approximation

LUMO: Lowest Occupied Molecular Orbital

MP2: Møller-Plesset second order Perturbation Theory

MOs: Molecular Orbitals

NPDR: Non-proliferative diabetic retinopathy

PAD: Peripheral artery disease

PDR: Proliferative diabetic retinopathy

QSAR: Quantitative Structure–Activity Relationship

SCF: Self-Consistent Field

STOs: Slater Type Orbitals

PES: Potential energy surface

ZPE: Zero Point Energy

List of figures

List of tables

Table of contents

Chapter 1

Introduction

This chapter provides information about the objectives and justification of the study presented in this thesis, the computational methods utilised, and the organization of the material in this thesis.

1.1. Background information

This thesis presents the results of a computational study of selected sulfonylureas (figure 1.1). Sulfonylureas are synthetic organic compounds which are used in medicine as antidiabetic drugs. They are used for the treatment of type 2 diabetes [1]. They are commonly classified as first and second-generation sulfonylureas [2]. These compounds stimulate the production of insulin in the body. Some of them were found to have severe side effects; therefore, there is a need to search for new compounds which will work effectively with minimal or no side effects. The search for new antidiabetic drugs is very important because diabetes can lead to severe or life-threatening complications, including blindness and amputations.

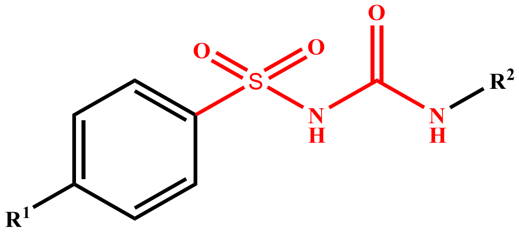


Figure 1.1. General structure of the sulfonylureas molecules

Since the biological activities of molecules depend on their molecular properties, it is essential to find detailed information about the molecular properties of the compounds of interest. This information is relevant to understand the action of the given molecules, and in the development of new molecules (from drug design), and it is obtained through computational studies.

This work focuses on the computational study of 36 new selected sulfonylureas. These compounds are being considered for synthesis by organic chemistry researchers at the University of Venda.

Figures 1.2 shows the general structures of the two classes of sulfonylureas molecules investigated in this study. Six different substituents are considered for the R group (substituent attached to the sulfonylurea moiety) and three different substituents are considered for the R′ group (substituent attached to a carbon atom chain attached to an oxygen atom bonded to the benzene ring). Although the nitrogen atom (N) is part of R′, it is indicated individually in the structures for clarity reasons.

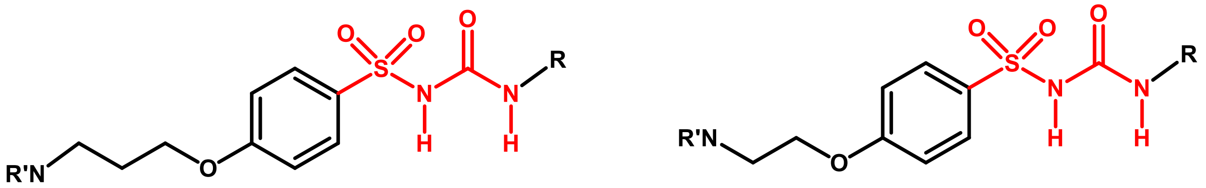


Figure 1.2. General structures of the sulfonylureas molecules considered in this study. The two structures differ by the length of the chain between the oxygen atom attached to the benzene ring and the nitrogen atom belonging to R′.

1.2. Objectives of the study

The broad objective of the study is to obtain information about the selected sulfonylureas molecules. The specific objectives are the following:

- To identify the stable conformations of the selected sulfonylureas molecules, considering all the possible geometries obtainable by rotations about relevant single bonds.
- To identify the conformers’ stabilizing factors.
- To determine the molecular properties of these molecules, such as conformational preferences, characteristics of intramolecular hydrogen bonds (IHBs), dipole moments, HOMO-LUMO energy difference, and IR vibrational frequencies of relevant bonds.
- To compare the molecular properties of different molecules in order to identify the effects of the various R and R′ substituents considered and, possibly, also to identify trends or patterns in these effects.

1.3. Justification of the study

Research on drugs for the treatment of diabetes is important because of the high number of people affected by the disease and the high number of deaths it causes. This work falls within a world-wide active search for improved sulfonylureas molecules for the treatment of diabetes, where 'improved' refers mostly to a decrease in the drawbacks of currently-used sulfonylureas, i.e., the occurrence of hypoglycemia episodes and the gradual decrease in the pancreas response to the drugs. An option for trying to improve on known drugs involves modifications of the molecular structure by using different substituents.

As already mentioned, the biological activity of molecules depends on their molecular properties; therefore, it is important to know as much as possible about these properties. In modern chemistry, there is an increasing tendency to interface experimental and computational research, as computational research can provide information that is useful for the interpretation of experimental findings. This work follows this trend and aims at providing new information which will add to the information currently available on sulfonylureas and may also contribute to the interpretation of the results of an experimental project conducted by other researchers in the same institution.

1.4. Computational methods and materials used

Electronic structure methods are selected for the molecular calculations in this study because they give more reliable information than non-quantum methods [3]. Both ab initio and Density Functional Theory (DFT) methods were used. This is because the use of different methods provides more complete information through the comparison of their results. For the ab initio calculations, the Hartree-Fock (HF) method was used with the 6-31G(d,p) basis set. The B3LYP functional with the 6-31+G(d,p) basis set was used for the DFT calculations. All the calculations were carried out with full geometry optimization (fully relaxed geometry), to identify stable conformations for each input geometry.

The Gaussian 16 [4] software was used for all the calculations, and GaussView [5] was used for visualization.

1.5. Organization of the materials

This thesis is organized in 6 chapters and an appendix, with the following roles:

Chapter 1 provides a quick background information about sulfonylureas, the justification and the objectives of the study and the tools and methods used for it.

Chapter 2 provides the theoretical background of the computational methods used in the study of molecules and information about molecular properties that can be calculated.

Chapter 3 provides information from literature on diabetes and on the sulfonylureas molecules.

Chapter 4 provides the results obtained in this study and their analysis and discussions.

Chapter 5 provides overall discussions and conclusions based on all the observation noted during the analysis of the results reported in chapter 4, and considerations for future studies on the same class of molecules.

Chapter 6 presents most of the tables reporting numerical results, and most of the figures showing the obtained optimized molecular geometries, selected molecular orbitals, and comparison diagrams for relevant values. They are grouped in a separate chapter because they are very bulky, and they would disrupt the readability of the text if inserted in it.

Literature references for the whole thesis are listed after chapter 6.

Appendix A presents additional tables that may be useful for the analysis of some results.

Chapter 2

Theoretical background

2.1. Importance of the computational study of molecules

The computational study of molecules is important for determining molecular properties such as conformational preferences, geometry (bond lengths, bond angles and dihedral angles), dipole moments, molecular orbitals, and others. This study is important for molecules that are biologically active because biological activities depend on the molecular properties. It is particularly useful for the determination of molecular properties that are inaccessible experimentally, and it can help establish better understanding of the activities of biologically active molecules. It can also enable us to predict the molecular properties of molecules that have not yet been synthesized.

2.2. The description of molecules

A molecule is a stable assembly of nuclei and electrons. We can see it as being made of atoms. Each molecule is characterized by its composition (type and number of atoms), by its structure (arrangement of atoms in the molecule) and by properties that depends on the structure [6, 7]. The molecular structure can be determined experimentally using different spectroscopic techniques [8-11]. The chemical and physical properties of substances are different due to different molecular properties [12].

A molecule can take many geometries, with each geometry defined by three sets of parameters, i.e., bond length, bond angles and dihedral angles.

A bond length is defined as the average distance between the nuclei of two bonded atoms and it is expressed in Angstrom (1 Å = 10^{-10} m) or pico-meter (1 pm = 10^{-12} m) [9]. In a molecule, we consider a bond length for each pair of bonded atoms. For example, the bond lengths of the ethane molecule (figure 2.1) are the following distances: C1–C2, C1–H3, C1–H4, C1–H5, C2–H6, C2–H7, C2–H8. The bond length is influenced by the size of the bonded atoms and by the multiplicity of the bonds. The bigger the atom size, the longer the bond length, and the smaller the atom size, the shorter the bond length. When the number of bonds between two bonded atoms increases, the bond length between them decreases [13, 14]. For instances, the length of the C–C single bond (1.54 Å) is greater than the length of the C=C double bond (1.34 Å), which is greater than the length of the C≡C triple bond (1.20 Å).

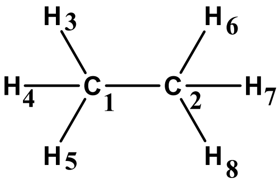


Figure 2.1. Structure of the ethane molecule.

A bond angle (θ) is the average angle between two consecutive bonds, that is, it is the angle identified by three subsequently bonded atoms [13, 15]. For example, the bond angles of the ethane molecule (figure 2.1) are the following: C1–C2–H6, C1–C2–H7, C1–C2–H8, C2–C1–H3, C2–C1–H4, C2–C1–H5, H3–C1–H4, H3–C1–H5, H4–C1–H5, H6–C2–H7, H6–C2–H8, H7–C2–H8. Bond angles are influenced by the hybridization of atomic orbitals, the presence of lone pairs of electrons and the electronegativity of the atoms. When the s- character of hybrid orbitals increases, the bond angle between two consecutive bonds increases. For example, the angle between two sp^3 hybrid orbitals is 109.5°, the angle between two sp^2 hybrid orbitals is 120° and the angle between two sp hybrid orbitals is 180°. The lone pairs of electrons tend to occupy more space than the pairs engaged in a bond; therefore, each lone pair tries to "squeeze" the bonded pairs closer to each other and the bond angle decreases. The higher the number of lone pairs, the smaller the angle between the bonds. An example is shown in figure 2.2: the $H\hat{C}H$ bond angle in the methane molecule (with no lone pairs) is 109.5°; the $H\widehat{N}H$ bond angle in the ammonia molecule (with one lone pair) is 107.0°; and the $H\hat{O}H$ bond angle in the water molecule (with two lone pairs) is 104.5° [15-18].

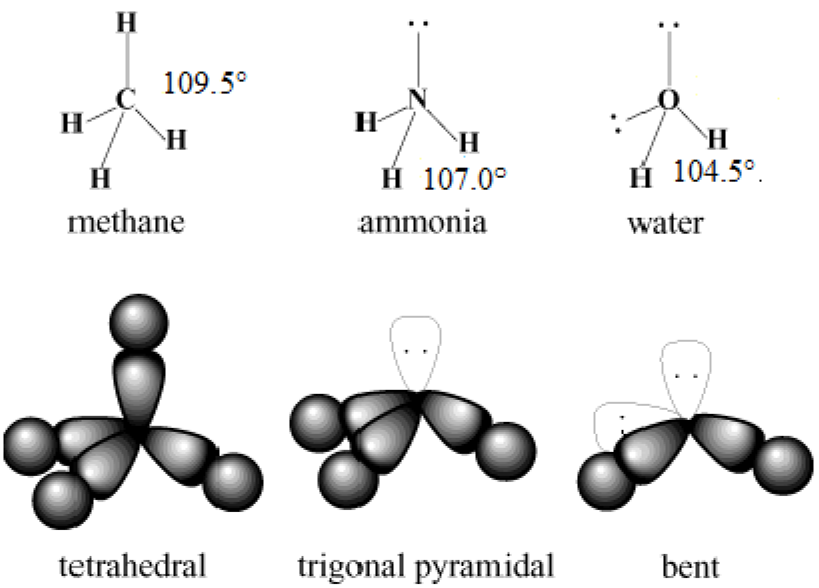


Figure 2.2. Decrease in the bond angle as the number of lone pairs of electrons in the molecule increases. Methane has no lone pair; ammonia has one lone pair and water has two lone pairs [19].

A dihedral or torsion angle is defined for groups of four atoms subsequently bonded in a chain [13]. If we number the four atoms as atoms 1, 2, 3 and 4, the dihedral angle can be defined as the angle between the plane identified by the first three atoms (atoms 1, 2 and 3) and the plane identified by the last three atoms (atoms 2, 3 and 4); it can also be seen as the angle by which the 3–4 bond must be rotated so as to eclipse the 1–2 bond. In the case of the ethane molecule (figure 2.1), we can identify the following dihedral angles: H3–C1–C2–H6, H3–C1–C2–H7, H3–C1–C2–H8, H4–C1–C2–H6, H4–C1–C2–H7, H4–C1–C2–H8, H5–C1–C2–H6, H5–C1–C2–H7, H5–C1–C2–H8.

A molecule can take several different geometries. It can change from one geometry to another by rotation around a single bond. Some of these geometries correspond to minima on the potential energy surface (PES, a multi-dimension diagram obtained by changing molecular parameters such as bond length, bond angles or dihedral angles by specific amounts [20, 21]). The geometries corresponding to the minima on the PES are called conformers [22]. A search for the conformers of a given molecule is referred to as conformational search.

Bond lengths, bond angles and dihedral angles are the internal coordinates of a molecule [3]. When preparing inputs for calculations, we can describe the starting geometry of the molecule in terms of the internal coordinates (Z matrix), or we can give the cartesian coordinates (x, y, z) of each atom. Each atom in a molecule has three coordinates and, therefore, it has 3 degrees of freedom. If there are N atoms in a molecule, the total number of degrees of freedom is 3N. In this work, all the inputs were prepared using the cartesian coordinates of the atoms [23].

As already mentioned, the PES is a multi-dimension diagram. It shows how the energy changes when some of the parameters of the molecule are changed. It can be visualized only in two or three dimensions [3, 23]. A two-dimension PES shows how the energy changes when one parameter is changed. A three-dimension PES shows how the energy changes when two parameters are changed. The stationary points on the PES are the points where the first derivative of the energy with respect to the parameter that is being changed is zero [3]. They can be minimum, maximum or saddle points. In order to know whether a stationary point identified by an optimization procedure is a minimum, we consider the vibrational frequencies. If all the vibrational frequencies are real for that geometry, then that point is a minimum point. There can be more than one minimum in the PES. Figure 2.3 shows an example of a two-dimension PES, where there are several local minima. The minimum which correspond to the lowest energy is called global minimum. There can be also several maxima and saddle points.

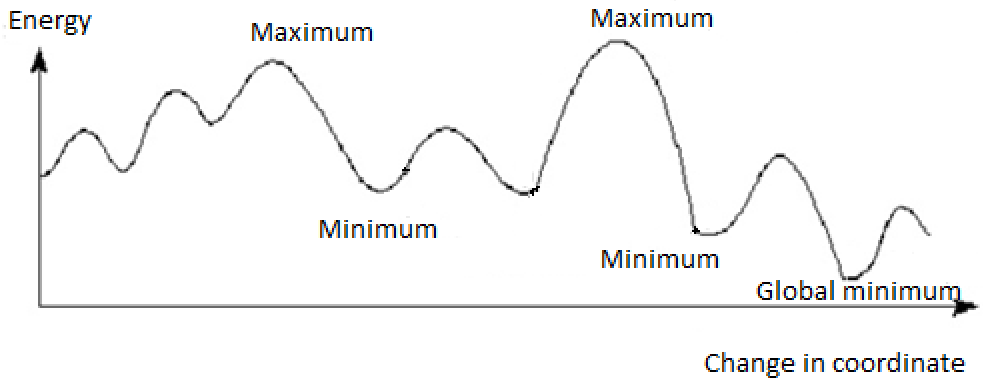


Figure 2.3. Example of a two-dimension potential energy surface (PES) showing local minima, the global minimum and a maximum [24].

The PES can also be considered for chemical reactions [25]. The equilibrium geometries of the reactants and products correspond to minimum points and the transition states are represented by first order saddle points, as illustrated in figure 2.4.

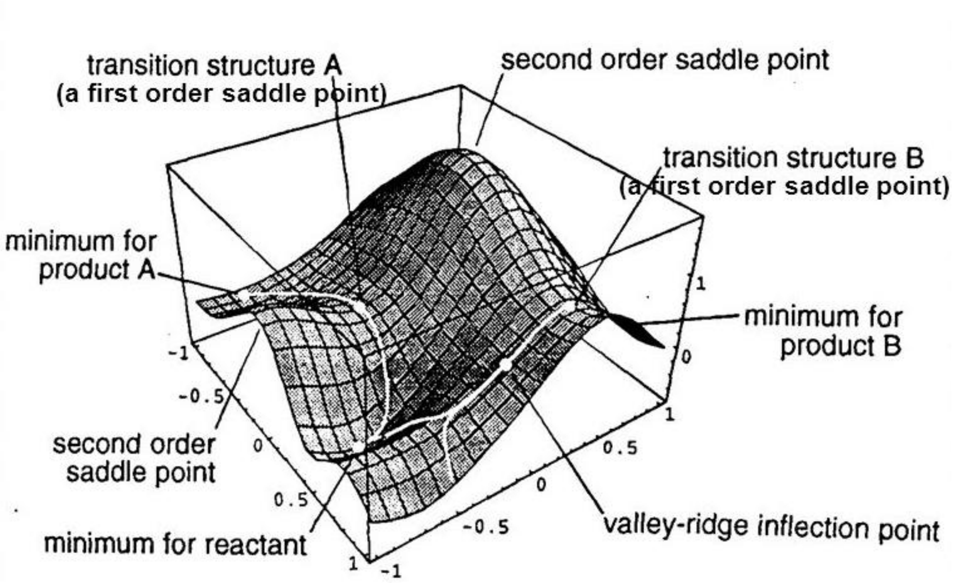


Figure 2.4. Example of a three-dimensional PES also considering a chemical reaction [20]

2.3. Computational methods for the study of molecules

Molecules can be studied using different methods. These methods can be classified into electronic structure methods and molecular mechanics [26]. The electronic structure methods comprise *ab initio*, semi-empirical and Density Functional Theory methods. This works uses electronic structure methods and, therefore, these are the methods discussed in the next sections. The electronic structure methods consider solving the Schrödinger equation.

2.3.1. The Schrödinger equations

In quantum mechanics, an atom or a molecule is described by the solutions of its Schrödinger equation [27–30]. The general form of the Schrödinger equation is the following:

$$\hat{H}\,\psi_i = E_i\,\psi_i \tag{1}$$

where $\hat{H}$ is the Hamiltonian operator, i.e., the energy operator

ψ_i is the total wavefunction of the i^{th} state (eigenfunction)

E_i is the energy value corresponding to ψ_i (eigenvalue corresponding to ψ_i).

The solution of the Schrödinger equation for a molecule are the molecular orbitals (MOs) of that molecule.

The Hamiltonian operator contains all the energy terms of the system, comprising both kinetic and potential energies. The kinetic energy terms are expressed in the form:

$$E_{kinetic} = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right) \tag{2}$$

where m is the mass of the particle, ħ is the Planck's constant divided by 2π ($\hbar = \frac{h}{2\pi}$) and the terms in parentheses are the Laplacian operator ∇^2

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \tag{3}$$

The potential energy terms are the terms expressing the electrostatic attractions or repulsion between the particles.

The complete Hamiltonian for the study of a molecule can be expressed by [29]:

$$\hat{H} = -\sum_i^N \frac{\hbar^2}{2m_e} \nabla_i^2 - \sum_k^M \frac{\hbar^2}{2m_k} \nabla_k^2 - \sum_i^N . \sum_k^M \frac{e^2 Z_k}{r_{ik}} + \sum_{i<j}^M \frac{e^2}{r_{ij}} + \sum_{k<p}^M \frac{e^2 Z_k Z_p}{r_{kp}} \tag{4}$$

where: i and j are electrons

k and p are nuclei

ħ is the Planck's constant divided by 2π

m_e is the mass of the electron

m_k is the mass of nucleus k

e is the charge of the electron

N is the number of electrons in the molecule

M is the number of nuclei in the molecule

Z_k is the atomic number of nucleus k

Z_l is the atomic number of nucleus l

r_{jk} is the distance between electron i and nucleus k

r_{ij} is the distance between electron i and electron j

r_{kl} is the distance between nucleus k and nucleus l

∇_{i}^2 is the Laplacian operator of electron i

∇_{k}^2 is the Laplacian operator of electron k

The first term in the Hamiltonian (equation 4) represents the kinetic energy of the N electrons in the molecule and the second term represents the kinetic energy of the M nuclei. The third term is the potential energy of the electrostatic attraction between the nuclei and the electrons, the fourth term is the potential energy of the electron-electron repulsion and the last term is the potential energy of the nuclei-nuclei repulsion [31].

The Schrödinger equation grows more complex as the number of electrons in the system increases. It can be solved exactly (analytically) only for one-electron systems. In all the other cases, we need to use approximations.

2.3.2. The Born-Oppenheimer approximation

All the terms in the Hamiltonian are necessary for a full description of a molecule. On the other hand, it is not possible to solve the equation exactly. Approximations of different types are introduced, and the most common approximation is the Born-Oppenheimer approximation. In a molecule, the nuclei move much more slowly than the electrons because they have much greater mass. The Born-Oppenheimer approximation considers the nuclei as stationary and the Schrödinger equation is written only for the motion and the energy terms pertaining to the electrons [32–34]. Therefore, within this approximation, the Hamiltonian is the electronic Hamiltonian and is expressed by:

$$\hat{\mathrm{H}}_{\mathrm{el}} = -\sum_{i}^{N} \frac{\hbar^2}{2m_{\mathrm{e}}} \nabla_{\mathrm{i}}^{2} - \sum_{i}^{N} . \sum_{k}^{M} \frac{e^2 Z_{\mathrm{k}}}{r_{\mathrm{ik}}} + \sum_{i<j}^{N} \frac{e^2}{r_{\mathrm{ij}}} \qquad (5)$$

When we study a molecule, we consider a certain set of nuclear distances and calculate the energy. Afterwards, we change the nuclear distances and other parameters and calculate the energy again.

The procedure is repeated until we find the geometry that give the lowest energy.

2.3.3. *Ab initio* methods

Ab initio means "from the beginning" [35]. It involves solving the Schrödinger equation analytically, which means that all the integrals are solved with mathematical methods, whether they are solved exactly, or whether they are solved using mathematical approximations, but without including any experimental values [36, 37]. The most common *ab initio* methods are Hartree-Fork (HF), Møller-Plesset Perturbation Theory (MP2) and a variety of configurations interaction (CI), which are usually post Hartree-Fock methods. In this work, MP2 and CI are not used, so they will not be discussed in detail.

2.3.3.1. The Hartree-Fock method

The HF method is a recursion procedure, i.e. a series of steps are repeated, with each of them giving better results than the previous step. The easiest way to explain a recursion procedure is by considering all the steps of the Hartree procedure for the study of a multi-electron atom with atomic number Z, i.e. an atom with Z electrons [38–42]:

- Step 1: We consider the Z electrons to be moving independently; we can then consider a guess potential as a sum of a set of Z identical net potentials, with each set depending on the radial coordinate (r) of only one electron.
- Step 2: We use the net potential to express the Hamiltonian operator and the Schrödinger equation for the atom.
- Step 3: By applying the separation of variables technique to solve the Schrödinger equation, we obtain Z identical differential equations, each of them depending on the coordinates of one electron.
- Step 4: Each of the obtained differential equation is solved, and we obtain the wavefunctions and the corresponding energy values.
- Step 5: We consider the filling of the newly found quantum states and write the electronic configuration of the ground state of the atom.
- Step 6: The charge distribution of each electron is evaluated as a product of its charge and the probability density function.
- Step 7: The charge distribution of Z-1 electrons is then added to the nuclear charge in order

to find the total charge distribution of the atom as seen by a typical electron.

- Step 8: On the basis of the charge distribution, we can calculate the produced electric field by using Gauss's law of electrostatics.
- Step 9: The integral of the electric field is evaluated, and it is a more accurate estimate of the net potential experienced by a typical electron.
- Step 10: The obtained net potential is compared with the value of the potential used at the beginning of the loop. If the difference is greater than a preselected value, the new potential is used to write the Hamiltonian and the Schrödinger equation (as in step 2), and the series of steps (3 to 10) is repeated. If the difference is less than the preselected value, then we say that the procedure has converged. The net potential is the self-consistent solution and the obtained wavefunctions describe the ground state of the atoms. The self-consistency is related to the fact that we obtain the results by using several cycles of steps.

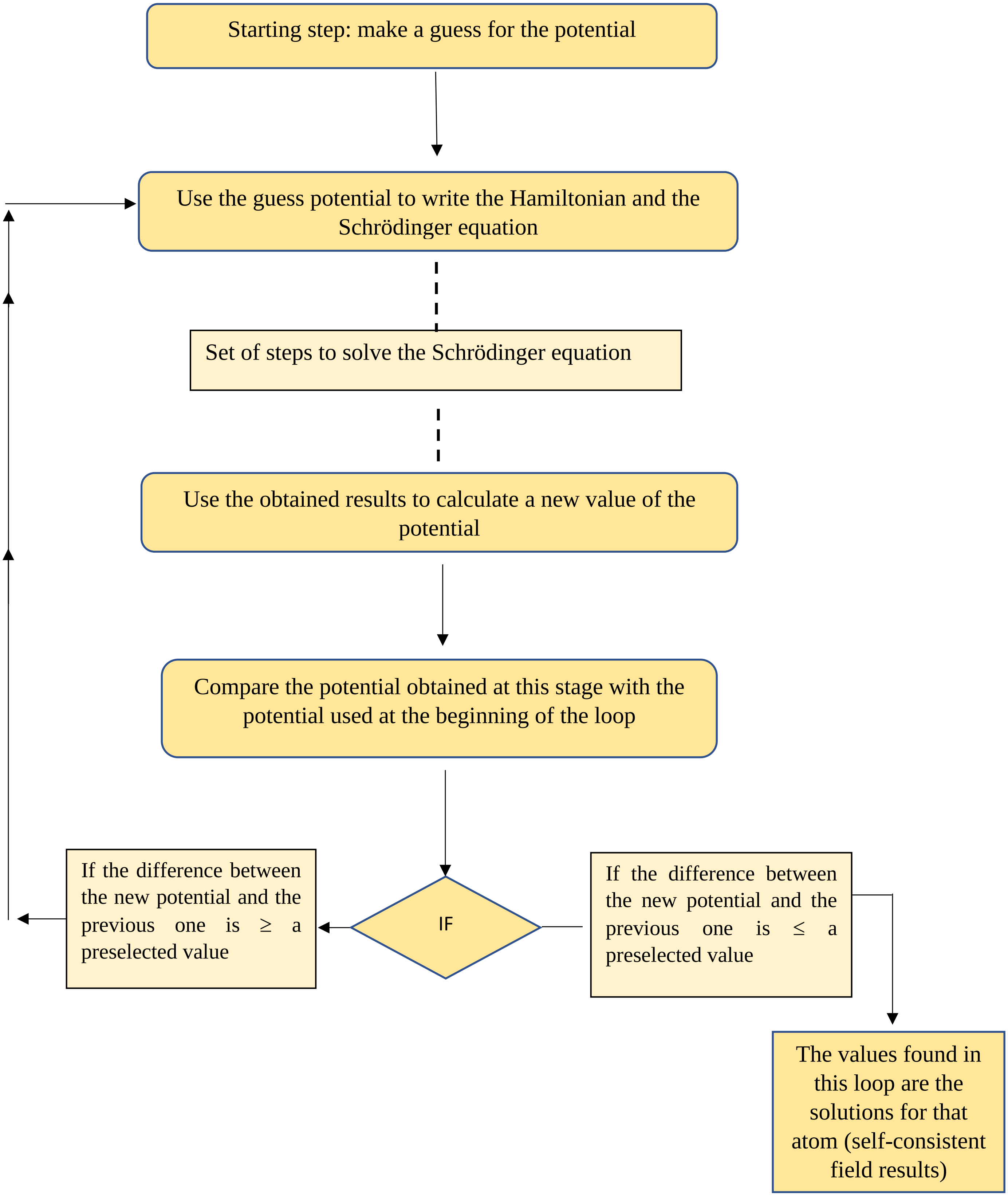


Figure 2.5. A flow chart showing the steps involved in the HF method [43]

2.3.3.2. Linear combinations of atomic orbitals (LCAO) and the variational principle

The solutions of the Schrödinger equations for a molecule are the molecular orbitals. Since we cannot solve the Schrödinger equation exactly, we have to use approximation methods. One of the approximations concerns the way of expressing the molecular orbitals. It is convenient to express them in terms of the atomic orbitals of the atoms of which a given molecule consists [44–46]. Therefore, this approximation expresses the molecular orbitals as a linear combination of atomic orbitals (LCAO).

$$\psi = \sum_{i} c_i \chi_i \tag{6}$$

where, ψ is a molecular orbital (MO)

χ_i are the atomic orbitals used for the expansion of ψ

c_i are the atomic orbital coefficients.

We consider atomic orbitals for each atom in the molecule. All the χ_i used for the MOs of a molecule constitute the basis set of the expansion. The atomic orbitals coefficients c_i are related to the contribution of a given orbital (χ_i) to the whole molecular orbital [47].

As already mentioned, whenever we solve a Schrödinger equation, we are looking for a minimum in the potential energy surface of the system considered (section 2.2). This means that we want to minimize the energy. In order to do this, we write the expression of the energy, we express the wavefunction in terms of equation 6, and we consider the conditions for the energy to be minimum. This will enable us to find the value of the coefficients c_i in the expansion. The variational principle ensures that, by using this method, we do not find energy values that are lower than the real value [48].

The variational principle states that, if a trial wavefunction is used to calculate the energy, the obtained values will not be less than the true energy value. The function expressed in terms of equation 6 is the trial function in the LCAO procedure. The energy value is expressed as an expectation value:

$$E = \frac{\int \psi^* \hat{\mathrm{H}} \psi d\tau}{\int \psi^* \psi d\tau} \tag{7}$$

If we consider real wavefunctions, we can then write:

$$E = \frac{\int \psi \hat{\mathrm{H}} \psi d\tau}{\int \psi^2 d\tau} \tag{8}$$

By substituting equation 6 into equation 7, the expectation value of the energy can be written as

$$E = \frac{\int (\sum_i c_i \chi_i) \hat{\mathrm{H}} (\sum_i c_i \chi_i) d\tau}{\int (\sum_i c_i \chi_i)^2 d\tau} \tag{9}$$

In order to find the minimum energy, we have to take the first derivative of the expectation value with respect to each of the coefficients and set it to be equal to zero. In this way we obtain a set of equations having the mathematical form

$$\left(\frac{\partial E}{\partial c_i}\right)_{j,\, j \neq i} = 0 \tag{10}$$

By replacing the expression of E from equation 9 in each of these equations, we obtain a set of equations where the unknown quantities are the coefficients c_i and the energy E. These equations that are called the secular equations. In order to solve them, we have to set the determinant of the coefficients of the unknown quantities equal to zero. The determinant is called the secular determinant [41, 42].

For illustration purpose, we can consider the case of two atoms, i.e. the case of a heteronuclear diatomic molecule consisting of two atoms, A and B. The wavefunction can be expressed as

$$\psi = c_A \psi_A + c_B \psi_B \tag{11}$$

where ψ_A and ψ_B are the atomic orbitals contributing to the molecular orbital ψ, and c_A and c_B are the coefficients to be determined.

By substituting equation 11 into equation 7, the expectation value becomes

$$E = \frac{\int (c_A\psi_A + c_B\psi_B)\hat{\mathrm{H}}(c_A\psi_A + c_B\psi_B)d\tau}{\int (c_A\psi_A + c_B\psi_B)^2 d\tau} \tag{12}$$

By expanding the expressions of the numerator and the denominator, we obtain certain integrals that are given specific names; these are the Coulomb integrals (α), the resonance integrals (β) and the overlap integrals (S). They are defined as follows:

$$\alpha_A = \int \psi_A \, \hat{\mathrm{H}} \, \psi_A d\tau \tag{13a}$$

$$\alpha_B = \int \psi_B \, \hat{\mathrm{H}} \, \psi_B d\tau \tag{13b}$$

$$\beta = \int \psi_A \, \hat{\mathrm{H}} \, \psi_B d\tau \tag{14}$$

$$S_{AB} = \int {\psi^*}_A \, \psi_B d\tau \tag{15}$$

In order to solve the secular equations, we set the secular determinant equal to zero.

$$\begin{vmatrix} \alpha_A - E & \beta - ES \\ \beta - ES & \alpha_B - E \end{vmatrix} = 0 \tag{16}$$

The determinant is expanded to a quadratic equation in E and then solved. The roots obtained are the energies of the bonding and antibonding molecular orbitals formed from the basis sets considered. The introduction of those energy values into the secular equation yields the coefficients c_A and c_B.

2.3.3.3. Complying with the antisymmetry requirements

For any multi-electron system, we have to consider the spin of the electrons. Therefore, the total wavefunction is a function of the space coordinates of the electrons and the total spin angular momentum [30, 38, 47–51].

total wavefunction = (space wavefunction) x (spin wavefunction) (17)

In the case of molecules, these wavefunctions are called spinorbitals. The spinorbitals can be expressed in the form:

$$\chi(\vec{x}_i) = \phi(\vec{r})\sigma \tag{18}$$

where $\phi(\vec{r})$ is a function depending on the space coordinates of the electron, $\vec{r}$ is a vector of the space coordinates of the electron and σ is a spin component taking into account the spins of all the electrons. For N electrons, the wavefunctions are written as the product of the spinorbitals, and this is called the Hartree product.

Since the electrons are fermions, we have to consider the Pauli's exclusion principle. The principle can be expressed through any of the following conditions [38]:

- Weaker condition: in a multi-electron atom, there can never be more than one electron in a given quantum state.
- Stronger condition: a system with several electrons must be described by an antisymmetric total wavefunction.

A function is antisymmetric if it changes sign when the two particles are exchanged (this is equivalent to changing the labelling of the two electrons). In the case of two particles, we can have only one exchange of the particles, so, there is only one permutation and the function can change sign. The total wavefunction can be antisymmetric with one of the two following options:

(antisymmetric total wavefunction) = (symmetric space wavefunction) x (antisymmetric spin wavefunction) (19a)

(antisymmetric total wavefunction) = (antisymmetric space wavefunction) x (symmetric spin wavefunction) (19b)

In the case of many electrons, there are many options for permuting two of them. Therefore, it is possible to have many permutations of two particles simultaneously. Each permutation implies a change in the sign of the wavefunction. Whether the overall sign of the wavefunction changes depends on the number of permutations considered. If the number of permutations is odd, the overall result is the change of sign [49, 52, 53]. If the number of permutations is even, there will be no change in sign in the overall result. In order to consider the overall outcome, the wavefunction is written in the form of a Slater determinant [52]:

$$\Phi_{\mathrm{SD}}=\frac{1}{\sqrt{\mathrm{N!}}}\begin{bmatrix} \chi_1(\vec{x}_1) & \chi_2(\vec{x}_1) & \cdots & \chi_N(\vec{x}_1) \\ \chi_1(\vec{x}_2) & \chi_2(\vec{x}_2) & \cdots & \chi_N(\vec{x}_2) \\ \vdots & \vdots & \ddots & \vdots \\ \chi_1(\vec{x}_N) & \chi_2(\vec{x}_N) & \cdots & \chi_N(\vec{x}_N) \end{bmatrix} \tag{20}$$

where: the electrons are numbered 1, 2,.., N

Φ is the wavefunction

$\frac{1}{\sqrt{\mathrm{N!}}}$ is the normalisation coefficient.

N is the total number of electrons

$\vec{x}_i$ are coordinate vectors

$\chi_i(\vec{x}_j)$ is the function of the electron i considered for the coordinate vector $\vec{x}_j$

The Hartree-Fock approximation uses a single Slater determinant for the description of electronic wavefunctions [54]. The Hartree-Fock energy can be written in terms of integrals. Considering two-electron operators, it is expressed as

$$E_{HF} = \langle \Phi_{\mathrm{SD}} | \hat{\mathrm{H}} | \Phi_{\mathrm{SD}} \rangle = \sum_i^N \langle i | \hat{h} | i \rangle + \frac{1}{2} \sum_i^N \sum_j^N \langle ii \,|\, jj \rangle + \langle ii \,|\, jj \rangle \tag{21}$$

where $\langle ii \,|\, jj \rangle = \iint |\chi_i(\vec{x}_1)|^2 \frac{1}{r_{12}} |\chi_i(\vec{x}_2)|^2 d\vec{x}_1 d\vec{x}_2$ (22)

$\langle \Phi_{\mathrm{SD}} | \hat{\mathrm{H}} | \Phi_{\mathrm{SD}} \rangle = \int \Phi_{\mathrm{SD}}\ \hat{\mathrm{H}}\ \Phi_{\mathrm{SD}} d\tau$ (assuming that the wavefunction is normalized)

The resulting two-electron integral is given by

$$\langle ii | jj \rangle = \iint \chi_i(\vec{x}_1)\chi_j^*(\vec{x}_1)\frac{1}{r_{12}}\chi_j(\vec{x}_2)\chi_i^*(\vec{x}_2)d\vec{x}_1 d\vec{x}_2 \tag{23}$$

2.3.3.4. Electron correlation

In the HF method, the motion of each electron is viewed as not being influenced by the motion of the other individual electrons (the repulsion with the other electrons is averaged). In reality, electrons influence each other’s motions. It is said that their motions are correlated [55]. The energy associated with this correlation is called correlation energy and it is viewed as the difference between the exact energy and the energy of the best possible HF calculation (energy of the HF limit).

2.3.3.5. Basis sets

A basis set is defined as a set of functions used to create molecular orbitals [47, 56]. The MOs are expanded as a linear combination of atomic orbitals with coefficients to be determined (eqn. (6); section 2.3.3.2). Choosing the right basis set is very critical for the quality of the results.
Atomic orbitals contributing to the formation of molecular orbitals include:

- **Core orbitals,** which are the orbitals of the inner, closed shells of the atom
- **Valence orbitals,** which are the orbitals of the valence shell of the atom
- **Virtual orbitals,** which are orbitals that are unoccupied in the ground state of the atom [57, 58].

Basis sets may include different numbers and types of orbitals (sections 2.3.3.5.2–2.3.3.5.4).

2.3.3.5.1. Types of functions involved in basis sets

The most straightforward way would be to use atomic orbitals directly, for example, the solution of the hydrogen atom. The difficulty was that they have to be supplemented for completeness. The Slater type orbitals (STOs) were used in the early days in quantum chemistry as basis functions due to their similarities with the wavefunctions of the hydrogen atom [54, 59, 60].

$$R(r) = Nr^{n-1}e^{-\xi r} \tag{24}$$

where R is the radium of the atomic nucleic distance
N is a normalisation constant
n is a natural number representing a principal quantum number, n = 1, 2….,
ξ is a constant related to the effective charge of the nucleus
r is the distance of the electron from the atomic nucleus

An advantage of the STOs was their direct physical interpretation [60–65]. However, STOs had a severe shortcoming, because the integrals required during the SCF procedure must be calculated numerically, which reduces the computational speed.

Gaussian type orbitals (GTO) were then introduced to approximate the STOs, by expressing them as linear combinations of gaussian orbitals. GTOs are referred to as gaussian primitives, which are usually obtained from quantum calculations of atoms [62, 66].

$$G_{nlm}(r,\theta,\varphi) = N_n r^{n-1} e^{-\alpha r^2} Y_l^m(\theta,\varphi) \tag{25}$$

where: n, m, l are the quantum numbers
θ, φ are the angular coordinates.

The exponents are varied until the lowest possible energy is obtained.

2.3.3.5.2. Minimal basis set

A minimal basis set is a basis set containing only the functions necessary to accommodate the electrons in the atom [47, 67]. Usually, a single basis function is used in the Hartree-Fock calculations of a free atom (for instance, 1s for the H atom). The most common minimal basis set is STO-nG, where n is an integer representing the number of GTOs used to approximate the STOs for both the valence and core orbitals. Since this basis set is not flexible, the use of additional functions is considered a better option to represent orbitals more accurately. For example, the 1s, 2s, $2p_x$, $2p_y$, $2p_z$ functions will be used for a lithium atom.

2.3.3.5.3. Polarized basis set

Polarisation refers to the distortion in the shape of an atomic orbital when the molecule is formed, due to the attraction of the electrons by the other nuclei [47, 69]. To take this phenomenon into account, basis functions with higher angular momentum quantum number (*d* and *f* type) are added so as to increase the flexibility of the resulting MOs. The additional flexibility provided by the polarization functions enables the MO to be asymmetric about the nucleus [69]. This allows for more accurate description of the bonding between atoms by removing the spherical symmetry around an atom. The polarisation functions are essential for a better description of chemical bonding and should be considered in all calculations where electron correlation is important. An asterix (*) is used to inform that a polarization function has been added to the heavier atom, and a double asterix (**) is used to inform that the polarisation function is added to both the heavier and the lighter atoms. For example, 6-31G* (or 6-31G(d)) informs that the polarization function has been added to the heavier atoms, that is, d orbitals have been added for carbon and other atoms of the second period. 6-31G** (or 6-31G(d, p)) informs that the polarisation function has been added to both the heavier and the lighter atoms, that is, d orbitals have been added for atoms of the second period and the p orbital have been added for hydrogen atoms.

2.3.3.5.4. Diffuse basis set

Diffuse basis sets are basis sets which contain diffuse functions. The diffuse functions are usually of the s and p type orbitals [70]. They are considered important for the description of anions and weak bonds correctly and are relevant in the calculation of molecular properties such as dipole moments. The presence of diffuse function is denoted by +. For example, the basis set 6-31+G** is a basis set in which polarisation functions have been added for both the light and heavy atoms and the diffuse functions have been added for heavy atoms. The basis set 6-31++G** is a basis set in which polarisation functions have been added for both the light and heavy atoms and the diffuse functions have also been added for both the light and heavy atoms.

2.3.3.4. Post-Hartree-Fock methods

The post HF methods are methods that are developed as an improvement on the HF results. They include electron correlation as a more accurate way to consider the electron-electron repulsions than in the HF method [65, 70]. Some of the methods are MP2 and CCSD(T), (coupled cluster methods); they will not be discussed here because they have not been used in this work.

2.3.4. Density functional theory (DFT)

2.3.4.1. General features of DFT

The DFT method is one of the most commonly used computational method for predicting the properties of chemical systems [71, 72]. Since the energy of the molecule can be determined in its ground state (E_0) from the electron density (ρ), DFT attempts to calculate the ground state molecular properties from the ground state electron density without using the wavefunction of the system [73, 74]. DFT considers the energy as a function of the electron density

$$E = E(\rho) \tag{26 a}$$

Since ρ is a function of the position [$\rho = \rho(r)$], the energy is a function of a function (functional), as expressed by the equation:

$$E = E[\rho(\vec{r})] \tag{26 b}$$

DFT takes into account electron correlation (section 2.3.3.4.) and it has the advantage that it requires less computing power in comparison to most of the post HF-methods. The DFT theory is also based on the idea that an external potential (V_{ext}) originating from a position of the nuclei in a molecule is a function of the electron density [75–79]. Due to this, two different external potentials can only yield different ground state electron densities.

The Hamiltonian ($\hat{H}$), is a functional of the electron density given by [29]:

$$\hat{H} = \hat{T} + \hat{V}_{ee} + \hat{V}_{ext} \tag{27}$$

where: $\hat{T}$ is the kinetic energy of the non-interacting electrons

$\hat{V}_{ee}$ is the external potential related to the classical electron-electron repulsion

$\hat{V}_{ext}$ is the external potential related to the nuclear-electron interaction

The energy of a molecule in its ground state (E_0), generated from the ground state electron density, can be expressed by the equation:

$$E_0 = E\,[\rho(r)] \qquad (28)$$

By re-writing E [ρ(r)] as functionals of the electron density ρ(r), one obtains:

$$E_0\,(\rho_0) = T\,[\rho_0] + E_{ee}\,[\rho_0] + E_{ne}\,[\rho_0] \qquad (29)$$

The terms T [ρ_0] and E_{ee} [ρ_0] in equation 29 are system independent, whereas E_{ne} [ρ_0] represents the potential energy due to the attractive interaction between nuclei and electrons and it is system dependent. Equation 29 can be split into specific components as follows

$$E\,[\rho(r)] = T_{ni}\,[\rho(r)] + V_{ne}\,[\rho(r)] + V_{ee}\,[\rho(r)] + \Delta T\,[\rho(r)] + \Delta V_{ee}\,[\rho(r)] \qquad (30)$$

where: T_{ni} is the kinetic energy of non-interacting electrons

V_{ne} is the potential energy corresponding to the nucleus-electron interaction

V_{ee} is the potential energy corresponding to the electron-electron interaction

ΔT is the change in kinetic energy

ΔV_{ee} is the change in potential energy of the electron-electron interaction

All these terms are written in equation 30 as functionals of the probability density.

2.3.4.2. The Hohenberg and Kohn theorem

Hohenberg and Kohn developed two theorems. The first Hohenberg-Kohn theorem considers the ground state energy generated from the Hohenberg-Kohn functional when the ground state electron density is specified [74, 75, 80]. The second Hohenberg-Kohn theorem considers the ground state electron density and any guess electron density, and uses the variational principle. The first three terms in equation 30 form the Hohenberg-Kohn functional (F_{HK} [ρ_0]), and they are system independent, while the last two terms are system dependent.

$$F_{HK}\,[\rho_0]) = T_{ni}\,[\rho(r)] + V_{ne}\,[\rho(r)] + V_{ee}\,[\rho(r)] \qquad (31)$$

The guess electron density [ρ_{trial}] results in an external potential giving a higher energy value than that of the ground state electron density

$$E\,[\rho_{trial}] = T\,[\rho_{trial}] + E_{ee}\,[\rho_{trial}] + E_{ne}\,[\rho_{trial}] \geq E_0 \qquad (32)$$

The application of DFT within the Hohenberg-Kohn approximation failed because the kinetic energy expression from the Hohenberg-Kohn functional was not well established.

2.3.4.3. Kohn and Sham method

Kohn and Sham develop a method yielding the Kohn-Sham equations. The theory focused on a system of non-interacting electrons (in general, the wavefunction and electron density of non-interacting electrons differ from those of interacting electrons). This approach includes the construction of a non-interacting system in a way that the density is the same as that of the interacting electrons. After discovering a correspondence of the Slater determinant which approximates the N-electron wavefunction with the true wavefunction for a non-interacting electron system from the HF approximation, they could conclude that [77]

$$T_{HF} = \langle \chi_i | \nabla^2 | \chi_i \rangle \qquad (33)$$

where χ_i are the spinorbitals

T_{HF} is the HF approximation

The ground state wavefunction can then be expressed using the Slater determinant Θ_s.

$$\Theta_s = \frac{1}{\sqrt{N!}} \begin{bmatrix} \varphi_1(\vec{x}_1) & \varphi_2(\vec{x}_1) & \cdots & \varphi_N(\vec{x}_1) \\ \varphi_1(\vec{x}_2) & \varphi_2(\vec{x}_2) & \cdots & \varphi_N(\vec{x}_2) \\ \vdots & \vdots & \ddots & \vdots \\ \varphi_1(\vec{x}_N) & \varphi_2(\vec{x}_N) & \cdots & \varphi_N(\vec{x}_N) \end{bmatrix} \qquad (34)$$

The orbitals (φ_i) in the Kohn-Sham theory are similar to those considered in the HF theory, and are related to the eigenvalue, ε_i, through the eigenvalue equation:

$$\hat{f}^{KS}\,\varphi_i = \varepsilon_i \varphi_i \tag{35}$$

where $\hat{f}^{KS}$ is the Kohn-Sham operator, which contains the effective potential $V_S(\vec{r})$:

$$\hat{f}^{KS} = \frac{1}{2}\nabla^2 + V_S(\vec{r}) \tag{36}$$

Consequently, the Hohenberg-Kohn function within the Kohn-Sham approach can be written as

$$E_{DFT}[\rho] = T_s[\rho] + E_{ne}[\rho] + J[\rho] + E_{xc}[\rho] \tag{37}$$

where: $T_s[\rho]$ represent the kinetic energy of non-interacting electrons

$E_{ne}[\rho]$ represent potential nucleus-electron interaction potential energy

$J[\rho]$ is the electron-electron interaction potential energy

$E_{xc}[\rho]$ is the exchange correlation energy

$E_{xc}[\rho]$ is calculated with an exchange-correlation functional and takes into account part of the electron correlation energy [74–80].

2.3.4.4. DFT functionals

The DFT method is focused towards the design of functionals which relate the electron density to the energy of the system. These functionals are classified based on their level of sophistication. The simplest functional is the LDA (Local Density Approximation), which is based on the assumption that the exchange correlation energy at any point in space is the only function of the electron on that point in space [81]. Consequently, LDA functional systems can be represented by a homogenous electron gas of the same density [82, 83]. Another functional is the GGA (Generalized Gradient Approximation) method which depend on both the electron density and the gradient. Since most molecular systems are spatially inhomogeneous and are different compared to a homogeneous electron gas, GGA is considered a significant improvement with respect to LDA.

Meta-GGA methods, which are methods which incorporate the kinetic energy density, and the hybrid density functionals combining the exchange-correlation of GGA with some level of HF exchange, have been developed. The hybrid functionals include the dependence on the kinetic energy density. One of the most commonly used hybrid functionals in quantum chemistry is the exchange correlation functional, B3LYP [84–87].

2.4. Molecular properties considered in this work

2.4.1. Conformers' relative energies

In the conformational study of molecules, it is interesting to compare the energy of the conformers whenever a molecule has more than one conformer). The outputs give the energies in Hartree, and these values are not convenient for comparisons to use in analysis. The easiest way to compare the energies of the conformers is by considering their relative energies. This is done by assigning zero value to the energy of the lowest energy conformer and considering the differences of the other energy values with respect to it. These differences are the relative energies of the individual conformers. Because of the way in which they are calculated, relative energies are always positive.

2.4.2. Vibrational frequencies and thermodynamic properties

In a molecule, different types of motions are possible and can influence its energy and physical properties [88, 89]. The motions comprise:

- translational motion: concerns the motion of the whole molecule in space
- rotational motion: concerns the rotation of molecules around the three axes (x, y, z) in space
- vibrational motion: it is related to the periodic motion of the atoms within a molecule.

These motions are a major contribution to the energy of the molecule [50, 89]. Their contributions sum up and yield the thermal energy (E_{th}) of a molecule

$$E_{th} = \varepsilon^T+\varepsilon^R+\varepsilon^V \tag{38}$$

where ε^T corresponds to the translation contribution

ε^R corresponds to the rotational contribution

ε^V corresponds to the vibrational contribution

The total energy of the molecule (E) is given by the sum of the thermal energy and the electronic energy (ε^E) and can be written as

$$E = \varepsilon^T+\varepsilon^R+\varepsilon^V+\varepsilon^E \tag{39}$$

The degrees of freedom of a particle are defined as the number of variables needed to give a complete description of its motion. They are expressed in terms of the coordinates in space (x, y, z). The motion of an atom moving in three-dimensions (translational motion) is described by three coordinates; therefore, the atom will have three degrees of freedom. For a molecule with N atoms, the total number of degrees of freedom is 3N, because each atom has 3 degrees of freedom. Three of these 3N degrees of freedom correspond to the translational motion of the molecule, which is the motion of the whole molecule in space. To know the degrees of freedom for rotational motion, we need to distinguish whether a molecule is linear or non-linear. For a non-linear molecule, there are three degrees of freedom for rotation because rotation is possible around all the three axes. For a linear molecule, the rotation around the molecular axis is not allowed; therefore, there are two degrees of freedom for rotation.

The degrees of freedom for vibrational motion are given by

Vibrational motion degrees of freedom = total degrees of freedom - translational degrees of freedom - rotational degrees of freedom (40)

Therefore, the vibrational degrees of freedom are 3N-6 for non-linear molecules and 3N-5 linear molecules [90].

Vibrational motions of a molecule can occur in all phases of matter (solid, liquid and gas). The simplest description for a molecular system with more than one vibrational mode considers the vibrations of a tri-atomic molecule, i.e. a molecule with only two bonds. The type of vibrations possible are

- **symmetric stretching:** the two bond lengths alternatingly increase and decrease simultaneously by the same amount
- **asymmetric stretching**: alternatingly, one bond lengths increase as the other decreases by the same amount
- **bending**: the bond angle between the two bonds changes

As the number of atoms increases, the type and number of vibrations also increases. Vibrational motions can also change the shape of a molecule. The lower energy vibrational motions can also change the shape of the benzene ring.

A molecular vibration is excited when a molecule absorbs a quantum of energy corresponding to the given vibrational frequency [91, 92]. Since the vibrations in a molecule are periodic motions, the harmonic approximations (harmonic oscillator) is the simplest approach. Using this approximation, the motion in a normal vibration can be described as a simple harmonic motion. The energy of a particle oscillating harmonically has two components, the kinetic energy and the potential energy. The vibrational potential energy (V) is a quadratic function with respect to the atomic displacement [50, 52].

$$V = \frac{1}{2}kx^2 \tag{41}$$

where: k is the restoring force constant
x is the displacement along the x direction

Therefore, the Schrödinger equation for a particle with a mass *m* oscillating harmonically is given by the equation

$$-\frac{h^2}{2m}\frac{\partial^2\psi}{\partial x^2} + \frac{1}{2}kx^2\psi = \mathrm{E}\psi \tag{42}$$

The first term on the left-hand side corresponds to the kinetic energy of the particle and the second term to its potential energy. By solving the Schrödinger equation, we obtain the energy values, given by

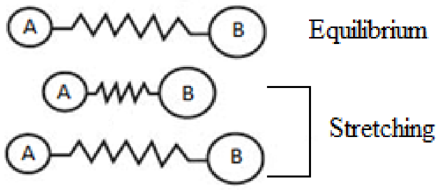
$$E_v = (v + \frac{1}{2})\hbar\omega \tag{43}$$

where v is the vibrational quantum number

ω is related to the force constant by the equation

$$\omega = \frac{1}{2\pi}\sqrt{\frac{k}{m}} \tag{44}$$

Considering the harmonic oscillator potential (figure 2.6), the spacing between the energy levels is constant and is equal to $\hbar\omega$. This is one of the limitations of the harmonic approximation, which would imply that all the transitions between two neighboring levels occur at the same frequency ($\Delta E_{v+1,v} = \hbar\omega$) [52]. Anharmonic corrections may be introduced to improve the results with respect to the harmonic oscillator. A frequent approximation is the Morse potential, which also takes into consideration bond dissociation. As the quantum number increases, the spacing between neighboring energy levels decreases. The Morse potential is a better representation of the potential energy for the vibrations in a molecule.



Strectching motion of a bond

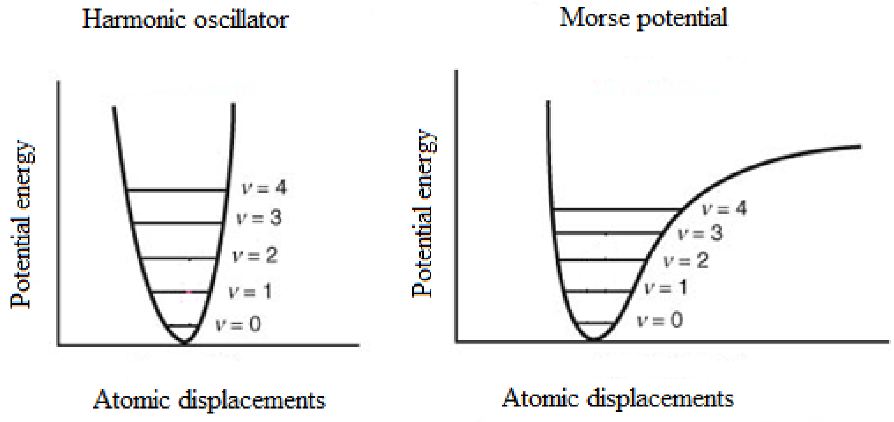


Figure 2.6. Harmonic oscillator potential and the Morse potential [93]

2.4.3. Zero-point corrected energy

The frequency calculations also give us the zero-point energy (ZPE), that is the difference between the lowest part of the potential (V = 0) and the first vibrational energy level (corresponding to v = 0). This energy difference is equal to $\frac{1}{2}\hbar\omega$ for the harmonic oscillator. This correction must be included to get the total energy of the molecule. When we consider the energy with this correction, we call it the zero-point corrected energy [52, 94, 95].

2.4.4. Molecular orbitals (HOMO and LUMO)

Molecular orbitals are the solutions of the Schrödinger equations and are built with the LCAO approximations (section 2.3.3.2). Molecular orbitals can be either bonding or antibonding [96, 52]. A bonding molecular orbital, when occupied, decreases the energy of the system with respect to the separated atoms. An antibonding molecular orbital, when occupied, increases the energy of the system with respect to the separated atoms. Therefore, the bonding molecular orbital has a stabilizing effect on the system, when they are occupied, and the antibonding molecular orbital has a destabilizing effect on the system.

Two molecular orbitals are particularly important for the description of a molecule because they relate to its properties: the Highest Occupied Molecular Orbital (HOMO) and the Lowest Unoccupied Molecular Orbital (LUMO). The energy difference between these molecular orbitals (HOMO-LUMO energy gap) is related to some molecular properties, including the reactivity of the molecules [97–100]. The most stable molecules have a higher energy gap, and the less stable molecules have a smaller energy gap. Molecules with smaller energy gaps may undergo chemical reactions more easily. The energy gap also relates to the ability of a substance to conduct electric current; a smaller gap is related to better conductivity [101].

2.4.5. Dipole moments

The electric dipole moment (μ) is defined for a pair of opposite charges of magnitude q, as the magnitude of the charge multiplied by the distance between them. The direction of the resulting dipole moment vector ($\vec{\mu}$) is toward the positive charge [102, 103]. A bond is polar when the two bonded atoms have different electronegativities. Each polar bond has a dipole moment. There is a dipole moment for the whole molecule if the sum of the vectors of all the dipole moments of the bonds is not zero. The sum is given by the equation.

$$\vec{\mu} = \sum_i q_i \vec{r}_i \tag{45}$$

where: $\vec{\mu}$ is the resulting dipole moment vector of the molecule

$q_i\vec{r}_i$ is the dipole moment of bond i

Water molecule   Carbon dioxide

Figure 2.7. Dipole moments of individual bonds and dipole moment of the water molecule and the carbon dioxide molecule.

The sum of the vectors depends on their mutual orientations. Figure 2.7 shows the case of water and the case of carbon dioxide (CO_2). Both molecules have two polar bonds, but, in the water molecule, the sum of the vectors is not zero because the two vectors form a non-zero angle, whereas in the CO_2 molecule, the sum of the vectors is zero because the two vectors are opposite and equal (angle equal to 180º) [103, 104].

2.4.6. Hydrogen bonds

Hydrogen bond is considered as a type of dipole-dipole attraction which occurs when a hydrogen atom (H) is bonded to a more electronegative and small-size atom (X), and another electronegative atom is available in the vicinity (100-102). A hydrogen bond can be illustrated as an interaction between a donor X–H and an acceptor Y (figure 2.8). X can be an electronegative atom such as oxygen (O), nitrogen (N) and fluorine (F) but, in some instances, it can be a carbon (C) atom. The acceptor Y can be an electronegative atom such as O, N or F. The Y atom usually has at least one electron pair available. Hydrogen bonds are usually denoted by denoted segments.

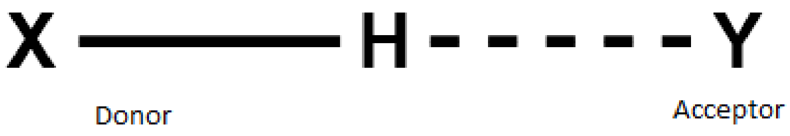


Figure 2.8. Illustration of a hydrogen bond

Different hydrogen bonds have different characteristics according to the nature of X and Y, and also to the molecular context. We usually describe the hydrogen bonds through their parameters: bond length, donor···acceptor distance (X···Y), and $X\hat{H}Y$ bond angle. The parameters also provide information about the hydrogen bond strength. The stronger hydrogen bonds are characterized by 1.2–1.5 Å H···Y bond length, with 2.2–2.5 Å X···Y donor···acceptor distance, and 170–180° $X\hat{H}Y$ bond angles. Moderate hydrogen bonds are characterized by 1.5–2.2 Å H···Y bond length, with 2.5–3.2 Å X···Y donor···acceptor distance, and 130–150° $X\hat{H}Y$ bond angles. Weaker hydrogen bonds are characterized by 2.2–3.2 Å H···Y bond length, with 3.2–4.0 Å X···Y donor···acceptor distance, and 90–120° $X\hat{H}Y$ bond angles [105–107]. An example of a weak hydrogen is shown in figure 2.9. The sp^2 O of the COOH group forms a hydrogen bond with the hydrogen on the OH group; this hydrogen bond is weak because of the small $O\hat{H}O$ bond angle [108].

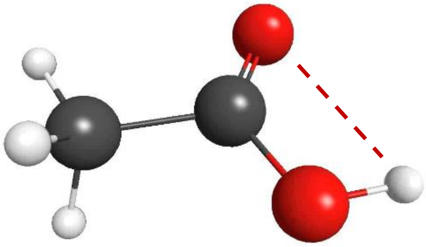
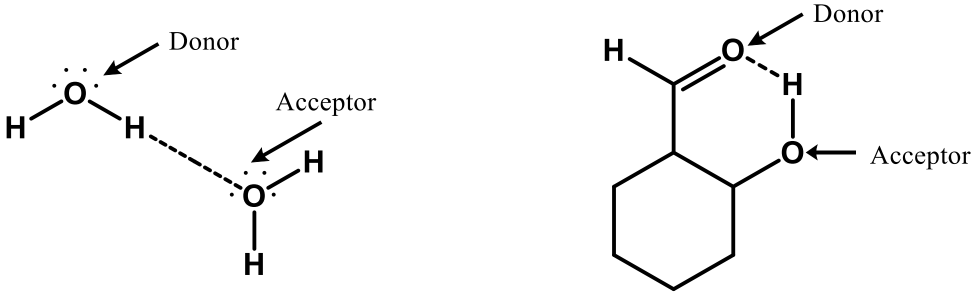


Figure 2.9. The weak hydrogen bond present in the carboxylic (COOH) group. The acetic acid molecule is selected as illustrative example.

There are two types of hydrogen bonds: intermolecular hydrogen bonds and intramolecular hydrogen bonds [109].

Intermolecular hydrogen bonds are hydrogen bonds which occurs between separate molecules. The donor belongs to one molecule and the acceptor belongs to another molecule. An example is given by a hydrogen bond between two water molecules (figure 2.10).

Intramolecular hydrogen bonds (IHBs) are hydrogen bonds which occur within a molecule. Both the donor and the acceptor belong to the same molecule. For such a hydrogen bond to form, the donor and the acceptor atoms must be able to come close to each other. An example is the hydrogen bond present in the salicylaldehyde molecule (Figure 2.10). IHBs are important in biomolecules, for example, proteins and DNA [109, 110]. It is important to consider the IHBs when studying a molecule because they stabilize a molecule and also influence its geometry. They are also particularly important for the study of biologically active molecule because they may be involved in the mechanism by which the biologically active molecules interact with the biological target .



Intermolecular hydrogen bond
between two water molecules

Intramolecular hydrogen bond in
salicylaldehyde [111]

Figure 2.10. Examples of intermolecular and intramolecular hydrogen bonds

There are instances in which two hydrogen bonds share the same donor or acceptor; such bonds are termed **bifurcated hydrogen bonds** [112, 113]. For example, one hydrogen bond donor can be bonded to two hydrogen bond acceptors (e.g. C=O···H···O=C); this is called a bifurcation on the hydrogen. Figure 2.11 shows an example of hydrogen bonds bifurcated on the hydrogen atom. It may also happen that two hydrogen bond donors are bonded to the same hydrogen bond acceptor (e.g., N—H···O···H—N); this is called a bifurcation on the oxygen atom. In some cases, the acceptor may be over coordinated.

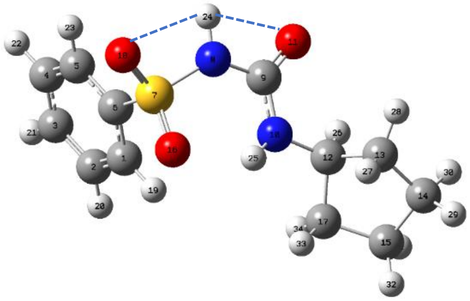


Figure 2.11. Example of hydrogen bonds bifurcated on the hydrogen atom.
The H atom bonded to the N which is bonded to the S atom is IHB donor to two O atoms – the O atom bonded to the S atom and the O atom bonded to the C atom between the two N atoms. The two IHBs are represented by dashed segments.

2.4.7. Red shift in the vibrational frequencies of the donor

The red shift is the decrease in the IR vibrational frequency of the bonds involved in the hydrogen bonding. The red shift is related to the elongation of the X–H (proton donor) bond length in the X–H···Y system. The red shift is correlated to the strength of an IHB [114].

Chapter 3

Literature review

This chapter presents information about diabetes as a disease and about the sulfonylureas molecules which are used for its treatment.

3.1. Diabetes mellitus

Diabetes mellitus [1, 115, 116], commonly referred to as diabetes, is a group of metabolic diseases characterized by high blood sugar (glucose) levels that result from defects in insulin secretion, or in its action, or both [1, 117]. Insulin is a hormone that the body needs to get glucose from the bloodstream into the cells of the body [118]. Diabetes mellitus was first (in the ancient world) identified as a disease associated with "sweet urine" and excessive muscle loss. The occurrence of diabetes is rapidly increasing in recent times and diabetes has become a worldwide health threat in the past decades. According to a statistical report, it is estimated that 382 million people worldwide, or 8.3% of the adult population, had diabetes in 2013; if these trends continue, the number will rise to 592 million by 2035 [117]. Furthermore, diabetes creates a favorable situation for the development of cardiovascular diseases, which are currently the first cause of death worldwide.

3.1.1. Different types of diabetes

There are three main types of diabetes, namely, type 1 diabetes, type 2 diabetes and gestational diabetes.

3.1.1.1. Type 1 diabetes

Type 1 diabetes is usually diagnosed in children and young adults and was previously known as juvenile diabetes [1]. Only 5–10% of diabetes cases are of this type. In this type of diabetes, the body does not produce insulin. People with type 1 diabetes rely on insulin injections or on continuous infusion of insulin via an insulin pump. There has been a rapid evolution in the care and treatment for people with type 1 diabetes, such as genetically engineered insulin and glucose monitoring devices, to control the blood glucose levels and to prevent or delay the diabetes-related complications [119, 120].

Figure 3.1 outlines the various phenomena which are involved in type 1 diabetes. The process includes various stages. The carbohydrates entering the body with food are converted to glucose (stage 1). The glucose then enters the blood stream to help the pancreas in the production of insulin (stage 2). If the pancreas produces little or no insulin (stage 3), the insulin that gets into the bloodstream is insufficient (stage 4). Then, not enough glucose is removed from the bloodstream to the cells. As a consequence, glucose builds up in the bloodstream (stage 5), thus resulting in type 1 diabetes [117].

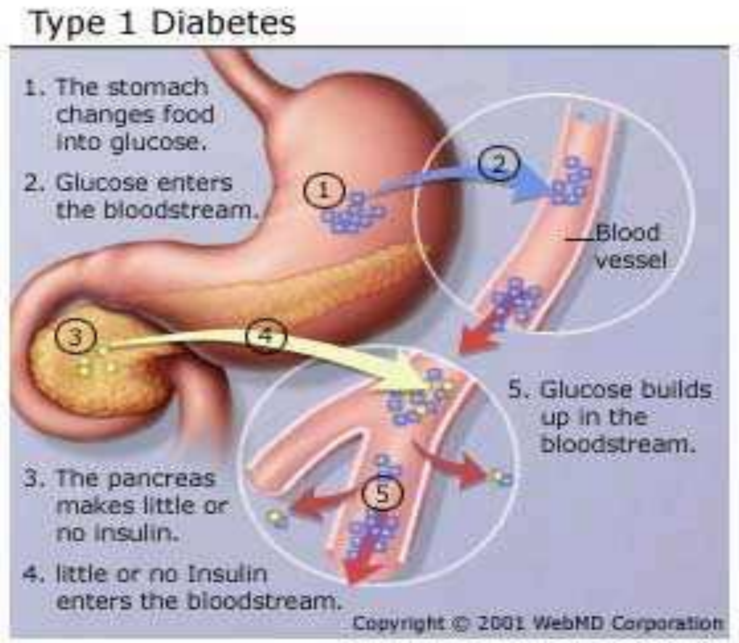


Figure 3.1. Phenomena involved in type 1 diabetes [117]

3.1.1.2. Type 2 diabetes

Type 2 diabetes constitutes the vast majority (about 90%) of the cases of diabetes [115]. It is commonly diagnosed in the population over the age of 45 years [121, 122]; in recent decades, it is increasingly developing also in younger people, even children under 14 years of age. It is a long term metabolic disorder that is characterized by high blood sugar levels caused by lack of insulin, in turn due to insulin resistance. In the early stages of the disease, the insulin levels in the blood are mostly normal or slightly elevated; at this early stage, people can usually manage their conditions so as to delay – and, in some cases, even prevent – the disease, by adopting a healthy lifestyle, including regular physical activities, healthy food intake and losing excess body weight [123]. However, at a later stage of the disease, patients become insulin-deficient and may require oral medications; eventually, when other medications fail to control the blood glucose level adequately, they need insulin injections. In the worst scenarios, diabetes may cause gangrene of the lower limbs, which results in the need for their amputation. It can also lead to blindness, and to heart and kidney failure.

3.1.1.3. Gestational diabetes

Gestational diabetes is a form of diabetes characterised by high glucose levels in the blood during the later stages of pregnancy [120, 124]. Gestational diabetes is said to affect about 4% of pregnancies worldwide and can cause complications to both mother and baby [1]. Gestational diabetes usually resolves after the delivery of the baby, but women with gestational diabetes and their children are at a higher risk of developing type 2 diabetes [124]. Approximately half of the women with a history of gestational diabetes have developed type 2 diabetes within five to ten years after delivery [125]. Since gestational diabetes can affect both mother and baby, it is important for it to be treated as early as possible. Treatments for gestational diabetes include special dietary plans and regular physical activities to keep normal blood glucose level, which are similar to those pregnant women should do [126]. In more serious cases, the treatment may also include daily blood glucose testing and insulin injections.

3.1.2. Diabetes in South Africa

According to a 2017 report based on the information released by Statistics South Africa on the causes of deaths in the country, there has been a significant increase in deaths due to diabetes [127]. The report says that the majority of people with diabetes have type 2 diabetes. The prevalence of type 2 diabetes was estimated at 4.5 % in 2010 [128, 129]. Over the past years, diabetes moved from being the 5th biggest killer (in 2013) to be the second biggest killer in South Africa (responsible for 5.4% deaths in 2015, [130-132]) and the leading cause of death among females. Diabetes was found to have been the number-one cause of death in the Western Cape Province. The reports suggest that in 2016 women were 36% more likely to die due to diabetes than from the combination of other causes [133]. Experts suggested that up to 7% of South Africans aged 21 to 79 (3.85 million people) had diabetes by then [129, 130]. The increase in the cases of people getting sick with diabetes is due to poor diet (unbalanced diet) and obesity. Excessive consumption of calories and sedentary lifestyles, and high consumption of soft and energy drinks, are also main contributors to the development of diabetes, because of their high sugar content [133].

Type 2 diabetes is said to be placing a large burden on the healthcare system. This is because of the costs associated with the management of diabetes, which may effectively require daily treatment and a regular monitoring, a healthy diet and lifestyle and diabetes-based education to ensure awareness [130]. The costs may also include hospital and medication costs and government provided disability grants. The health expenditure in relation to diabetes is said to be increasing yearly since 2010, and the costs are becoming alarming. A high presence of diabetes in the country can also affect work productivity in an indirect way, as healthy employees remain absent in order to care for sick relatives. Reports indicate that 76% of diabetes-related deaths occur amongst people below the age of 60, which is said to be the economically productive population [131, 132].

3.1.3. Most common symptoms of diabetes

The symptoms may develop gradually, not in direct relationship to whether an individual has insulin resistance. The body may manage with lower insulin levels for a certain period, but some symptoms eventually begin to be noticed; these include [134-138]:

- **Fatigue**: the body may not be getting the needed energy from the consumed foods, which results in a person feeling tired;
- **Extreme thirst**: the tissues get dehydrated when there is too much glucose in the blood, because the body will often pull the fluids from the tissues to the blood in an attempt to keep the blood diluted and to also counteract the high glucose levels. Consequently, the dehydrated tissues will relay a message that more water is needed;

- **Frequent urination**: it is due to drinking a lot of water to stay hydrated; it is also an attempt by the body to get rid of the excess glucose through urination;
- **Extreme hunger**: due to the body's insulin resistance, the glucose is prevented from entering the muscles and providing energy; therefore, the muscles and other tissues will relay a hunger message even after the individual has eaten, because they are not getting the needed energy;
- **Weight loss**: when the body does not get the energy it needs from food, it breaks down the fat and the muscles in order to create some energy, and this results in weight loss;
- **Infections**: the body may experience frequent infections due the effects of type 2 diabetes. Bacteria are known to flourish when the levels of glucose in the blood are high, and this makes it difficult for the body to fight off infections;
- **Slow wound healing**: the functionality of the white blood cells, which are responsible for wound healing, is affected by the high levels of glucose in the blood; therefore, it may take longer for wounds to actually heal;
- **Blurry vision**: the body may pull fluids from the eyes in an attempt to counteract the high levels of glucose in the blood; this may cause problems with focusing, resulting in blurry vision.

3.1.4. Diabetes related complications

When diabetes is present in the body for many years, it can result in several complications including heart (cardiomyopathy) and kidney (nephropathy) diseases, diabetic eye diseases (including retinopathy), and problems to the nervous system (neuropathy) [115]. Some of these complications can become extremely damaging to the body if left untreated. For instance, retinopathy can result in blindness [139]. The interference of diabetes with wound healing may result in ulcerations, leading to amputations in the worst cases [140, 141].

3.1.4.1. Diabetic nephropathy

Diabetic nephropathy is a kidney disease which is as a result of diabetes [142]. It affects the kidney's ability to do their usual work of waste products and extra fluid removal from the body.

Diabetes affects the tiny blood vessels in the glomerulus, a key structure in the kidney composed of capillary blood vessels and critical for the filtration of blood to remove waste products [142-147]. Diabetic nephropathy is a leading cause of kidney failure worldwide. More than 40% of the people with diabetes are likely to develop diabetic nephropathy.

The association of kidney disease and diabetes is worse than the presence of kidney diseases alone. This is because there is a high possibility that people with diabetes have also other diabetes-related medical conditions such as high blood pressure, high cholesterol, blood vessel diseases, and progressively impaired kidney function. People with diabetes are also more likely to have kidney-related diseases such as nerve damage to the bladder and bladder infections [146, 147]. When diabetic nephropathy is severe, an individual may experience kidney failure (end-stage renal disease) and, as a result, he/she may require kidney dialysis or worse, a kidney transplant [148]. It is said that about 1 in 4 women and 1 in 5 men with type 2 diabetes develops diabetic nephropathy.

3.1.4.2. Diabetic cardiomyopathy

Diabetic cardiomyopathy is a major cause of heart failure among people with diabetes. It is one of the cardiovascular diseases which are leading cause of death amongst diabetic patients [146, 149]. People with diabetes are 2–5 times more likely to develop heart failure as compared to non-diabetic patients [150, 151]. Diabetic cardiomyopathy is known as a specific form of heart disease which is promoted by resistance in the heart tissue to the metabolic actions of insulin (insulin resistance). It is defined as the presence of abnormal cardiac structure and performance in the absence of coronary artery disease, hypertension, and significant valvular disease [152, 153].

3.1.4.3. Diabetic eye diseases

Diabetic eye diseases are a group of eye conditions affecting people with diabetes [154, 155]. These conditions may affect different parts of the eye including the retina, macula, lens and the optic nerve. They are often differentiated based on the parts of the eye that is mostly affected. They include diabetic retinopathy, diabetic macular oedema (DME), diabetic cataract and glaucoma. They can potentially cause severe vision loss and blindness.

3.1.4.3.1. Diabetic retinopathy

Diabetic retinopathy is a very serious sight-threatening complication of diabetes [156, 157]. It is the most common cause of the loss in vision, and a leading cause of blindness and vision impairment, amongst the people with diabetes and the working-age adults. It affects the retina – a light sensitive tissue lining the back of the eye, which is responsible for detecting and converting light to signals sent through the optic nerve to the brain. Retinopathy is a result of the damage caused by diabetes on the tiny blood vessels located in the retina [158]. The damage to these blood vessels is also associated with chronically high levels of glucose in the blood. As a result, the retinal blood vessels may end up leaking fluid into the macula, which is the part of the retina enabling us to see different colours and fine details and, therefore, is the part responsible for clear vision. The macula may swell because of the excess fluid, and this results in blurred vision.

New blood vessels may form on the surface of the retina as an attempt to improve the blood circulation. Since these new blood vessels are very fragile, they can possibly bleed into the back of the eye resulting in the blockage of vision [159, 160].

Diabetic retinopathy can be classified into two types: non-proliferative and proliferative. Non-proliferative diabetic retinopathy (NPDR) is the earlier stage of the disease, where the symptoms are mild. During this stage, the tiny blood vessels in the retina are weak. There are tiny bulges in the blood vessels (microaneurysms) which may begin leaking fluid into the retina. Due to this leakage, the macula may swell.

Proliferative diabetic retinopathy (PDR) is the most advanced stage of the disease, where there are circulation problems which can deprive the retina of oxygen. Cosequently, there is a growth of new and fragile tiny blood vessels in the retina and into the vitreous fluid (the gel-like fluid filling the back of the eye). These tiny blood vessels may leak blood into the vitreous, resulting in a clouded vision [159-162].

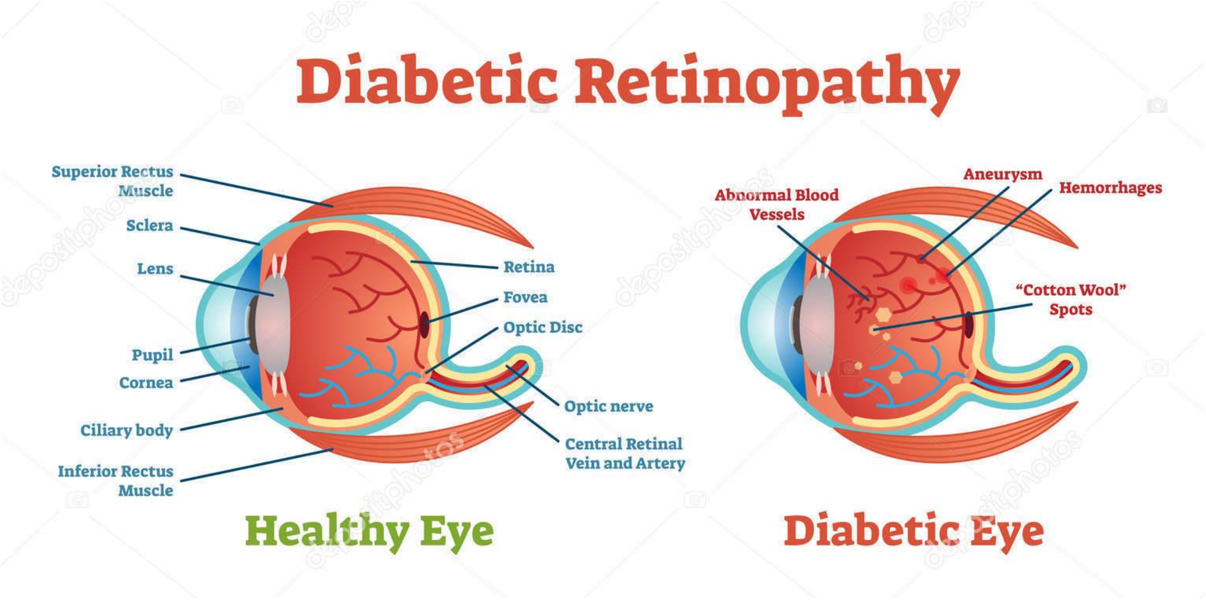


Figure 3.2: Difference between a healthy eye and a diabetic eye [1163].

Figure 3.2 shows the difference between a heathy eye and an eye affected by diabetic retinopathy and other diabetic eye conditions. It also shows the presence of the abnormal tiny blood vessels which are most likely to form on the surface of the retina in an attempt to increase the circulation of blood.

3.1.4.3.2. Diabetic macular edema

Diabetic macular oedema (DME) is characterized by the presence of retinal thickening or the accumulation of fluid in the macula from the damaged blood vessels. DME is the most common cause of vision loss among the people with diabetic retinopathy, and it is said that about half of the people with diabetic retinopathy may develop DME [164]. It is most likely to occur in a worsened case of diabetic retinopathy, but can also occur in any stage of the disease [156, 162, 165].

3.1.4.3.3. Glaucoma

Glaucoma is a group of eye conditions which damages the optic nerve (bundle of nerve fibres connecting the eye and the brain). It is also associated with elevated pressure inside the eye [158, 166]. Glaucoma is known to affects adults, but its risk is doubled for people with diabetes.

3.1.4.3.4. Cataract

Cataract is the clouding of the eye's lens. It is more likely to develop in adults with diabetes than in those without it. It can also develop in people with diabetes at a younger age than for people without diabetes [167, 168].

3.1.4.4. Diabetic neuropathy

Diabetic neuropathy is a very serious and most common complication of diabetes. It is a type of nerve damage which can occur among the people with diabetes [169]. It most commonly affects the nerves of the legs and feet. There are many symptoms of diabetic neuropathy, depending on the nerves damaged, and some damages to the nerves can lead to disability in the worst cases [170].

3.1.4.4.1. Types of diabetic neuropathy

There are four different types of diabetic neuropathy, and it is highly possible for a person to have more than one type. The symptoms develop gradually; therefore, an individual may not notice the damage until a considerable damage to the nerves has already occurred.

These diabetic neuropathy types differ according to the part of the body where the affected nerves are [169-171]:

- **Peripheral neuropathy** is the most common type of neuropathy and it mostly affects first the legs and feet and then the hands and arms. Its symptoms include tingling, sharp pains and increased insensitivity. It may lead to the need for amputation.
- **Autonomic neuropathy** affects the autonomic nervous system, which is the one that controls the heart, stomach, intestines, bladder and the eyes. The nerves in any of these

areas may be affected, resulting in bladder problems, persons' lack of awareness of the low blood sugar levels and increased heart rate.

- **Radiculoplexus neuropathy** affects the nerves in the hips, thighs and legs. It is most common among people with type 2 diabetes and adults. It usually affects only one side of the body.
- **Mononeuropathy** (also referred to as focal neuropathy), is the damage due to diabetes to a specific nerve in the face, middle body and the legs. It is most common among adults and can cause severe pain but not long-term problems. It can also cause problems in the eyes resulting in double vision.

3.1.4.4.2. Complications related to diabetic neuropathy

Diabetic neuropathy may lead to severe complications. They are outlined in the next paragraphs.

3.1.4.4.2.1. Amputations (mostly loss of a foot or leg)

Diabetes has been found to be one of the leading causes of amputation of the lower limbs throughout the world [115, 141]. *Charity Diabetes UK* noted that foot problems are the most frequent reasons for hospitalization amongst patients with diabetes [172]. Reports suggests that people with diabetes are up to 30 times more likely to undergo amputations than those who don't have it [172-175]. Amputations are more common among the elderly and their rate increases with age [141].

Diabetes can lead to peripheral artery disease (PAD) due to elevated blood glucose levels [176, 177]. PAD causes the narrowing of the blood vessels and also a reduction in the amount of blood flowing to the legs and feet [178]. This may result in the nerve damage known as peripheral neuropathy and can prevent a person from feeling pain. This means that individuals may not realize if they have a wound or ulcer on the feet. Continued pressure on the affected area can then cause the ulcer to grow and become infected [177]. Reduced blood flow can slow wound healing and make the body less effective in fighting infections, which results in healing failure for that wound. Tissue damage or gangrene may also inset, and the existing infection may spread to the bones. If the infection does not respond to treatment, or if it is irreparable, then amputation may be necessary. Amputations of toes, feet, and lower legs are the most common [178].

3.1.4.4.2.2. Other complications

Urinary tract infections and urinary incontinence: Damage to the nerves that control the bladder may cause an individual to be unable to empty the bladder fully. There can also be a build-up of bacteria in the bladder and kidneys, causing urinary tract infections. An individual may also be unable to feel the need to urinate or also be unable to control the muscles that release urine which may results in the leakage of urine (incontinence) [171].

Digestive problems: If the nerves in the digestive tract are damaged, an individual may experience diarrhoea or constipation. The nerve damage due to diabetes cause gastroparesis, which is a condition in which the stomach is very slow to empty wastes or even fails to do it. As a consequence, there might be an interference with the digestion, which may severely affect the levels of glucose in the blood. The symptoms may include vomiting and bloating.

Joint damage: Diabetes-related nerve damage can also cause the joints to deteriorate [179]. The deterioration usually occurs in the feet and affects the small joints. The symptoms may include sensitivity loss and swelling, instability and deformity of joints.

Increased or decreased sweating: The nerve damage due to diabetes can cause disruption of the functionality of the sweat glands; therefore, the body may have difficulties controlling the temperature properly. People with autonomic neuropathy may experience excessive sweating during the night or even when they are eating. Too little or no sweating at all may be life-threatening [169, 170].

Sharp drops in blood pressure: If the nerves that controls the flow of blood are damaged due to diabetes, the body’s ability to adjust blood pressure may be affected. This may result in sharp drops in the blood pressure when an individual stands and may cause dizziness and even fainting [170].

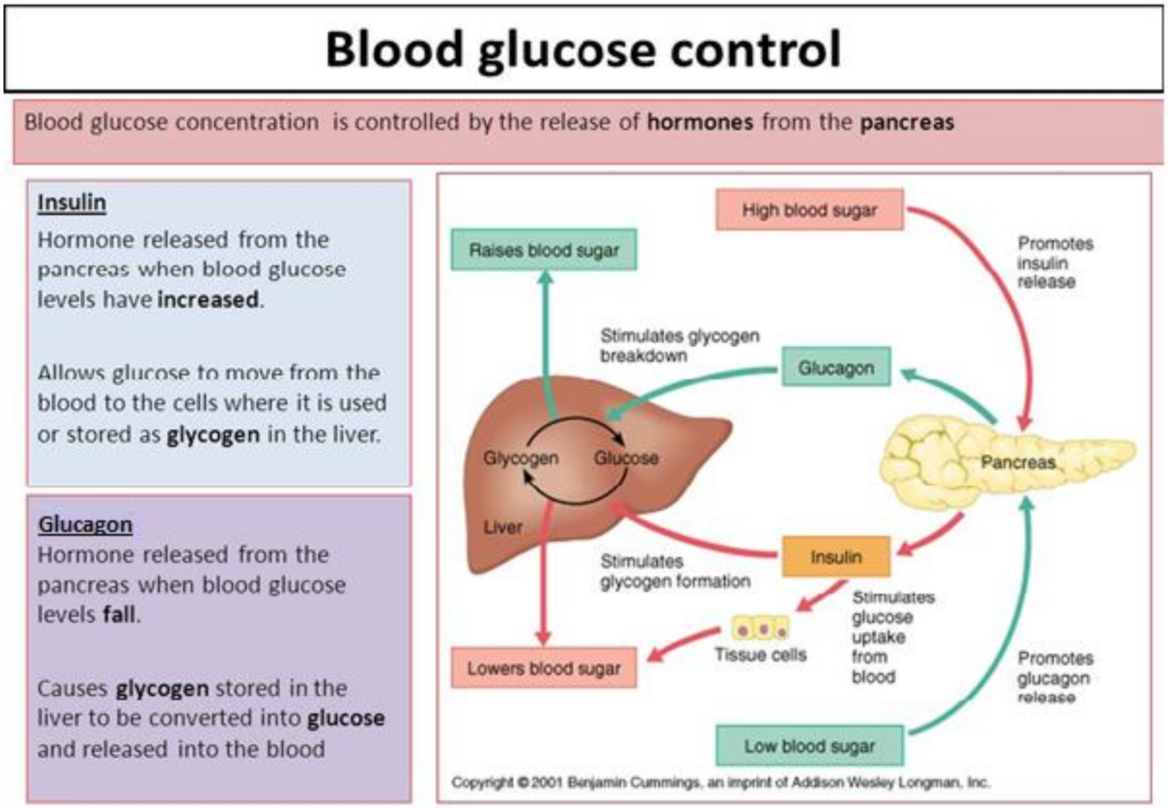
3.1.5. Insulin

3.1.5.1. The action of insulin

Insulin is a major metabolism-regulating hormone which is secreted by β-cells in the pancreas

[180]. The major function of insulin is that of countering the actions of some of the hormones which generate hyperglycaemia and also maintaining low levels of glucose in the blood. In addition to its role in regulating glucose metabolism, insulin stimulates lipogenesis and increases the transportation of amino acids into cells [181]. Insulin also has a role in promoting the storage of dietary calories, thus lowering the circulating levels of glucose coming from carbohydrate throughout the whole body.

Figure 3.3 outlines some of the phenomena that occur in the body and some pathways involving insulin. The liver, skeletal muscles, and adipose tissues are the main target tissues of insulin. Insulin increases the activity of enzymes enhancing glycogen, lipid and protein synthesis in the liver. At the same time, insulin also suppresses the activity of enzymes catalyzing gluconeogenesis and glycogenolysis, which break down the glycogen stored in the liver and muscles into glucose [181, 182]. Insulin stimulates the uptake of glucose, fatty acids and amino acids from the blood, permitting synthesis and storage of glycogen, carbohydrates, lipids, and proteins in the skeletal muscles.



Blood glucose control

Blood glucose concentration is controlled by the release of **hormones** from the **pancreas**

Insulin
Hormone released from the pancreas when blood glucose levels have **increased**.

Allows glucose to move from the blood to the cells where it is used or stored as **glycogen** in the liver.

Glucagon
Hormone released from the pancreas when blood glucose levels **fall**.

Causes **glycogen** stored in the liver to be converted into **glucose** and released into the blood

Figure 3.3. Blood glucose control including the actions of insulin and glucagon and their pathways [183].

Insulin also promotes lipogenesis to store substrates and inhibits lipolysis (breakdown and release of fatty acids by adipose tissue) in adipose tissue. Most of the glucose (80%) that is taken up by peripheral tissues is utilized by muscles with a relatively smaller amount being turned into fat or deposited in the liver [182, 184].

3.1.5.2. Insulin resistances

Insulin resistance is a condition in which the cells in the body are resistant to the effects of insulin; this means that there is a reduction in the response to a given amount of insulin [185]. As a consequence, higher amount of insulin will be required for it to affect the body properly, the pancreas then compensates by producing even more insulin. The resistance may be caused by genetic factors and also some medications can be contributing factors, and is common in people with obesity and during pregnancy. It may occur in response to the body's own insulin or when insulin is administered by injection.

3.1.6. Classification of antidiabetic drugs/agents

Different types of medicines involved in the treatment of diabetes are referred to as antidiabetic agents [186]. These agents aim at reducing the blood sugar levels to an acceptable range and relieving symptoms of diabetes such as thirst, excessive urination, and ketoacidosis [187]. Antidiabetic agents also prevent or slow down the development of diabetic complications, including neuropathy and retinopathy [188].

Table 3.1 outlines the main classification of known antidiabetic agents, including the known drugs for each class and their principal modes of action. Different classes of antidiabetic drugs have different modes of action and are applied in the treatment of different types of diabetes [186–189]. The current work focusses on sulfonylureas.

Table 3.1: Classes of antidiabetic medications against type 2 diabetes

Class	Examples	Principal mode of action
Sulfonylureas	Glimepiride, Glipizide Gliclazide, Tolbutamide, Glyburide, chlorpropamide	Stimulate insulin secretion
Thiazolidinediones	Pioglitazone, Rosiglitazone	Increase insulin action
Alpha-glucosidase inhibitors	Acarbose, Miglitol	Slow down the rate of carbohydrate ingestion
Biguanides	Metformin, Buformin, Phenformin	Improve insulin action
Amylin analogs	Pramilintide	Decrease glucose levels
Sodium Glucose CO - Transporter 2 inhibitors	Remogliflozin, Dapagliflozin	Reduce glucose reabsorption in the proximal renal tubules and lowers renal glucose threshold

3.2. Sulfonylureas

3.2.1. Description of Sulfonylureas

Sulfonylureas are a class of organic compounds used in medicine as antidiabetic drugs [190]. Figure 3.4 shows their general molecular structure. It comprises a benzene ring with two mutually para substituents: an R^1 group and the thiourea group (a sulphonyl group to which a urea group is attached). A substituent R^2 may be attached to the urea group. Different molecules differ by the nature of R^1 and R^2, which can be either cyclic or acyclic organic groups [191].

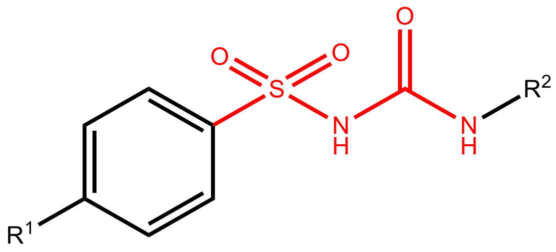
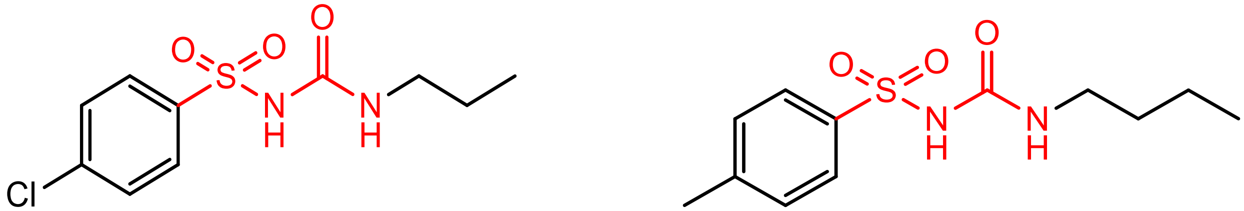


Figure 3.4. General structure of sulfonylureas molecules

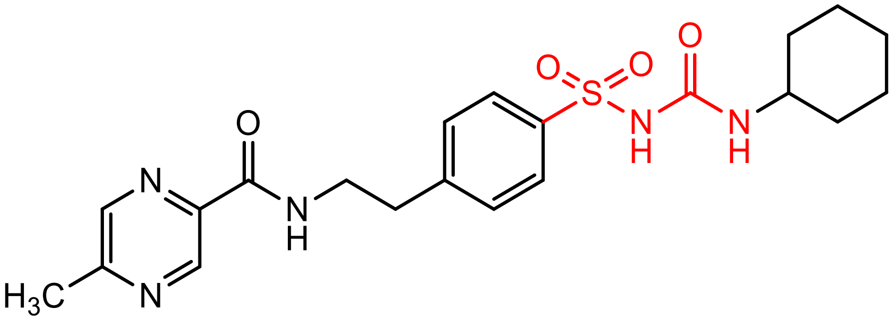
The sulfonylureas molecules are further divided in two categories, namely, first-generation and second-generation sulfonylureas molecules [192]. The main difference between the two classes is the way in which they bind to the sulfonyl receptor, with the second generation binding more tightly and thus requiring a lower dose to stimulate the secretion of the same amount of insulin [2, 193]. First generation sulfonylureas include chlorpropamide and tolbutamide (figure 3.5). The second-generation sulfonylureas include glipizide and glimepiride (figure 3.6) [192].



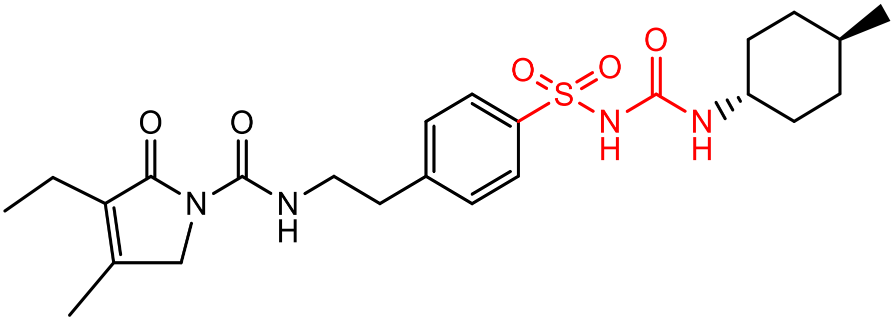
Chlorpropamide

Tolbutamide

Figure 3.5: Examples of first-generation sulfonylureas



Glipizide



Glimepiride

Figure 3.6: Examples of second-generation sulfonylureas

3.2.2. Mechanism of action of sulfonylureas

Sulfonylureas are widely used in the management of type 2 diabetes mellitus, when it is still possible to manage it without insulin injections. Sulfonylureas lower blood glucose levels by stimulating insulin release from the β-cells of the pancreas [194]. Their action depends on the presence of functioning β-cells; so, they are ineffective where there is absolute deficiency of insulin production, such as in type 1 diabetes, or in post-pancreatectomy situations.

Sulfonylureas stimulate insulin release by blocking ATP (adenosine triphosphate) sensitive potassium channels in the β-cells, thus reducing potassium permeability. They bind to an ATP-dependent K^+ (KATP) channel on the cell membranes of pancreatic β-cells, thus inhibiting a tonic, hyperpolarizing outflux of potassium, which would cause the electric potential over the membrane to become more positive. This causes depolarization of the cell membrane and increases calcium entry [195]. The rise in intracellular calcium leads to increased fusion of insulin granules with the cell membrane and, therefore, increases the secretion of insulin.

Sulfonylureas can also sensitize β-cells to glucose, in such a way that they limit the production of glucose in the liver in order to decrease lipolysis (breakdown and release of fatty acids by adipose tissue) and also decrease the clearance of insulin by the liver [196, 197]. Moreover, they inhibit glucagon secretion and sensitize target tissues to the action of insulin. These drugs rapidly lower the blood sugar level but also run a risk of causing hypoglycaemia.

Chapter 4

Results

This chapter presents the results of the calculations on the sulfonylureas molecules considered in this study. The chapter analyses the results according to selected criteria. The conclusions will then be summarised in chapter 5.

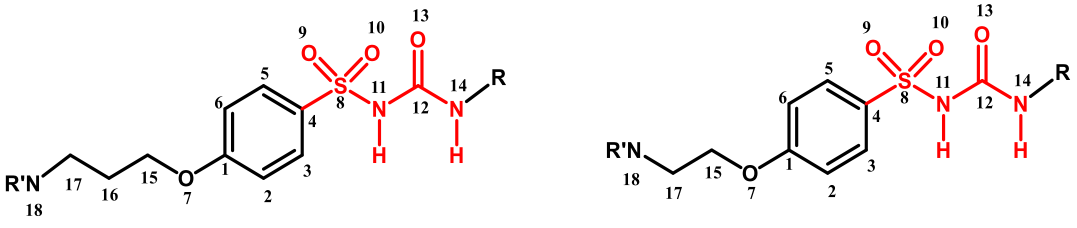
4.1. Molecules considered

4.1.1. Description of the molecules considered

The molecules considered in this work are sulfonylureas (section 3.2) with specific characteristics. Figure 4.1. shows the general structure of the considered sulfonylureas molecules and the atom numbering for the atoms that are present in all these molecules. It is considered important to give the same numbers to the atoms present in the same positions in all the molecules to facilitate descriptions and comparisons.

All the molecules have the sulfonylurea moiety attached to a benzene ring (a group typical of sulfonylureas molecules) and an oxygen atom (O7) attached to the benzene ring in para position with respect to the sulfonylurea moiety; furthermore, a group R is attached to the outer nitrogen atom of the thiourea group, and an alkylic chain is attached to O7 and ends with a nitrogen atom (N18), to which another group, R′, is attached. Substituents R and R′ can be either cyclic or acyclic. The length of the chain between O7 and N18 is not constant, as the chain may contain either two or three carbon atoms. The general atom numbering (figure 4.1) is referred to the case where the chain contains three carbon atoms (figure 4.1 left). When it contains only two carbon atoms, the number 16 is not present (figure 4.1, right.). The hydrogen atoms take the numbers of the atoms to which they are attached; for instance, H2 is a hydrogen atom attached to the C2 carbon atom.

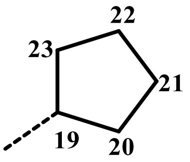
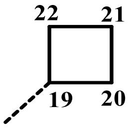
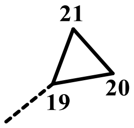
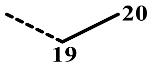
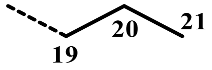
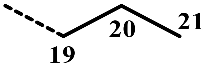
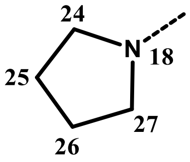
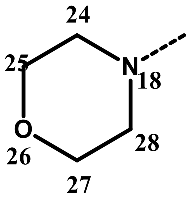
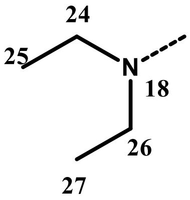
R and R′ may have different nature and, therefore, different numbers of atoms. The atoms of R are numbered before the atoms of R′. The lowest atom number in 19 for all the R groups; the highest atom number (23) pertains to the pentagonal R. In order to ensure that the same R′ has the same atom numbering in all the compounds (whichever the R), the numbering of the atoms of R′ starts with the number 24. Table 4.1 shows the numbering of the atoms of the different R and R′.



Three carbon atoms between O7 and N18 Two carbon atoms between O7 and N18

Figure 4.1. General structure of the sulfonylureas molecules considered in this work and atom numbering utilized for the atoms that are present in all the molecules. The sulfonylurea moiety is coloured in red.

Table 4.1. Atom numbering of the different R and R′ appearing in the compounds considered.

Group	Structures of the groups with atom numbering		
R			
			
R′			

4.1.2. Classification and naming of the molecules considered

The molecules considered were classified on the basis of their differences. This yields three criteria, namely, the nature of R, the nature of R′, and the length of the chain between O7 and N18. The classification hierarchy is illustrated by the flow chart in figure 4.2.

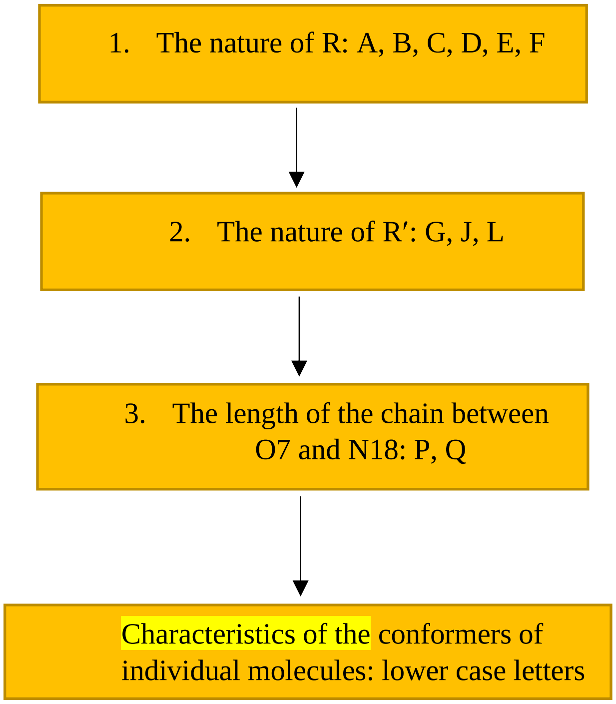


Figure 4.2. Illustration of the hierarchy of the classification criteria used for the sulfonylureas molecules and letters selected to denote the characteristics for each criterion.

The compounds and their conformers are concisely denoted by acronyms, in which each of the features corresponding to the classification criteria is denoted by an upper-case letter, as shown in figure 4.2 and table 4.2. Using acronyms reflecting this classification is important because it facilitates comparisons of compounds with one or more similar characteristics.

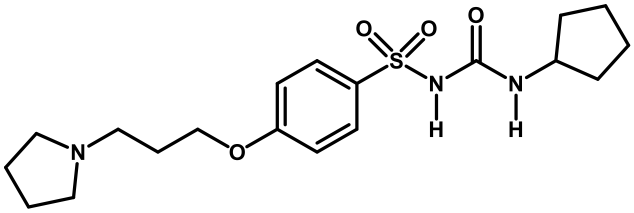
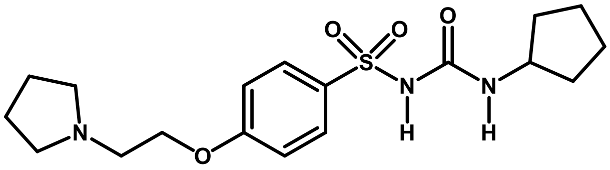
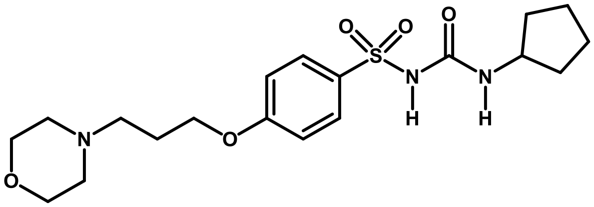
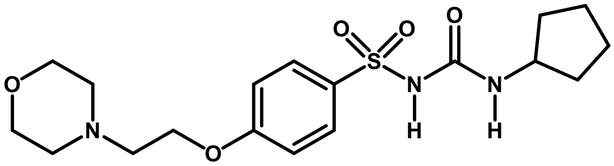
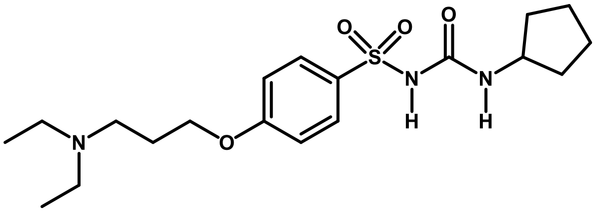
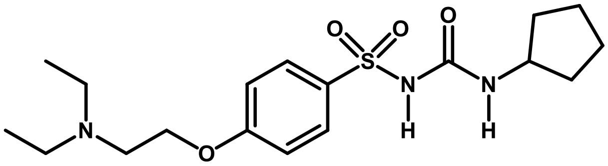
Table 4.2. Letters used to denote the characteristics related to the classification of the compounds considered in this work.

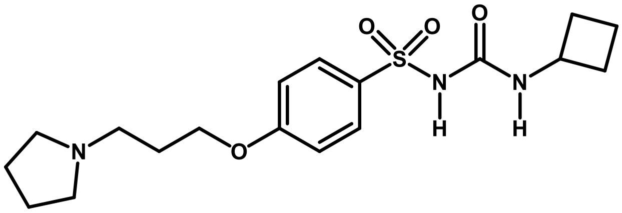
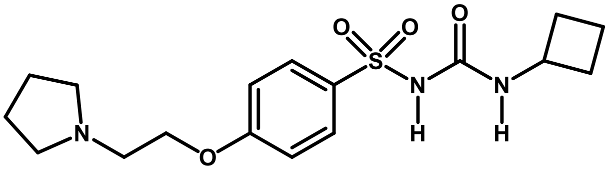
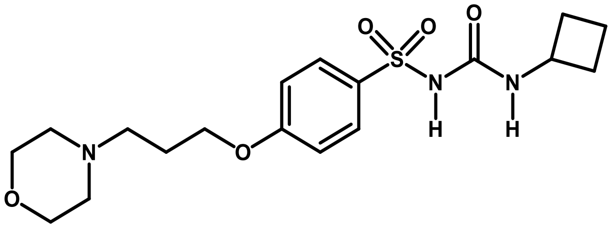
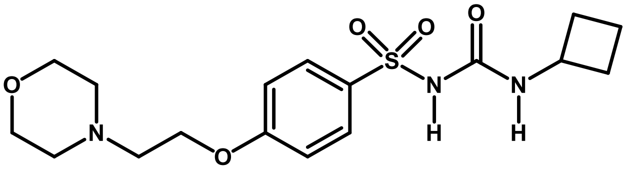
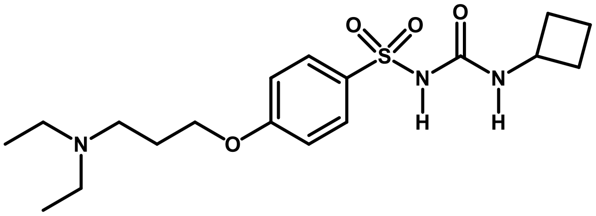
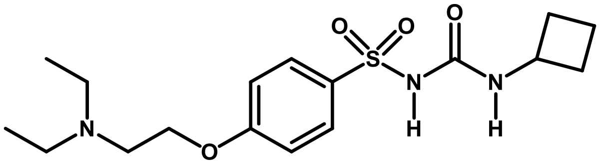
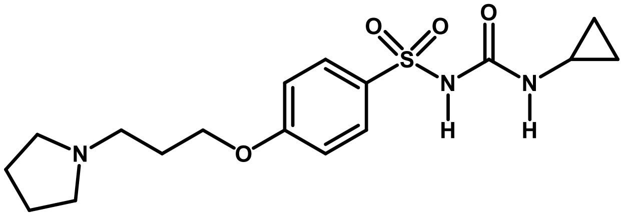
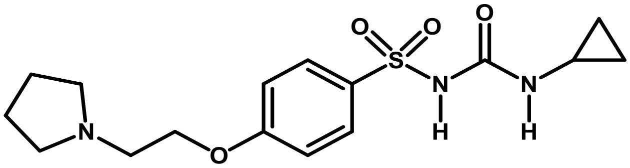
Characteristics	Letter	Description	Characteristics	Letter	Description
Nature of R	A	Cyclopentane	Nature of R′	G	Pyrrolidine
	B	Cyclobutene		J	Morpholine
	C	Cyclopropane		L	Diethylamine
	D	Methane			
	E	Ethane	Length of chain between O7 and N18	P	3 carbons
	F	Propane		Q	2 carbons

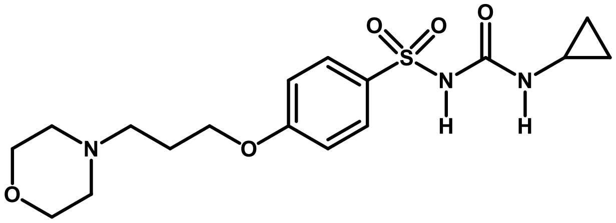
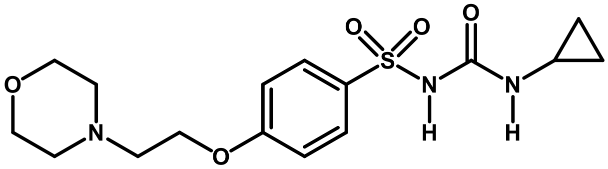
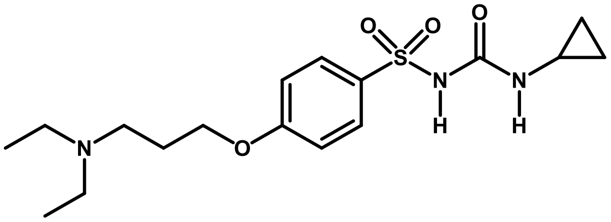
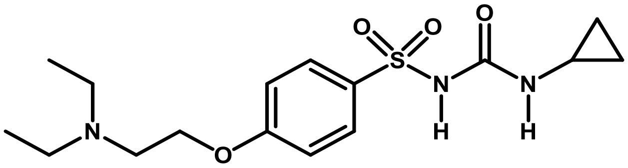
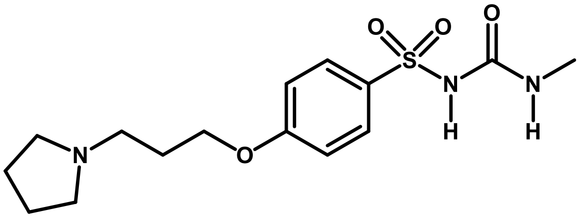
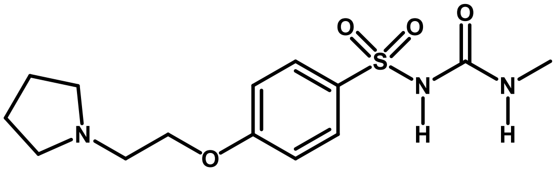
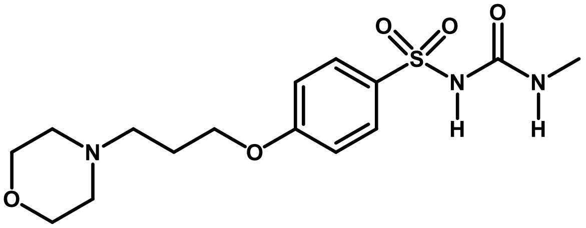
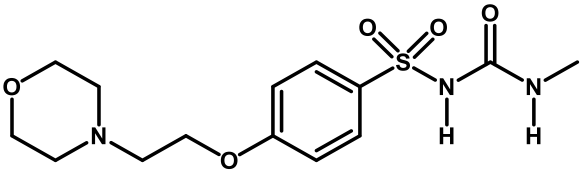
4.1.3. List of the molecules considered

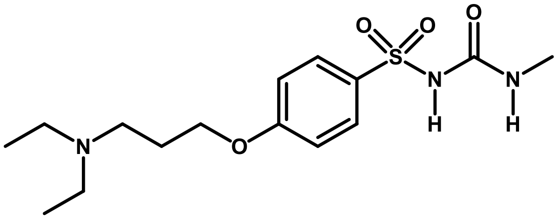
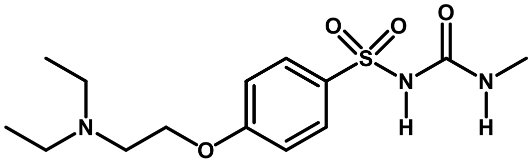
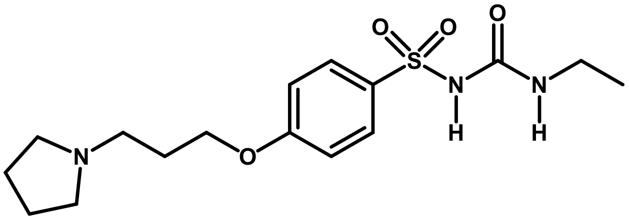
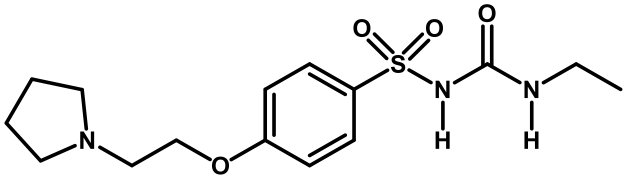
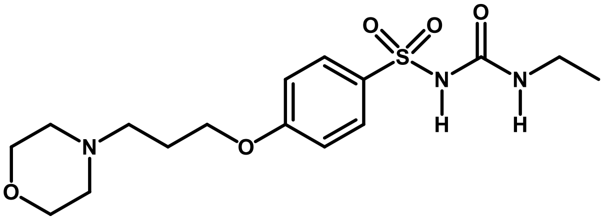
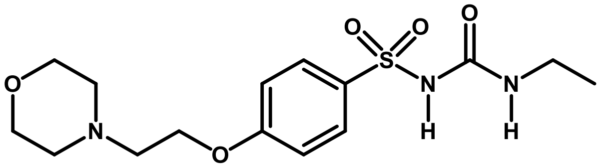
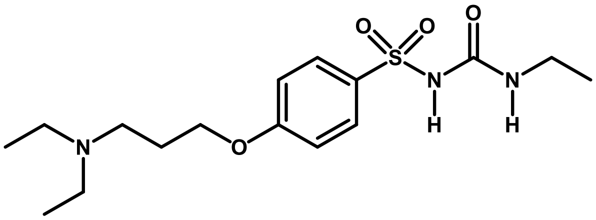
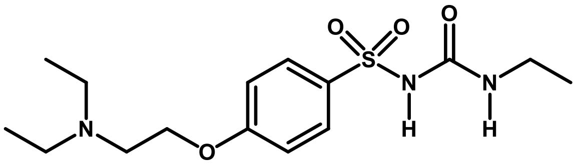
36 compounds were considered in this work. Table 4.3 lists all the compounds, showing their structures and giving their chemical names and the acronyms used in this work to denote them concisely. The molecules are grouped into 6 groups on the basis of the nature of R (groups A, B, C, D, E and F, table 4.2).

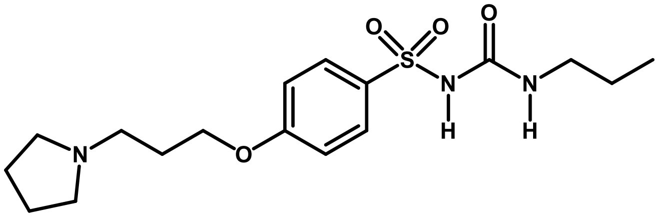
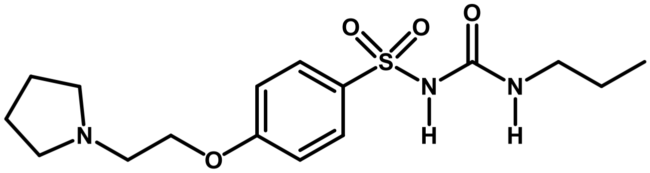
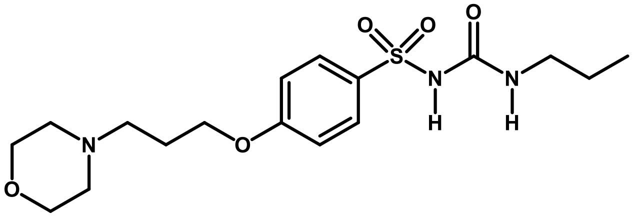
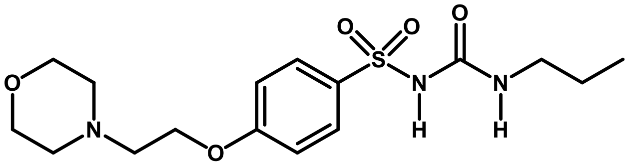
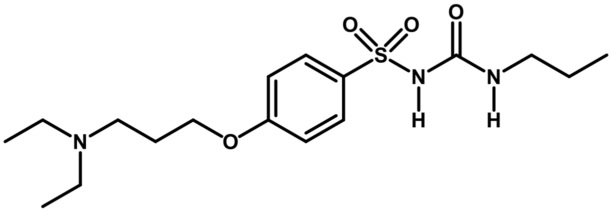
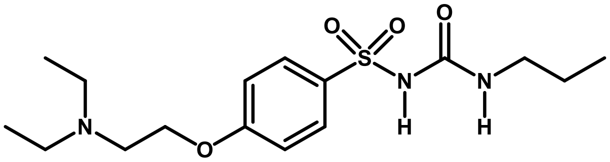
Table 4.3. List of the compounds considered in this work. The space under each structure reports the IUPAC name of that structure, and (in a separate line) the acronym used in this work

Group A molecules	
	
N-(cyclopentylcarbomyl)-4-(3-(pyrrolidin-1-yl) propoxy) benzosulfamide AGP	N-(cyclopentylcarbomyl)-4-(2-(pyrrolidin-1-yl) ethoxy) benzosulfamide AGQ
	
N-(cyclopentylcarbomyl)-4-(3-morphilinopropoxy) benzosulfamide AJP	N-(cyclopentylcarbomyl)-4-(2-morphilinoethoxy) benzosulfamide AJQ
	
N-(cyclopentylcarbomyl)-4-(3-(diethylamino)propoxy) benzosulfamide ALP	N-(cyclopentylcarbomyl)-4-(2-(diethylamino)ethoxy) benzosulfamide ALQ

Group B molecules	
	
N-(cyclobutylcarbomyl)-4-(3-(pyrrolidin-1-yl) propoxy) benzosulfamide BGP	N-(cyclobutylcarbomyl)-4-(2-(pyrrolidine-1-yl) ethoxy) benzosulfamide BGQ
	
N-(cyclobutylcarbomyl)-4-(3-morphilinopropoxy) benzosulfamide BJP	N-(cyclobutylcarbomyl)-4-(2-morphilinoethoxy) benzosulfamide BJQ
	
N-(cyclobutylcarbomyl)-4-(3(diethylamino)propoxy) benzosulfamide BLP	N-(cyclobutylcarbomyl)-4-(2-(diethylamino)ethoxy) benzosulfamide BLQ
Group C molecules	
	
N-(cyclopropylcarbomyl)-4-(3-(pyrrolidin-1-yl) propoxy) benzosulfamide CGP	N-(cyclopropylcarbomyl)-4-(2-(pyrrolidine-1-yl) ethoxy) benzosulfamide CGQ

	
N-(cyclopropylcarbomyl)-4-(3-morphilinopropoxy) benzosulfamide CJP	N-(cyclopropylcarbomyl)-4-(2-morphilinoethoxy) benzosulfamide CJQ
	
N-(cyclopropylcarbomyl)-4-(3(diethylamino)propoxy) benzosulfamide CLP	N-(cyclopropylcarbomyl)-4-(2-(diethylamino)ethoxy) benzosulfamide CLQ
Group D molecules	
	
N-(methylcarbomyl)-4-(3-(pyrrolidin-1-yl) propoxy) benzosulfamide DGP	N-(methylcarbomyl)-4-(2-(pyrrolidine-1-yl) ethoxy) benzosulfamide DGQ
	
4-(3-(morphilinopropoxy)-N-(methylcarbomoyl) benzosulfamide DJP	4-(2-morphilinoethoxy)-N-(methylcarbomoyl) benzosulfamide DJQ

	
4-(3-(diethylamino)propoxy)-N-(methylcarbomoyl) benzosulfamide DLP	4-(2-(diethylamino)ethoxy)-N-(methylcarbomoyl) benzosulfamide DLQ
Group E molecules	
	
N-(ethylcarbomyl)-4-(3-(pyrrolidin-1-yl) propoxy) benzosulfamide EGP	N-(ethylcarbomyl)-4-(2-(pyrrolidine-1-yl) ethoxy) benzosulfamide EGQ
	
4-(3-(morphilinopropoxy)-N-(ethylcarbomoyl) benzosulfamide EJP	4-(2-morphilinoethoxy)-N-(methylcarbomoyl) benzosulfamide EJQ
	
4-(3-(diethylamino) propoxy)-N-(ethylcarbomoyl) benzosulfamide ELP	4-(2-(diethylamino)ethoxy)-N-(ethylcarbomoyl) benzosulfamide ELQ

Group F molecules	
	
N-(propylcarbomyl)-4-(3-(pyrrolidin-1-yl) propoxy) benzosulfamide FGP	N-(propylcarbomyl)-4-(2-(pyrrolidine-1-yl) ethoxy) benzosulfamide FGQ
	
4-(3-(morphilinopropoxy)-N-(propylcarbomoyl) benzosulfamide FJP	4-(2-morphilinoethoxy)-N-(propylcarbomoyl) benzosulfamide FJQ
	
4-(3-(diethylamino)propoxy)-N-(propylcarbomoyl) benzosulfamide FLP	4-(2-(diethylamino)ethoxy)-N-(propylcarbomoyl) benzosulfamide FLQ

4.2. Selection of the computational methods

The selection of the computational methods for this study was based on a balance between results' accuracy and affordability of the computational cost.

All the calculations were done in *vacuo* using two methods with different nature: Hartree-Fock (HF), an *ab initio* method, and the Density Functional Theory (DFT) method. All the calculations were performed with full geometry optimization to identify the closest stable conformation for each input considered. The 6-31G(d,p) basis set was used for HF calculations. This level had proven to be the simplest, less expensive method capable of giving reasonable views of conformational preferences for other classes of molecules [198, 199].

The DFT calculations utilized the Becke, 3-parameter, Lee–Yang–Parr (B3LYP) functional [84–87] with the 6-31+G(d,p) basis set. It was decided to use a basis set containing also the diffuse functions on the heavy atoms because this contributes to a better description of hydrogen bonding.

Frequency calculations were performed at both the HF/6–31G(d,p) and the DFT/B3LYP/6-31+G(d,p) levels. They were performed as single point calculations on the corresponding (HF and DFT) optimized geometries. The calculated frequencies were scaled by 0.8992 for HF calculations and 0.9648 for DFT calculations [200].

4.3. Preparation of inputs

Different inputs were prepared considering the relevant aspects by which the conformers may differ, resulting in criteria for identifying the conformers. These include considering different orientations of the thiourea group with respect to the benzene ring by rotation of the C4–S8 bond; different orientations of the atoms in the thiourea group by rotating single bonds; and different orientations of the chain between O7 and N18 with respect to the benzene ring, by changing the C6–C1–O7–C15 dihedral angle. The geometry of the rest of the chain between O7 and N18 was taken as linear, as the usually preferred one.

4.4. Computational results

4.4.1. Identification and naming of conformers

The energy and the geometry of the conformers are influenced by the following factors: the presence of intramolecular hydrogen bonds (IHBs); the orientation of the chain between O7 and N18 with respect to the benzene ring (C6–C1–O7–C15 dihedral angle); the orientation of R with respect to the sulfonylurea moiety. The orientation of the sulfonylurea moiety with respect to the benzene ring and the geometry of the sulfonyl urea moiety itself are determined by the IHBs and, therefore, they are not considered separately.

The description of a conformer must specify all these characteristics. In order to specify them concisely, lowercase letters are utilized to denote each of them. The letters are combined into acronyms used to denote individual conformers. Letters in combination with numbers are used to denote identified different orientations of R with respect to the benzene ring, in correspondence to the different dihedral angles. All the letters and their meanings are listed in table 4.4.

Table 4.4. Characteristics of the conformers of the molecules considered and letters utilized to denote them concisely.

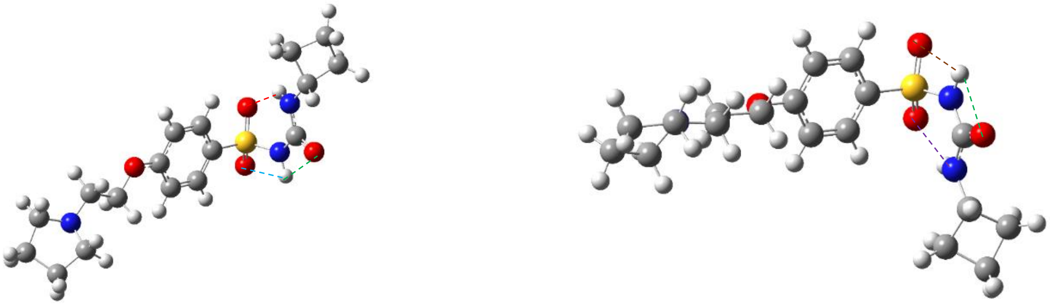
Symbol	Meaning
m	Three simultaneous IHBs present (H11····O10, H11····O13 and H14····O9); the C4–S8–N11–H11 dihedral angle is ≈ 86°
p	Three simultaneous IHBs present (H11····O9, H11····O13, H14····O10); the C4–S8–N11–H11 dihedral angle is ≈ -86°
k	Two simultaneous IHBs present (H11····O13, H14····O10); the C4–S8–N11–H11 dihedral angle is ≈ -55°
g	One IHB present (H11····O9); the C4–S8–N11–H11 dihedral angle is ≈109°
j	The C4–S8–N11–H11 dihedral angle is ≈ -42°
q	The C6–C1–O7–C15 dihedral angle is ≈180°
r	The C6–C1–O7–C15 dihedral angle is ≈ 0°
s	The C6–C1–O7–C15 dihedral angle is ≈ 90°
t	The C6–C1–O7–C15 dihedral angle is ≈ -90°
u1	The H14–N14–C19–H19 dihedral angle is ≈ 163° for A
u2	The H14–N14– C19–H19 dihedral angle is ≈ 12° for A
u3	The H14–N14– C19–H19 dihedral angle is ≈ -163° for A
u4	The H14–N14– C19–H19 dihedral angle is ≈ -12° for A
v1	The H14–N14– C19–H19 dihedral angle is ≈ 163° for B
v2	The H14–N14– C19–H19 dihedral angle is ≈ 12° for B
v3	The H14–N14– C19–H19 dihedral angle is ≈ -163° for B
v4	The H14–N14– C19–H19 dihedral angle is ≈ -12° for B
v5	The H14–N14– C19–H19 dihedral angle is ≈ 98° for B
w1	The H14–N14– C19–H19 dihedral angle is ≈ 133° for C
w2	The H14–N14– C19–H19 dihedral angle is ≈ 19° for C
w3	The H14–N14– C19–H19 dihedral angle is ≈ -113° for C
w4	The H14–N14– C19–H19 dihedral angle is ≈ -19° for C
w5	The H14–N14– C19–H19 dihedral angle is ≈ 90° for C
w6	The H14–N14– C19–H19 dihedral angle is ≈ -90° for C
x1	The H14–N14– C19–C20 dihedral angle is ≈ 40° for E and F
x2	The H14–N14– C19–C20 dihedral angle is ≈ 90° for E and F
x3	The H14–N14– C19–C20 dihedral angle is ≈ -40° for E and F

x4	The H14–N14– C19–C20 dihedral angle is ≈ -90° for E and F

Five different types of IHBs can be present in these molecules, for a maximum of three in each conformer. These IHBs are: N11–H11····O9, N11–H11····O10, N11–H11····O13, N14–H14····O9 and N14–H14····O10. The N11–H11····O9 and N11–H11····O10 IHB cannot be present simultaneously in the same conformer; similarly, the N14–H14····O9 and N14–H14····O10 IHBs cannot be present simultaneously in the same conformer.

When three IHBs are present simultaneously in a conformer, the two following combinations are possible: N11–H11····O9, N11–H11····O13 and N14–H14····O10 or N14–H14····O9, N11–H11····O13 and N14–H14····O9. They are denoted as m and p respectively, and they correspond to opposite orientations of the C4–S8–N11–H11 dihedral angle. Therefore, these conformers are symmetrical. The three simultaneous IHBs involve bifurcation on the H11 hydrogen atom (N11–H11····O9 and N11–H11····O13, or N11–H11····O10 and N11–H11····O13). Figure 4.3 shows these two combinations. Altogether, all the five different IHBs are shown in the figure 4.3.

When two IHBs are present simultaneously in a conformer, the following options are possible: N11–H11····O13 and N14–H14····O9 or N11–H11····O13 and N14–H14····O10; there is no bifurcation. The N11–H11····O13 IHB is always present when two or three IHBs are present simultaneously in a conformer. When only one IHB is present in a conformer, it is either N11–H11····O9 or N11–H11····O10.



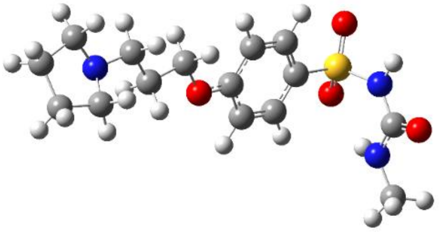
m

p

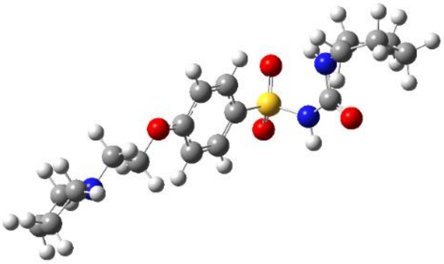
Figure 4.3. Examples of conformers containing three IHBs simultaneously.

The figure shows the two possible combinations, respectively denoted as m and p. The IHBs are indicated by dotted segments and different colours are used for each IHB: blue for H11····O10, red for H14····O9, green for H11····O13, purple for H14····O10, dark orange for H11····O9.

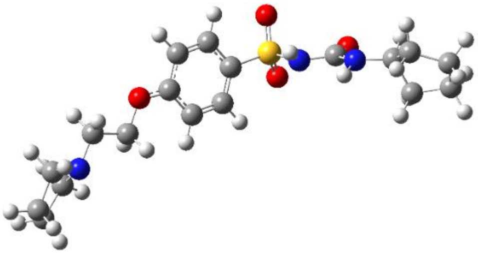
Five different orientations are possible for the thiourea group with respect to the benzene ring. They differ by the value of the C4–S8–N11–H11 dihedral angle (table 4.3, figure 4.4).



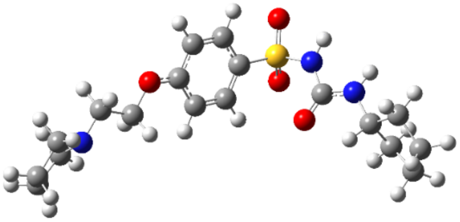
C4–S8–N11–H11 ≈ -86º (p)



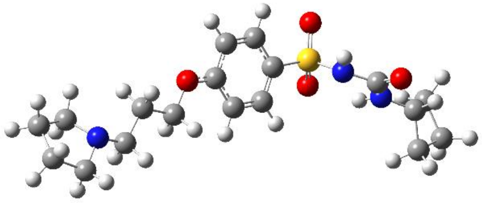
C4–S8–N11–H11 ≈ 86º (m)



C4–S8–N11–H11 ≈ -55º (k)



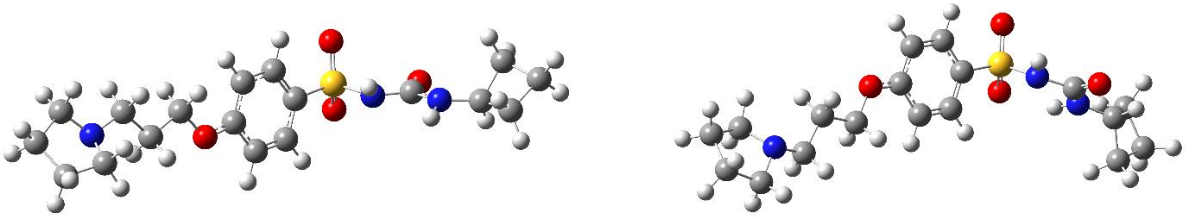
C4–S8–N11–H11 ≈109º (g)



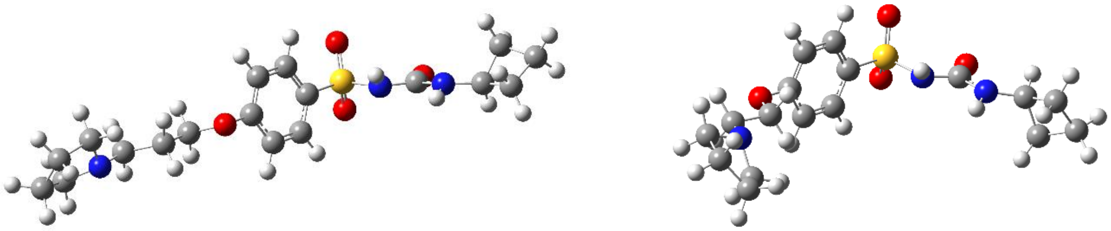
C4–S8–N11–H11 ≈ -42º (j)

Figure 4.4. Different orientations of the thiourea group with respect to the benzene ring and corresponding values of the C4–S8–N11–H11 dihedral angles. The letters denoting the given orientations in the conformers' acronyms are indicated in parentheses.

Four different orientations of the chain between O7 and N18 with respect to the benzene ring are possible, corresponding to four different values of the C6–C1–O7–C15 dihedral angle. The orientations are denoted by the letters q, r, s and t (table 4.3) as illustrated in figure 4.5. The orientations corresponding to the letters q and r are the most frequent.



C6–C1–O7–C15 ≈ 180º (q)   C6–C1–O7–C15 ≈ º0 (r)



C6–C1–O7–C15 ≈ 90º (s)   C6–C1–O7–C15 ≈ -90º (t)

Figure 4.5. Illustration of the different geometries of the chain between O7 and N18 with respect to the benzene ring. The value of the C6–C1–O7–C15 dihedral angle is shown under each image, followed by the letter denoting these features in the conformers' acronyms.

The conformational preferences of individual molecules are mostly influenced by the intramolecular hydrogen bonds (IHBs), and therefore, the characteristics of the IHBs will be given specific attention (section 4.4.3.3). On comparing different molecules, it is clear that the nature of R and R′ have greater influence than the length of the chain between O7 and N18. Therefore, this influence will be analysed more in detail. Since two computational methods have been used in this study, it is also interesting to compare the trends identified by the results of the two methods.

4.4.2. Organization of the material presenting results

4.4.2.1. Organisation criteria

The data obtained for the computational results are organized in tables, and those that require images are also organized in figures. All these tables and figures are at the end of the thesis in a separate chapter (chapter 6); including them in the text would make readability difficult because they are bulky. Only tables and figures that are sufficiently small and essential for the comprehension of the text are inserted in the text. Tables presenting the ranges of each of the molecular properties considered in the analysis are included at the end of this chapter (tables 4.5–4.15).

Both in the tables and in the figures, the compounds are listed according to their groups (A, B, C, D, E and F). Within each group, the compounds are listed in alphabetical order based on the letters denoting the different R′ (G, J, L) and the letters denoting the different O7 to N18 chain lengths (P and Q). For example, in group A, the compounds are listed as follows: AGP, AGQ, AJP, AJQ, ALP, ALQ. The conformers of the same compound are listed in order of increasing DFT relative energies.

4.4.2.2. Summary of tables in chapter 6

In all the tables reporting numerical values, both the HF and DFT results are included. The tables are grouped according to the properties considered, and, for each property, there is one table for each compound. The contents of the tables are as follows:

- Table 6.1–6.36 report the relative energies, the HOMO-LUMO energy gaps and the dipole moments of individual conformers for each of the compounds considered. These properties were grouped together in order to avoid increasing the number of separate tables for different properties, and also to be able to easily identify possible relationship or correspondences between the relative energies and the other two properties. As will be explained later, in many cases, conformers with very close, almost identical relative energies were obtained from different inputs, with both calculation methods; all these conformers were included in the tables to present all the results obtained.

- Tables 6.37–6.72 report the relative energies corrected for zero-point energy and the Gibbs free energies (sum of electronic and thermal free energies) from the frequency calculations. The uncorrected energies (from tables 6.1–6.36) are reported in the first column for comparison purposes.
- Tables 6.73–6.108 report the ZPE corrections and the corrections to the Gibbs free energies.
- Tables 6.108–6.144 report the parameters of the hydrogen bonds (bond lengths, N····O distances (donor····acceptor distances), and N$\hat{H}$O bond angles). All the IHBs present in the conformers are included. The conformers without any IHB are not included in these tables.
- Tables 6.145–6.180 report the vibrational frequencies (harmonic approximation) of the N11–H11 and N14–H14 bonds for all conformers in each of the molecules considered.
- Tables 6.181–6.216 show the red shifts (section 4.3.3.6) in the vibrational frequencies of the N11–H11 and N14–H14 bonds for all the cases in which these two bonds are engaged in an IHB.

4.4.2.3. Summary of figures in chapter 6

There are four sets of figures, namely:

- Figures 6.1–6.36, showing the optimized geometries of the calculated conformers of each compound
- Figures 6.37–6.72, showing the shapes of the HOMO and LUMO molecular orbitals of the calculated conformers of each compound
- Figures 6.73–6.108, showing graphs comparing the relative energies from the DFT and HF results.
- Figures 6.109–6.144, showing graphs comparing the uncorrected relative energies, the relative energy corrected for ZPE, and the Gibbs free energies from DFT and HF results.

4.4.2.4. Appendix A

This appendix contains tables providing information about relations between inputs and outputs, to highlight cases where different inputs optimise to the same outputs:

- Tables A1–A36 shows the input geometries and the resulting outputs conformers for all the compounds.
- Table A37–A38 shows the types of conformers and what they optimized to for different R′ group.

4.4.3. Relative energies

4.4.3.1. Factors influencing conformers' relative energies

4.4.3.1.1. Conformers differing by the intramolecular hydrogen bonds present and the related geometry of the thiourea group

The relative energies of the conformers (tables 6.1–6.36) are greatly influenced by the types and numbers of the IHBs present and by the associated geometry of the thiourea group.

For most of the molecules considered, most conformers have relative energies below 4 kcal/mol and contain IHBs. The majority of the low energy conformers have three simultaneous IHBs (m and p conformers); others have two simultaneous IHBs (k conformers); and few conformers have only one IHB (g conformers). Most of the conformers whose relative energy is not much greater than 4 kcal/mol have one IHB (g conformers). The highest energy conformers have no IHBs (j conformers). Conformers of different types have different relative energy ranges, depending on the compound; the ranges are shown in table 4.5.

The lowest energy conformer of each of the molecules considered has three simultaneous IHBs, with the exception of the BLP-k-q-v1 conformer, with relative energies 0.000 kcal/mol/DFT and 0.132 kcal/mol/HF (table 6.11, figure 6.11), which has only two simultaneous IHBs.

Figure 4.5 shows a conformer (CJP-m-r-w1) with three simultaneous IHBs, visualized using a space filling model to better highlight the IHBs. The image shows all the IHBs possible for the m combination. The H14····O9 IHB appears in the bottom part of the image. The bifurcated H11····O10 and H11····O13 IHBs are seen in the top part of the image. The two sp^2 oxygen atoms O10 and O13 are on either side of H11and each of them forms an IHB with H11 (H11····O10 and H11····O13 respectively); in this way, H11 is donor to both O10 and O13. The image also shows the better directionality of the H14····O9 IHB and the poorer directionality of the two bifurcated

IHBs (H11····O9 and H11····O13). The directionality of the H14····O9 IHB suggests that it is stronger than the bifurcated IHBs. The fact that H14····O9 closes a six-member ring also suggests that it is stronger than the other two IHBs, which close four member rings. The conformer shown in fig. 4.6 is an m conformer; similar situations can be observed for the p conformers.

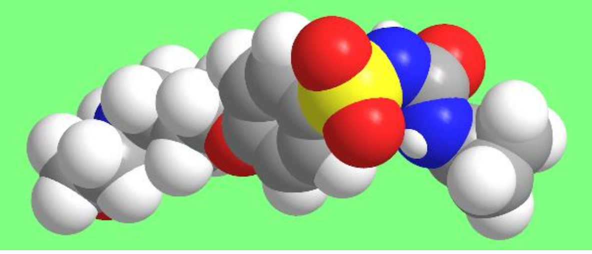
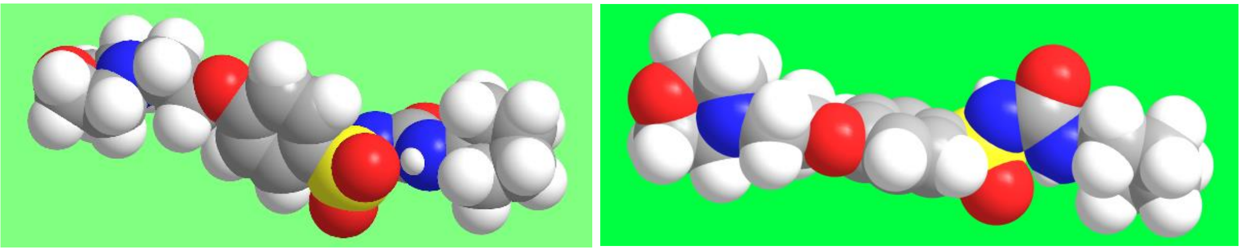


Figure 4.6. Space filling image of conformer CJP-m-r-w1, having three simultaneous IHBs. (Relative energy of this conformer: 0.229 kcal/mol/DFT and 0.664 kcal/mol/HF).

The m and p conformers differ only by the combinations of three simultaneous IHBs. They are symmetrical (section 4.4.1). They mostly have the same relative energies, or their energy difference is negligible. For example, conformers AJQ-p-r-u3 and AJQ-m-q-u1 have very close relative energies (0.615 kcal/mol/DFT, 0.707 kcal/mol/HF and 0.617 kcal/mol/DFT, 0.713 kcal/mol/HF respectively; table 6.4, figure 6.4). When conformers differ by other factors besides the IHBs, their energies can be significantly different. For example, the relative energies (kcal/mol) of CJP-p-q-w3 and CJP-m-q-w2 are 0.000/DFT, 0.000/HF and 2.830 /DFT, 3.663/HF respectively (table 6.15); this relative energy difference may be due to the different orientations of the R=cyclopentyl group (as indicated by the w3 and w2 symbols).

Figure 4.7 shows space filling models of a sample k conformer (AJQ-k-q-u1). The molecule is viewed from two different perspectives to better highlight the two IHBs. The directionality of the H14····O10 IHB is clearly better than the directionality of the H11····O13.



Focusing on the H14····O10 IHB showing both IHBs

Figure 4.7. Space filling images of conformer AJQ-k-q-u1, which has two simultaneous IHBs. (Relative energy of this conformer: 1.175 kcal/mol/DFT and 1.466 kcal/mol/HF).

In most cases, the k conformers have higher relative energies than the m and p conformers, although remaining in the range of the lower energy conformers. This is because the k conformers have one IHB less than the m and p conformers, implying that the m and p conformers are more stabilized than the k conformers. Their relative energies are comparatively close; for instance, the highest energy k conformer of compound AJQ (AJQ-k-r-u1) has relative energies 1.974 kcal/mol/DFT and 2.390 kcal/mol/HF (table 6.4) (the lowest energy k conformer of AJQ is shown in fig. 4.7).

The only case where a k conformer has the lowest relative energy concerns compound BLP, where the BLP-k-q-v1 conformer has 0.000 kcal/mol/DFT and 0.132 kcal/mol/HF relative energy.

There are also cases in which some k conformers have relative energies slightly lower than that of some m and p conformers. An example is offered by conformer ALQ-k-r-u1, with relative energies 1.365 kcal/mol/DFT 1.661 kcal/mol/HF, which is lower than that of conformer ALQ-m-r-u2, with relative energies 1.764 kcal/mol/DFT and 1.801 kcal/mol/HF, (table 6.6.). This may be related to the fact that the N14–H14····O9 IHB has shorter bond length in ALQ-k-r-u1 than in ALQ-m-r-u2, suggesting that the IHB is stronger in ALQ-k-r-u1 than in ALQ-m-r-u2. More detailed analysis of the IHBs and their stabilizing effect is presented in section 4.4.3.3.

Conformers with only one IHB (g conformers) are observed only in some of the molecules. Their relative energies still remain comparatively low, mostly between 3 kcal/mol and 5 kcal/mol. For example, the relative energies of FGP-g-r-x1 are 4.949 kcal/mol/DFT and 3.327 kcal/mol/HF; the relative energies of FGQ-g-r-x1 are 4.917 kcal/mol/DFT and 3.371 kcal/mol/HF; and the relative energies of DGP-g-r are 4.630 kcal/mol/DFT and 3.002 kcal/mol/HF.

Conformers with no IHB (j conformers) are the ones with the highest relative energies for all the compounds. For example, CLQ-j-r-w5 has relative energies 9.967 kcal/mol/DFT and 9.442 kcal/mol/HF. The space filling models in fig 4.8 illustrate the probable reasons. The model on the left indicates the presence of repulsion between the two nitrogen atoms because, with this geometry, they are very close to each other and their repulsion is not smoothed by an IHB between them. The model on the right indicates that the three oxygen atoms are also sufficiently close to each other to perceive mutual repulsion.

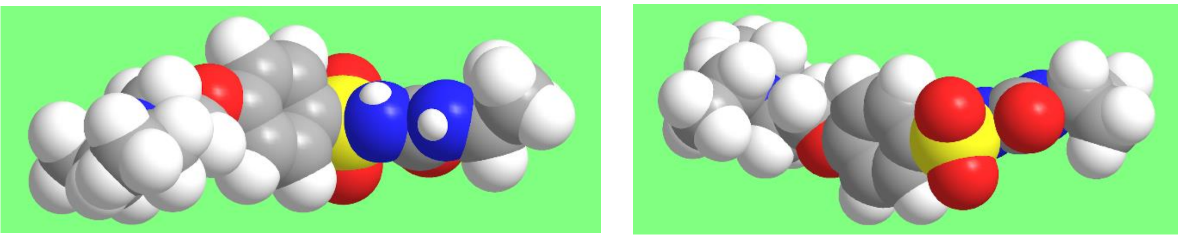


Figure 4.8. Space filling images of conformer CLQ-j-r-w5 – a conformer without any IHB.
The two images show two different perspectives.
(Relative energy of this conformer: 9.967 kcal/mol/DFT and 9.442 kcal/mol/HF).

The importance or the stabilizing effect of the IHBs is also shown by the fact that some of the inputs without IHBs optimized to conformers with one or more IHBs, yielding conformers which are mostly among those with the lowest relative energies. In this way, some low-energy conformers were obtained from more than one calculation, with different inputs, as indicated in the appendix (tables A1-A36). For example, conformer BJP-p-q-v3 was obtained from the calculations of different inputs (table A9). The fact that some conformers were obtained from different inputs supports the assumption that the conformational search that has been performed in this work is sufficiently complete to include all the low energy conformers.

4.4.3.1.2. Conformers differing by the orientations of the chain between O7 and N18 with respect to the benzene ring

For most molecules, the relative energies of the individual conformers also differ by the orientation of the chain between O7 and N18 with respect to the benzene ring (indicated by the C6–C1–O7–

C15 dihedral angle). In q and r type conformers, the chain is on the same plane as the benzene ring, and its orientations in the two conformers are symmetrical, as shown by the values of the C6–C1–O7–C15 dihedral angle (table 4.4). When the other characteristics are the same, the q and r conformers have very close relative energies. For example, the AJQ-m-q-u2 conformer has relative energies 0.465 kcal/mol/DFT and 0.456 kcal/mol/HF and the AJQ-m-r-u2 conformer has relative energies 0.470 kcal/mol/DFT and 0.455 kcal/mol/HF (table 6.4, figure 6.4).

In s and t type conformers, the chain between O7 and N18 is perpendicular to the plane of the benzene ring, and its orientations in the two conformers are symmetrical, as shown by the values of the C6–C1–O7–C15 dihedral angle (table 4.4). When the other characteristics are the same, the s and t conformers have very close relative energies. For example, the BGP-p-s-v3 conformer has relative energies 0.000 kcal/mol/DFT and 2.428 kcal/mol/HF and the BGP-p-t-v3 conformer has relative energies 0.000 kcal/mol/DFT, 2.454 kcal/mol/HF, (table 6.7, figure 6.7).

Both the q and the r conformers are present in all the considered compounds, whereas the s and t conformers may be present together, or only one for a given compound, or not present at all. The s conformers are mostly observed in the compounds with three carbons between O7 and N18 (P compounds) and the t conformers are mostly observed in the compounds with two carbons between O7 and N18 (Q compounds).

4.4.3.1.3. Influence of the nature of R′ on the conformational preferences of the compounds

Three different R′ groups may be present in the compounds considered in this work (figure 4.2): pyrrolidine, morpholine and diethylamine, respectively denoted as G, J and L in the compounds' acronyms (table 4.1). All of them contain a nitrogen atom (N18). Twelve compounds have been considered for each R′ group, and this enables reliable comparisons for the identification of the influence and effect of each R′ group.

The same geometry of the rest of the molecule has been used for inputs with each of the three different R′. The outputs show that R′ can influence the geometry of the thiourea group even if it is comparatively far away from it; therefore, the nature of R′ influences the types and number of

IHBs that can be formed and because of this, some conformers are not possible for certain compounds with a given R′ group.

Most of the compounds with R′=pyrrolidine can have all the conformer types; in few cases, some types are not possible, and inputs of that type optimized to other geometries (table A37). For the compounds with R′=morpholine and R′=diethylamine, the g conformers are not observed, and the g-type inputs optimized to different geometries (tables A38 and A39). This observation further highlights the influence of the R′ on the type of stable geometries of the given compound. It is also to be noted that the k conformers are not possible for the compounds of group C, regardless of the type of R′ present, whereas the m and the j conformers are possible for all the compounds.

4.4.3.1.4. Relative energies corrected for ZPE and Gibbs free energy

The calculation of vibrational frequencies also provides the relative energies corrected for ZPE (zero point energy) and the Gibbs free energies (sum of electronic and thermal free energies). The uncorrected relative energies, the relative energy corrected for ZPE and the Gibbs free energies are compared in tables 6.37–6.72 and their trends are highlighted in the diagrams of figures 6.109–6.144.

For most compounds, the energy increasing sequence is the same or very similar for the three cases; where there are reversals between energetically neighbouring conformers, they usually involve marginal differences, mostly below 0.1 kcal/mol; there are only few cases in which the difference is greater than 0.1 kcal/mol, but it remains smaller than 0.5 kcal/mol. These trends can be better illustrated through examples. Figures 6.122 and 6.128, concerning compounds CGQ and DGQ respectively, are here selected as illustrative examples. The energy difference among the first four conformers of these compounds is marginal. The energy differences between neighbouring conformers with different number of IHBs show correspondence of trends for the uncorrected relative energy, the relative energy corrected for ZPE and the Gibbs free energy. For all compounds, and for all these three types of energies, the energy difference between the highest energy conformer having at least one IHBs and the lowest energy conformer without any IHB is large, confirming the dominant role of IHB on conformational preferences.

The energy differences between neighbouring conformers with different number of IHBs (m/p, k, g and j conformers) are comparable for the uncorrected relative energies, relative energies corrected ZPE and the Gibbs free energy. This is the same for all the compounds considered. It can also be noted that the energy difference between the neighbouring conformers are mostly slightly smaller for the Gibbs free energy than for the ZPE-uncorrected and corrected relative energies. This is easily observed in most of the relative energies diagrams for most of the compounds considered (figures 6.109–6.144).

The three quantities often have close values for the lower energy conformers, with no regular pattern about which is greater. For instance, for compound BKLP (figure 6.119) the values of the Gibbs free energy are greater than the other two, except for the high energy conformers (conformers without IHBs). For high energy conformers, the uncorrected relative energy is mostly greater than the corrected one, and the Gibbs free energy is smaller than the other two.

Table 6.73–6.108 report the ZPE corrections for the electronic energy and the thermal corrections for the Gibbs free energy. They are also obtained from the frequency calculations. Their ranges are reported I table 4.6, to enable a comparison of these properties within the same group of molecules and also across all the group of all the molecules considered.

The ZPE corrections are different for different molecules, but very close for the individual conformers for each of the molecules considered. The values of the ZPE corrections are always greater than the values of the thermal corrections for the Gibbs free energy for each of the molecules considered. The corrections are greater for the conformers of the compounds of group A. The ZPE corrections of the individual conformers of the same compound differ by less than 3 kcal/mol for all the compounds considered, and the thermal corrections to the Gibbs free energy of the individual conformers differ by less than 5 kcal/mol.

4.4.3.2 Comparison of conformational preferences and energetics in the HF and DFT results

The comparison of the results obtained with the two methods follows a similar pattern (in terms of analysis terms) as the analysis in the previous section. Furthermore, these comparisons mostly utilise tables and diagrams already mentioned in the previous analysis, because they report both the DFT and the HF results.

4.4.3.2.1 Comparisons of the relative energies

For most of the molecules considered, the conformer with the lowest relative energy is the same for both DFT and HF (with the same or similar geometry in the two cases). An example is offered by the ALQ-m-r-u1 conformer (table 6.6, figure 6.6).

In other cases, the conformers with the lowest relative energies are different for the two methods. For example, for compound BLP, the conformer of with the lowest relative energy is BLP-k-q-v1 for DFT and BLP-m-r-v1 for HF.

For the other conformers besides for the lowest energy one, the conformers' relative energy sequence is the same in the HF and DFT results for most compounds, but there are reversals for some conformers. When the values of the relative energies are different, but very close, the geometries of the concerned conformers are identical. In most cases, the difference in the relative energies of the lower energy conformers is very small for both methods.

4.4.3.2.2. Comparison of the influence of the orientation of the chain between O7 and N18 with respect to the benzene ring

As already mentioned, (section 4.3.2.1.1), the pairs of q/r and s/t conformers of the same compound have the same or very close relative energies with both the methods. This is because the two conformers of a pair are symmetrical, and all their features are the same except for the different orientation of the chain – parallel to the plane of the benzene ring (q/r) or perpendicular to it (s/t).

Conformers not belonging to the same q/r or s/t pairs may have different relative energies with the two methods. This may happen for q and t, q and s, r and t or r and s conformers. For example, the BLP-k-r-v1 and the BLP-k-s-v1 conformers have the same relative energies with DFT (0.219 kcal/mol), but different relative energies with HF (0.377 kcal/mol and 2.755 kcal/mol respectively; table 6.11, figure 6.11) The two conformers are both k conformers with the same geometry of the R group, which may account for the similarity in their DFT relative energies, although in one of them the chain between O7 and N18 is perpendicular to the plane of the benzene ring and in the other is parallel, which may account for the different HF relative energies.

It also happens that s conformers may have the same DFT relative energies as either the r or the q conformers of the same compound, but very different HF relative energies. For example, the BJQ-p-r-v3 conformer has relative energies 2.133 kcal/mol/DFT, 2.171 kcal/mol/HF and the BJQ-p-s-v3 conformer has relative energies 2.133 kcal/mol/DFT, 4.589 kcal/mol/HF (table 6.10, figure 6.10). In BJQ-p-r-v3, the orientation of the chain between O7 and N18 is parallel to the plane of the benzene ring, and in BJQ-p-s-v3 conformer it is perpendicular. These cases suggest that the HF calculation method gives more importance to the orientation of the chain between O7 and N18 than DFT.

It happened that different inputs resulted in conformers with the same HF relative energies, but different DFT results. These conformers have symmetrical geometries. For example, BLP-p-q-v4 has relative energies 1.679 kcal/mol/DFT, 1.419 kcal/mol/HF and BLP-p-r-v4 has relative energies 1.708 kcal/mol/DFT, 1.419 kcal/mol HF, (table 6.11 and figure 6.11, table A11); the two conformers have symmetrical geometries.

There are also conformers with different geometries but very close or the same relative energies. For example, AGP-m-q-u1 has relative energies 0.036 kcal/mol/DFT, 0.031 kcal/mol/HF and AGP-p-r-u3 0.037 kcal/mol/DFT, 0.030 kcal/mol/HF (table 6.1, figure 6.1). This may be due to the fact that, in both conformers, the orientation of the chain between O7 and N18 is parallel to the plane of the benzene ring, and to the fact that geometry difference in the R group do not have much influence on the relative energies of the conformers.

There are also several cases where conformers with different geometries have the same or very close DFT relative energy. For example, AJQ-p-q-u3 has relative energy 0.583 kcal/mol/DFT, 0.000 kcal/mol/HF and AJQ-m-r-u1 r has relative energy 0.583 kcal/mol/DFT, 0.689 kcal/mol/HF (table 6.4, figure 6.4). The orientation of the chain between O7 and N18 is parallel to the plane of the benzene ring in both conformers. The difference in the geometry of the R group may be responsible for the difference in the HF relative energies of the two conformers.

4.4.3.2.3. Comparison of the influence of the nature of the R′ group

For most of the considered compounds (and for all the G, J and L compounds), the conformers with the lowest relative energy are the m/p conformers, with both DFT and HF methods. The only exception is BLP, whose lowest energy conformer is a k conformer for DFT and an m/p conformer for HF. For all these compounds, the relative energies of individual conformers having IHBs are mostly below 3 kcal/mol in the DFT results; however, for the G compounds, the g conformers may have DFT relative energies around 4 or 5 kcal/mol.

The corresponding HF relative energies of individual conformers are mostly close to the DFT ones. However, some s and t conformers have higher HF relative energies in all the compounds, and the difference can reach 3 or 4 kcal/mol with respect to the DFT results.

4.4.3.2.4. Comparisons of uncorrected relative energies, relative energy corrected for ZPE and Gibbs free energy.

Tables 6.37–6.72 report both the DFT and the HF results for the uncorrected relative energies, relative energies corrected for ZPE and Gibbs free energies (corrected for the sum of the electronic and thermal free energies) of the individual conformers for each of the molecules considered. Figures 6.109–6.144 report diagrams comparing the trends of these three quantities (uncorrected relative energies, relative energy corrected for ZPE and the Gibbs free energy). To facilitate the comparisons, the diagrams of the DFT and HF results for the same compound are reported in the same page (one page for each compound). The energy ranges are reported in table 4.5.

The comparison of the uncorrected relative energies, relative energy corrected for ZPE and Gibbs free energy, show that, in most cases, the conformer with the lowest energy is the same with both DFT and HF. The comparative diagrams show similar trends for the DFT and HF results in a number of cases. However, in other cases the low energy conformers have very close energy values in the DFT results, but not in the HF results; furthermore, it may happen that the three types of energy have very similar trends in the DFT results, but not in the HF results. For example, for compound CGP (figure 6.121), the DFT results show very close values for the first six conformers and similar trends for the three quantities, whereas this is not true for the HF results.

The comparative diagrams also show that the energy trends are more similar for the compounds with two carbon atoms in the chain between O7 and N18 (Q compounds), than for the compounds with three carbon atoms in the chain between O7 and N18 (P compounds) for both the DFT and HF results. This observation is true whether the DFT and HF results are similar or not, as highlighted, for example, by Figure 6.145 (compound FLP), where the trends of HF and DFT are identical, and figure 6.146 (compound FLQ) where there are some differences in the DFT and HF results.

Tables 6.73–6.108 reports the ZPE corrections for the electronic energy and the thermal corrections for the Gibbs free energy. The values of corrections for the individual conformers of the considered compounds are greater in the HF results than the DFT results.

4.4.3.3. Characteristics of the intramolecular hydrogen bonds

The IHBs have the strongest influence on the geometry preferences and the relative energies of the conformers and, therefore, they are given specific attention in this section. As already described in section 4.4.1., the IHBs that may be present in the calculated molecules are H14····O9 or H14····O10 (not present simultaneously), and H11····O13, which may be present simultaneously with either H11····O9 or H11····O10; in the latter case, the two IHBs are bifurcated on H11. When a conformer contains three simultaneous IHBs, it contains H14····O9 or H14····O10, H11····O13, and H11····O9 or H11····O10.

IHBs are described through their parameters: bond length, donor-acceptor distance, and bond angle. The parameters of the IHBs in the conformers of the calculated molecules are reported in tables 108–144. Their ranges are summarized in tables 4.7–4.11, devoting one table to each IHB, and the values are analysed in terms of the different compounds; since, for the two IHBs with H11 as donor, it is important to know whether there is bifurcation or not, the symbol α is used for the bifurcated cases and the symbol β to specify that there is no bifurcation.

When comparing IHBs, we consider that, generally, shorter bond length corresponds to greater strength. Comparisons of the parameters of the IHBs present in the calculated molecules shows that H14····O9 and H14····O10 have the shortest bond length and, therefore, they are the strongest IHBs. This is related to the fact that the acceptor is an sp^2 O atom (O9 or O10), and also to the fact that they close a six membered ring, which is a favourable ring-geometry. Although they are the strongest in these molecules, H14····O9 and H14····O10 cannot be considered strong IHBs, because their directionality (N$\hat{H}$O bond angle) deviates considerably from linearity. H14····O9 and H14····O10 are present in symmetrical conformers of the same molecule: H14····O9 is present in m conformers and H14····O10 in p conformers. H14····O9 is only present in m-type conformers, which are conformers with three IHBs present in all the molecules considered. It is stronger in the compounds of group C; for instance, its length-ranges for compounds CLQ are 2.058–2.065/HF and 2.025–2.034/DFT (table 4.6).

As for the IHBs for which H11 is the donor, H11····O13 has shorter bond lengths than either H11····O9 or H11····O10. All three of them (H11····O9, H11····O10 and H11····O13) are weak IHBs. Their situation seems analogous to that of the IHB between the OH and the sp^2 O in the carboxylic group (COOH): an IHB that closes a four membered ring with a very small bond angle (section 2.3.4). It may even be questioned whether they can be truly considered IHBs, because of the bond angle. They are considered IHBs here because the conformers' energy values show that they have a stabilising effect.

When three IHBs are present (i.e., when there is bifurcation on H11, like in the m conformers), the bond lengths of all the IHBs are longer than when only two IHBs are present, like in the k and the p conformers; this suggests that the bifurcation on H11 decreases the strength of the IHBs. For example, the length ranges (table 4.7) of the H14····O10 IHB in compound ELP are 1.974–1.977 Å/DFT and 2.028–2.033 Å/HF in conformers with two IHBs (no bifurcation) and 2.084–2.091Å/HF and 2.054–2.055Å/DFT in conformers with three IHBs (where there is bifurcation on H11); thus, it appears that the presence of bifurcation on H11 influences not only the two bifurcated IHBs, but also the other IHB present.

The H11····O9 IHB is present either simultaneously with H11····O13 (p-type conformers) or in conformers in which it is the only IHB present (g-type conformers). The ranges of its length are similar for molecules pertaining to the same group (same R), but slightly different for molecules of different groups. The length is also different in different conformer-types (p or g). For example, its bond lengths are 2.446Å/DFT, 2.396Å/HF for EGP-g-r-x1 and 2.595Å/DFT, 2.505Å/HF for EGP-p-q-x3.

The H11····O10 IHB is present only simultaneously with H11····O13 (m-type conformers), never alone. The ranges of its length are similar for molecules of the same group and slightly different in molecules of different groups. For example, the ranges of its bond lengths (table 4.10) in the compound AGP, AGQ and ALP are 2.590–2.598/DFT and 2.499–2.512/HF.

The H11····O13 IHB is present in the m, p and k conformers; it is never present alone in a conformer, but only simultaneously to at least another IHB. Its bond length differs in conformers of different types. For example, in the ALQ compound, its bond length is 2.386–2.390/ DFT and 2.354–2.364/HF for m-type or p-type conformers (where there is bifurcation on H11), and 2.347–2.348/DFT and 2.313–2.314/HF in k-type conformers, where the other IHB present is H14····O10.

For each of the groups of molecules considered, the parameters of each of the IHB present are very close in conformers of the same type, in the results of the same method. Comparison of the results from HF and DFT shows that, in most cases, the bond length in the DFT results is shorter than in the HF results. For instance, in the case of k conformers, the length of the H14····O9 IHB is mostly below 2.0 Å in the DFT results, and longer in the HF results. This is consistent with the known tendency of HF to underestimate the strength of hydrogen bonds and of DFT to overestimate it. However, there are cases where the bond lengths are longer in the DFT results than in the HF results; this is notable in cases where there is bifurcation.

Furthermore, the similarities of the parameters of the IHBs in a given set of molecules may differ in the results of the two methods. For instance, the N····O distances for the H11···O13 IHB are the same (2.280 Å) in the DFT results for the molecules of group D, whereas they are different in the HF results.

The parameters of hydrogen bonds are related to their strength. It is not easy to determine the energy of individual IHBs, because their removal would substantially change the geometry of the molecule. An idea of the stabilising effect of the IHBs could be given by the difference between the energy of the lowest energy conformer without any IHB and the energy of the highest energy conformer with at least one IHB (table 4.12). These differences are different for different types of compounds. The greatest differences are observed for the JP compounds (R′=morpholine, two carbons in the chain between O7 and N18) and the smallest for G compounds (R′=pyrrolidine). This shows that the length of the chain between O7 and N18has some influence on the relative energies of the conformers and on the stabilizing effects of the IHBs present in a conformer. The differences are very close for most of the L compounds (R′=diethylamine).

4.4.3.4. Influence of the nature of R

Investigating possible influences by the nature of R entails comparisons of molecules with different R and the same R′. Therefore, the comparisons in this section will be grouped according to the types of R′; for each R′, the compounds will be sub-grouped according to the length of the chain between O7 and N18 and also to similarities in some observations made.

4.4.3.4.1. Comparisons of compounds with different R and R′= pyrrolidine (G compounds)

The G type compounds with the chain between O7 and N18 containing three carbons (GP compounds) are AGP, BGP, CGP, DGP, EGP and FGP. The G type compounds with the chain between O7 and N18 are AGQ, BGQ, CGQ, DGQ, EGQ and FGQ. The analysis of the results confirms that the type of lowest energy conformer does not depend on R, as the conformers with the lowest relative energies are m/p conformers for all the compounds.

The nature of R may influence the types of conformers that are possible. For example, g conformers are observed only in G compounds, but not in all of them (they are not observed for compounds BGQ and CGQ). Compounds with R=cyclopropane do not have the k conformers.

4.4.3.4.2. Comparisons of compounds with different R and R′= morpholine or R′= diethylamine

The J type compounds (compounds with R′= morpholine) comprise JP compounds (AJP, BJP, CJP, DJP, EJP, FJP, with of the chain between O7 and N18 containing three carbons), and JQ compounds (AJQ, BJQ, CJQ, DJQ, EJQ and FJQ, with the chain between O7 and N18 containing two carbons). The L (R′ = diethylamine) type compounds comprise LP compounds (ALP, BLP, CLP, DLP, ELP and FLP, with the chain between O7 and N18 containing three carbons) and LQ compounds (ALQ, BLQ, CLQ, DLQ, ELQ and FLQ with the chain between O7 and N18 containing two carbons).

These two classes of compounds (J and L) are considered together in this part because of their similarities. Their relative energies show similar trends; there is not much influence of the nature of R on the type of lowest energy conformer (which is an m/p conformer, with the exception of compound BLP, whose lowest energy conformer is a k conformer). Most of the other conformers of these compounds are also m/p conformers; some compounds do not have k conformers. This shows that there is not much influence of the nature of R on the conformational preferences of the compounds of these two groups. The parameters of the IHBs are also very similar for these compounds.

4.4.3.5. IR Vibrational frequencies

The IR vibrational frequencies (harmonic approximation, section 2.4) were calculated for all the conformers of all the considered compounds. The analysis is particularly interesting for the bonds that can make IHBs, i.e., the N11–H11 and N14–H14 bonds. Their IR vibrational frequencies are reported in tables 6.180-6.216. The changes in their IR vibrational frequencies when they form IHBs are analysed in detail in section 4.3.3.6.

The vibrational frequencies of the N11–H11 bond are always greater when it forms IHBs than when it does not form any, and they are related to the types of IHBs it forms and to the presence or absence of IHB formed by N14–H14. The frequency is highest when it forms H11····O9 without bifurcation, and without the presence of IHBs formed by N14–H14; it is lowest when it forms H11····O13 without bifurcation and with the presence of H14····O10; it is intermediate in either of the two bifurcated cases, whether the IHB formed by N14–H14 is H14····O9 or H14····O10.

The vibrational frequencies of the N14–H14 bond are very close whether it forms H14····O9 (m-type conformers) or H14····O10 (p-type and k-type conformers); in the latter case, the frequency is slightly greater in the k conformers than in the p conformers.

The vibrational frequencies of the N11–H11 and N14–H14 bonds are very similar when neither of them is engaged in an IHB (j conformers).

The two bonds often have coupled vibrations when N11–H11 forms the H11····O9 IHB and N14–H14 is not engaged in IHBs (g conformers). In these cases, both the symmetric and asymmetric vibrations appear with the same frequency values for the two bonds; they are reported together for the two bonds in tables 6.145–6.180

The vibrational frequencies of N11–H11 and N14–H14 are comparatively close in the HF and DFT results, and the main differences may be related to the presence and the type of IHBs. The differences are also related to how HF and DFT estimate the strength of hydrogen bonds, and therefore they will be analysed in section 4.3.3.6.

4.4.3.6. Changes in the IR vibrational frequencies of the N11–H11 and N14–H14 bonds when they form IHBs

Tables 6.181–6.216 report the changes in the IR vibrational frequencies of the N11–H11 and N14–H14 bonds when they form IHBs, and table 6.217 reports their ranges. The changes are taken as the difference between the average vibrational frequency of the given N–H bond over the conformers where it does not form IHBs and its vibrational frequency in the considered conformer where it forms an IHB. In this way, a positive change indicates a decrease in the vibrational frequency and a negative change indicates an increase.

In most cases, the formation of a hydrogen bond causes a red shift in the vibrational frequency of the donor (section 2.3.5), i.e., the frequency decreases. This is also observed for N14–H14 when it is engaged in IHBs. However, the frequency of N11–H11 increases when it forms IHBs. The phenomenon is called blue shift [201–207]. The literature [206–207] reports a blue shift in the frequency of the amino N–H bond when it is involved in bifurcated hydrogen bonds, which is comparable to the case of N11–H11 in the compounds considered in this work. A blue shift is accompanied by a contraction of the donor X–H bond length in the X–H····Y system. Both red shifts and blue shifts can be related to the strength of the hydrogen bond [203]. For this reason, it is also interesting to compare the magnitude of the red shifts or the blue shifts with the IHB bond lengths, to have a better idea of the relative strengths of the various IHBs.

From the tables, it is clear that the blue shift is smallest (close to negligible) when N11–H11 forms the H11····O13 IHB and H14····O10 is also present (k conformers); it is greatest when N11–H11 forms the H11····O9 IHB and no other IHB is present (g conformers); and intermediate in all the cases where N11–H11 forms bifurcated IHBs whether H11····O13 plus H11····O9 or H11····O13 plus H11····O10, and whichever IHB is formed by N14–H14 (m/p conformers). In this way, the blue shift is greatest when H11····O9 is not bifurcated and smallest when H11····O13 is not bifurcated; it is intermediate when there is bifurcation on H11. The IHB bond lengths suggest that either H11····O9 or H11····O13 are stronger when they are not bifurcated (with H11····O13 always being slightly stronger than H11····O9, whether alone or bifurcated).

The red shifts for the vibration of the N14–H14 bond are all comparable, but slightly greater when N14–H14 forms the H14····O10 IHB and N11–H11 simultaneously forms H11····O13 (k conformers). The bond lengths of H14····O9 and H14····O10 are very similar when the IHBs bifurcated on H11 are also present, and so are their red shifts. However, the bond length of H14····O10 suggests that it is stronger when the IHBs bifurcated on H11 are not present, as indicated also by the greater red shift.

DFT and HF results show comparable trends for both blue shifts and red shifts for all the conformers except the k conformers. The increase for the blue shift or decrease for the red shift is much smaller in the HF results than in the DFT results because HF underestimates the strength of the hydrogen bonds while DFT/B3LYP overestimates it. In the case of k conformers, the DFT results show a small blue shift for N11–H11, whereas the HF results show a small red shift; however, the small values of these changes could be comparable to the overestimation or the underestimation of the strength of the hydrogen bonds by the two methods, with respect to the actual strength. Furthermore, there are cases in which N14–H14 shows red shift with the DFT results and blue shift in the HF results. For example, in compound AJP (table 6.183), there is a red shift with the DFT results and blue shifts with the HF results for conformers AJP-m-r-u2, AJP-m-s-u2 and AJP-m-q-u2.

4.4.3.7. Dipole moments

The dipole moments of all the conformers of all the studied molecules are included in tables 6.1–6.36. Their ranges can be analysed in terms of the different compounds (table 4.13), in terms of compounds and conformers (table 4.14), or in terms of conformer types across compounds (table 4.15).

For each compound, the dipole moments can vary significantly across conformers. The ranges of the dipole moment depend on the substituents and the type of IHBs present. The difference for different compounds is largely related to the number and type of polar bonds that are present. This also means that it is related mostly to the nature of R′ because that is the part that can differ by the type and number of polar bonds. For example, R′= morpholine (J compounds) contains two electronegative atoms (oxygen and nitrogen), R′= pyrrolidine (G Compounds) and R′= diethylamine (L compounds) contain one nitrogen atom. As a result, the dipole moments are lower in the J compounds than in the G and L compounds. For example, across the compounds of group B, the dipole moments ranges (Debye, DFT results) are 4.5103–8.2516 for BJP, 5.2828–9.9492 for BGP, 6.0489–9.7683 for BLP (table 4.12).

The dipole moments of the m and the p conformers (tables 4.14 and 4.15) are very close in most of the molecules in which they are both present. For example, in compound BGP, the ranges of the dipole moments are 6.3073–7.1291 Debye/DFT, 5.7919–6.9927 Debye/HF for m-type conformers and 6.2528–6.2533 Debye/DFT, 5.4640–5.8287 Debye/HF for the p-type conformers. This is related to the fact that the two conformer types are symmetrical and other geometrical differences do not have great effect on their dipole moments. The dipole moments of k conformers are very close to those of the m/p conformers. For example, in the same compound BGP, the ranges of the dipole moments of the k conformers are 6.2109–6.9481 Debye/DFT, 5.7070–6.8235 Debye/HF, which are close to those of the m and p conformers.

The dipole moments are highest for j conformers, that is, the conformers without any IHB. This highlights the influence of IHBs on the dipole moments, which somehow may partially compensate for the effects of the polarity on the donor. The lowest dipole moments pertain to the g conformers in G compounds (R′=pyrrolidine).

The dipole moments are comparable in both the DFT and HF results, both in terms of compound types and of conformer types.

4.4.3.8. The HOMO–LUMO energy gaps

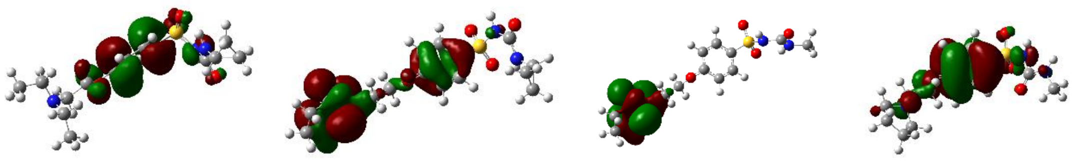
The HOMO–LUMO energy gaps for the considered compounds are also included in tables 6.1–6.36; the ranges of their values and the range-widths for each compound are reported in table 4.16. On analysing and comparing their values, it has to be taken into account that the DFT values are much smaller than the HF values, as a well-known phenomenon of the two methods; this is the reason for comparing the ranges-width. The overall ranges, considering the smallest value and the highest value of these energy gaps across all the compounds are 115.233–122.563 kcal/mol (compounds DLQ and BJQ respectively) in the DFT results and 272.301–286.263 kcal/mol (compounds BLQ and AGQ respectively) in the HF results. The width of the ranges for most of the molecules are below 8 kcal/mol; some exceptions in which the ranges are above 9 kcal/mol concern some of the J (R′=morpholine) and L compounds (R′=diethylamine).

The comparison of the ranges of the P (compounds with 3 carbons in the chain between O7 and N18) and Q compound (compounds with 2 carbons in the chain between O7 and N18) having the same R and R′ helps highlight possible dependence on R and R′. In the DFT results, the difference in the ranges for P and Q compounds is not large for G compounds (R′= pyrrolidine). Similarly, there is not much difference for the L compounds, except for B (R = cyclobutyl) and D (R = methyl) compounds. There is considerable difference for the J compounds, except for F compounds (R = propyl). For Q compounds, the gap is greatest for all the J compounds and for some of the L compounds (BLQ and DLQ).

The width of the ranges of the HOMO–LUMO energy gaps are comparable for the DFT and the HF results for all the compounds except for the J compounds, for which there is a big difference between P and Q in the HF results.

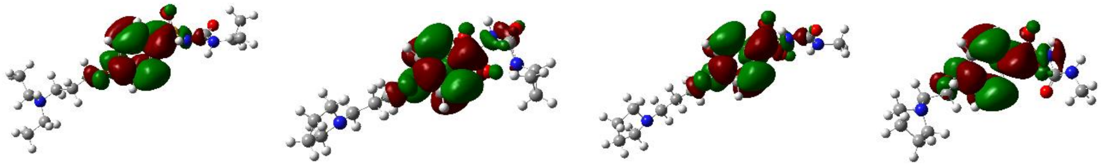
The calculation outputs also enable the visualization of the shapes of the HOMO and LUMO molecular orbitals, showing the distribution of the electron density for each orbital in the different parts of the molecule. Thus, it can be seen whether the distribution of the electron density is preferably on the benzene ring, on the thiourea moiety, or on the R and R′ of each molecule.

The shapes of representative HOMOs and LUMOs, with different distributions within the molecules, are shown in figures 4.9 and 4.10 respectively. The distribution of the electron density does not depend significantly on R and R′. For the HOMO, the distribution of the electron density depends mostly on the type of conformers and only slightly on the nature of R. For the majority of conformers across compounds, the distribution of the HOMO is similar to that of the CJP-p-s-w5 conformer (figure 4.9), that is, it is mostly on the benzene ring and also on the electronegative atoms of the thiourea group. For some conformers, the HOMO is distributed mostly on the benzene ring and the R′ group, similar to the CGP-p-q-w5 example (figure 4.9). There are also conformers in which the HOMO is distributed only on the R′ group, as in the DGP-k-s example (figure 4.9), or mostly on the benzene ring, but also on the thiourea group, and on some atoms on the R′ group, as in the DGQ-j-t example (figure 4.9). The distribution of the LUMO is similar in all the conformers across compounds, prevalently on the benzene ring and on the thiourea moiety.



CJP-p-s-w5 CGP-p-q-w5 DGP-k-s DGQ-j-t

Figure 4.9. Representative shapes of HOMOs of sulfonylureas.



CJP-p-s-w5 CGP-p-q-w5 DGP-k-s DGQ-j-t

Figure 4.10. Representative shapes of LUMOs of sulfonylureas.

Table 4.5. Ranges of relative energies not corrected for ZPE (ΔE), relative energies corrected for ZPE (ΔE$_{corr}$), and Gibbs free energy corrected for the sum of electronic and thermal free energies (ΔG$_{corr}$) of each conformer type for each of the compounds considered.

Molecules	Conformer type	ΔE (kcal/mol)		ΔE$_{corr}$ (kcal/mol)		ΔG$_{corr}$ (kcal/mol)	
		DFT	HF	DFT	HF	DFT	HF
AGP	m	0.000–1.763	0.000–2.428	0.010–2.014	0.000–2.143	0.023–2.820	0.000–2.951
	p	0.003–0.037	0.030–2.450	0.000–0.060	0.014–2.095	0.000–0.253	0.014–0.535
	k	1.154–1.379	1.440–1.679	1.099–1.251	1.364–1.576	0.326–0.653	1.035–1.189
	g	4.532–4.664	2.880–3.119	3.869–4.020	2.307–2.548	3.545–3.797	2.398–2.653
	j	10.245–10.351	9.554–11.782	9.671–9.746	9.008–10.886	9.266–9.445	8.948–9.733
AGQ	m	0.000–1.774	0.000–1.811	0.000–2.004	0.000–2.147	0.000–2.852	0.000–2.953
	k	1.082–1.238	1.441–1.660	1.082–1.239	1.373–1.567	0.454–0.459	1.038–1.176
	g	4.496–4.662	2.917–5.438	3.870–4.012	2.350–4.539	3.715–3.772	2.439–3.192
	j	10.248–10.279	9.564–12.269	9.679–9.689	9.024–11.163	9.236–9.544	8.950–12.163
AJP	m	0.000–1.842	0.000–4.220	0.000–2.058	0.000–4.196	0.000–2.838	0.000–3.761
	k	1.171–1.392	1.458–4.025	1.103–1.272	1.379–3.572	0.532–0.639	1.029–1.815
	j	17.994–18.137	17.097–19.349	17.129–17.238	16.299–18.199	16.398–16.545	15.854–16.648
AJQ	m	0.052–0.617	0.045–3.109	0.047–0.776	0.029–0.880	0.312–1.412	0.030–1.724
	p	0.000–0.615	0.000–3.115	0.000–0.793	0.000–0.927	0.000–1.721	0.000–1.733
	k	1.170–1.974	1.466–2.390	1.107–1.761	1.387–2.116	0.643–1.050	1.044–1.313
	j	8.670–8.838	8.027–8.271	8.234–8.352	7.630–7.839	7.812–7.942	7.543–7.680
ALP	m	0.000–1.780	0.000–4.242	0.000–1.993	0.000–4.219	0.000–2.682	0.000–3.747
	k	1.367–1.679	1.443–3.905	1.110–1.457	1.366–3.905	0.777–1.108	1.027–1.849
	j	10.540–10.647	9.899–12.129	9.856–9.932	9.325–11.206	9.708–9.857	9.595–10.358
ALQ	m	0.000–1.775	0.000–1.807	0.000–1.992	0.000–2.150	0.000–2.743	0.000–2.959
	k	1.315–1.365	1.444–1.661	1.602–1.227	1.337–1.570	0.377–0.484	1.028–1.167
	j	10.255–11.778	9.564–10.907	9.681–10.971	9.028–9.918	9.326–10.286	8.632–8.971
BGP	m	0.001–1.569	0.000–3.834	0.007–1.745	0.000–3.734	0.000–2.469	0.000–3.074
	p	0.000	2.428–2.454	0.000	2.070–2.098	0.080–0.082	0.540–0.782
	k	1.079–1.300	1.366–3.962	1.026–1.209	1.324–3.542	0.686–0.819	0.783–1.478
	g	4.572–4.712	2.940–3.183	3.848–4.000	2.350–2.595	3.243–3.620	2.373–2.631
	j	10.319–10.423	10.421–10.642	9.735–9.805	9.770–11.643	9.452–9.584	9.780–10.544
BGQ	m	0.000–1.558	0.000–1.400	0.000–1.748	0.000–1.655	0.000–2.337	0.000–2.250
	k	1.083–1.289	1.368–1.590	1.029–1.197	1.328–1.526	0.575–0.725	0.772–0.935
	j	10.327–10.353	9.649–12.362	9.738–9.745	9.093–11.441	9.265–9.503	9.010–12.223
BJP	m	1.548–1.621	1.399–3.817	1.763–1.813	1.659–3.717	2.436–2.439	2.234–3.047
	p	0.000–0.087	0.000–2.418	0.000–0.078	0.000–2.059	0.000–0.032	0.000–0.813
	k	1.095–1.312	1.384–3.959	1.040–1.226	1.341–3.538	0.482–0.808	0.778–1.483
	j	18.067–18.210	17.182–19.437	17.201–17.304	16.374–18.277	16.498–16.669	15.923–16.712
BJQ	m	1.518–1.570	1.380–3.897	1.364–1.724	1.361–3.435	1.370–2.265	1.394–2.242
	p	0.000–2.133	0.001–4.589	0.000–1.869	0.000–3.948	0.000–1.715	0.000–2.254

	j	10.261–10.427	0.000–9.816	9.676–9.727	9.030–9.239	9.387–9.409	8.961–9.093
BLP	m	0.133–0.168	0.000–2.448	0.166–0.169	0.000–2.088	0.511–0.589	0.718–1.515
	p	0.131–1.708	1.419–3.860	0.153–1.920	1.657–3.765	0.545–2.872	1.657–3.765
	k	0.000–0.219	0.132–2.755	0.000–0.174	0.014–2.257	0.000–0.063	0.000–0.657
	j	9.243–9.351	9.177–11.425	8.707–8.786	8.458–10.351	8.865–8.909	8.997–9.758
BLQ	m	1.465–1.479	1.225–1.236	1.288–1.259	0.757–0.766	0.688–1.118	0.000–0.124
	p	0.000–1.560	0.000–3.833	0.000–1.737	0.000–3.020	0.000–2.430	0.712–3.554
	k	1.081–1.290	1.358–1.597	0.992–1.194	1.320–1.534	0.576–0.892	1.486–1.646
	j	8.913–8.947	8.085–11.605	8.309–8.346	7.454–10.531	7.941–8.162	7.930–12.031
CGP	m	0.233–2.782	0.668–6.101	0.222–2.884	0.610–5.865	0.000–3.185	0.397–4.784
	p	0.000–0.029	0.000–2.415	0.000–0.039	0.000–2.059	0.105–0.114	0.000–0.732
	g	3.417–4.580	3.004–3.288	3.941–4.110	2.483–2.760	4.041–4.217	2.625–2.907
	j	9.899–9.994	9.312–11.552	9.413–9.505	8.843–10.732	8.971–9.365	8.788–9.575
CGQ	m	0.002–0.255	0.008–0.679	0.001–2.227	0.019–0.631	0.003–0.071	0.004–0.423
	p	0.000–0.014	0.000–0.012	0.000–0.006	0.000–0.023	0.000–0.051	0.000–0.008
	j	9.902–9.926	9.336–10.052	9.439–9.440	8.875–11.226	9.146–9.275	8.806–12.004
CJP	m	0.229–2.830	0.664–6.087	0.208–2.931	0.604–5.853	0.388–3.452	0.395–4.763
	p	0.000–0.036	0.000–2.405	0.000–0.005	0.000–2.046	0.000–0.371	0.000–0.798
	j	17.645–17.786	16.853–19.117	16.867–16.965	16.131–18.041	16.334–16.384	15.708–16.504
CJQ	m	0.000–2.378	0.000–5.282	0.000–2.100	0.000–4.585	0.000–1.682	0.000–2.270
	p	1.529–2.117	1.496–4.163	1.389–1.888	1.365–3.970	1.173–1.660	1.389–2.256
	j	9.841–10.002	9.272–9.512	9.390–9.515	8.819–9.024	9.159–9.167	8.772–8.902
CLP	m	0.231–2.789	0.667–6.109	0.229–2.877	0.611–5.875	0.115–3.202	0.398–4.772
	p	0.000–0.678	0.000–2.425	0.000–0.046	0.000–2.070	0.000–0.044	0.000–0.678
	j	9.590–10.841	8.948–12.611	9.258–10.047	8.508–11.493	8.980–9.207	8.121–9.977
CLQ	m	0.014–3.149	0.033–0.275	0.020–0.218	0.001–2.745	0.000–0.296	0.013–0.494
	p	0.000–2.471	0.000	0.000–0.001	0.000–2.127	0.331–0.332	0.000–0.783
	j	9.297–11.601	9.893–9.967	9.396–9.467	8.828–10.794	9.258–9.402	8.779–9.557
DGP	m	0.000–0.044	0.001–2.445	0.018–0.047	0.000–2.082	0.095–0.105	0.000–0.847
	p	0.002	0.000–2.460	0.000	0.000–2.100	0.000–0.005	0.002–0.754
	k	1.090–1.310	1.346–3.945	0.949–1.121	1.210–3.424	0.258–0.334	0.774–1.471
	g	4.630–4.775	3.002–3.250	4.068–4.215	2.472–2.721	3.948–4.090	2.620–2.875
	j	10.365–10.425	9.675–11.915	9.885–9.923	9.174–11.061	9.704–9.748	9.134–9.913
DGQ	m	0.000–0.031	0.000–0.016	0.024–0.033	0.000–0.008	0.000–0.216	0.008–0.023
	p	0.003	0.003	0.000	0.004	0.041	0.000
	k	1.093–1.299	1.351–1.573	0.961–1.126	1.218–1.145	0.452–0.539	0.781–0.934
	g	4.601–4.771	3.045–5.580	4.062–4.236	2.516–5.736	4.087–4.327	2.661–5.736
	j	10.374–10.399	9.690–12.411	9.898–9.910	9.191–11.545	9.849–9.860	9.146–12.319
DJP	m	0.000–0.041	0.003–0.031	0.000–0.053	0.000–0.021	0.000–0.338	0.000–0.074
	p	0.000–0.041	0.000–2.424	0.000–0.053	0.001–2.065	0.003–0.337	0.040–0.865
	k	1.108–1.320	1.363–3.940	0.939–1.135	1.226–3.420	0.114–0.478	0.808–1.518

	j	18.116–18.260	17.219–19.484	17.309–17.440	16.471–18.680	16.588–16.733	16.096-16.887
DJQ	m	0.000–2.144	0.000–4.593	0.000–1.873	0.000–3.942	0.000–1.570	0.000–4.471
	p	1.577–2.139	1.467–2.172	1.384–1.879	1.324–1.852	1.443–1.589	1.357–1.522
	k	1.088–1.291	1.349–1.584	0.949–1.111	1.212–1.422	0.416–0.473	0.769–0.918
	j	2.666–2.788	2.129–2.318	2.386–2.481	1.787–1.948	2.530–2.571	2.062–2.177
DLP	m	0.000–0.049	0.001–2.454	0.024–0.026	0.000–2.092	0.018–0.160	0.000–0.824
	p	0.002–0.051	0.000–2.470	0.000–0.030	0.001–2.109	0.000–0.034	0.006–3.070
	k	1.093–1.312	1.349–3.955	0.963–1.118	1.212–3.436	0.318–0.372	0.773–1.450
	j	10.365–10.476	9.676–11.917	9.886–9.955	9.176–11.065	9.763–9.810	9.138–9.901
DLQ	m	1.419–2.903	1.563–2.796	1.433–2.703	1.640–2.391	1.410–2.343	1.076–3.221
	p	0.000	0.000	0.000	0.000	0.000	0.000
	k	1.090–1.233	1.348–1.568	0.968–1.076	1.213–1.409	0.378–0.380	0.777–0.918
	j	10.374–10.412	9.686–12.444	9.899–9.927	9.186–11.584	9.728–9.821	9.142–12.437
EGP	m	0.000–0.359	0.000–2.754	0.000–0.223	0.000–2.278	0.068–0.363	0.008–1.359
	p	0.316	0.322–2.741	0.179	0.205–2.267	0.000–0.006	0.000–0.788
	k	1.159–1.374	1.662–4.311	1.047–1.225	1.507–3.722	0.747–0.911	0.914–1.662
	g	4.794–4.948	2.232–3.480	4.116–4.241	2.598–2.846	4.074–4.078	2.583–2.836
	j	10.527–10.628	9.908–12.141	9.900–9.963	9.288–11.170	9.799–9.839	9.089–9.869
EGQ	m	0.000–0.339	0.000–0.327	0.000–0.219	0.000–0.208	0.177–0.507	0.000–0.093
	p	0.358–0.375	0.378–0.379	0.276–0.294	0.307–0.317	0.000–0.189	0.236–0.260
	k	1.152–1.358	1.361–1.581	1.064–1.225	1.292–1.487	1.177–1.269	1.103–1.245
	g	4.764–4.939	3.276–5.806	4.110–4.266	2.639–2.846	4.302–4.379	2.605–3.166
	j	10.531–10.556	9.923–12.636	9.904–9.920	9.303–11.649	9.826–9.920	9.084–12.277
EJP	m	0.000–0.083	0.000–2.419	0.000–0.065	0.000–2.058	0.167–0.403	0.077–0.110
	p	0.083–0.361	0.321–2.733	0.065–0.248	0.204–2.258	0.000–0.401	0.000–0.809
	k	1.177–1.389	1.733–4.306	1.055–1.244	1.520–3.175	0.912–1.674	0.601–0.722
	j	18.275–18.423	17.452–19.709	17.363–17.440	16.581–18.485	16.552–16.740	16.000–16.791
EJQ	m	0.000–2.461	0.000-4.916	0.000–2.112	0.000–4.160	0.000–1.417	0.000–1.417
	p	1.833–2.457	1.801–4.922	1.606–2.106	1.551–4.164	1.142–1.417	1.285–2184
	k	3.286–3.435	3.558–3.788	2.957–3.106	3.182–3.389	2.198–2.402	2.501–2.691
	j	10.468-10.634	9.859–10.102	9.866–9.996	9.256–9.465	9.367–9.433	1.142–1.417
ELP	m	0.000–0.361	0.000–2.448	0.000–0.236	0.000–2.287	0.210–0.462	0.000–0.905
	p	0.315	0.321–2.751	0.177–0.178	0.205–2.277	0.000–0.004	0.001–0.709
	k	1.160–1.377	1.719–4.321	1.064–1.220	1.509–3.732	0.879–0.890	0.911–1.633
	j	10.223–10.630	9.544–12.142	9.711–9.982	8.953–11.172	8.411–9.846	9.564–9.928
ELQ	m	0.000–0.343	0.000–0.324	0.000–0.213	0.000–0.210	0.000–0.591	0.000–0.087
	k	1.147–1.359	1.349–1.589	1.076–1.233	1.283–1.495	1.169–1.252	1.096–1.247
	j	10.488–10.755	9.860–12.428	9.866–10.755	9.246–11.425	9.710–9.799	9.029–9.965
FGP	m	0.000–0.372	0.000–2.856	0.000–0.293	0.000–2.381	0.000–0.247	0.000–0.882
	p	0.337–0.374	0.427–2.843	0.248–0.300	0.311–2.369	0.002–0.131	0.004–0.763
	k	1.163–1.375	1.837–2.075	1.059–1.239	1.640–1.865	0.774–0.990	0.742–2.623
	g	4.949–5.099	3.327–3.575	4.227–4.379	2.684–2.933	3.823–3.998	2.562–2.818

	j	10.679–10.855	10.006-12.235	10.020–10.090	9.378–11.257	8.875–9.657	9.086–9.871
FGQ	m	0.000–0.350	0.000–0.434	0.000–0.270	0.000–0.314	0.000–0.199	0.000–0.163
	k	1.362	1.580	1.245	1.487	1.009	1.209
	g	4.917–5.094	3.371–5.898	4.227–4.395	2.726–4.920	3.715–3.983	2.596–3.301
	j	10.684–10.783	10.021–12.730	10.014–10.053	9.393–9.444	8.843–9.586	9.092–12.291
FJP	m	0.000–0.081	0.000–2.416	0.000–0.048	0.000–2.057	0.000–0.126	0.068–0.850
	p	0.342–1.394	0.427–0.461	0.264–1.254	0.309–2.360	0.032–0.713	0.000–0.815
	k	1.184–1.394	1.853–2.424	1.057–1.255	1.653–3.849	0.461–0.722	0.769-1.571
	j	18.429–18.573	17.549–17.802	17.463–17.570	16.670–18.571	16.401–16.464	16.003–16.793
	m	0.000–0.350	0.000–0.435	0.000–0.297	0.000–0.321	0.058–0.315	0.001–0.042
	p	0.338–0.347	0.372–0.438	0.272–0.278	0.292–0.326	0.000–0.126	0.000–0.167
	j	10.406–10.717	9.831–12.867	9.810–10.078	9.271–11.707	9.270–9.681	8.908–12.305
FLP	m	0.000–0.378	0.000–2.865	0.000–0.298	0.000–2.390	0.101–0.303	0.039–0.868
	p	0.337	2.427–2.853	0.253	0.310–2.378	0.000–0.004	0.004–0.730
	k	1.165–1.379	1.839–4.439	1.082–1.241	1.642–3.865	0.870–0.949	0.743–1.471
	j	10.374–10.779	9.641–12.236	9.839–10.114	9.041–11.258	9.306–9.750	8.416–9.850
FLQ	m	0.001–0.347	0.000–0.432	0.004–2.287	0.003–0.316	0.073–0.212	0.000–0.051
	p	0.000–0.353	0.007–0.439	0.000–0.284	0.000–0.315	0.000–0.168	0.002–0.181
	k	1.147–1.368	1.347–2.059	1.082–1.266	1.283–1.842	0.681–1.101	0.736–1.214
	j	10.635–10.769	9.958–10.166	9.989–10.095	9.337–9.516	9.409–9.474	9.037–9.174

Table 4.6. Ranges of the ZPE corrections to the energy and of the thermal correction to the Gibbs free energy for each of the compounds considered.

Molecule	ZPE correction (kcal/mol)		Thermal correction to G (kcal/mol)	
	DFT	HF	DFT	HF
AGP	297.544–298.459	319.911–321.150	256.341–258.452	279.031–282.230
AGQ	279.722–280.392	300.864–302.114	239.803–241.924	261.073–264.479
AJP	300.806–301.954	323.849–325.336	259.117–261.785	282.646–286.489
AJQ	283.022–283.836	305.131–268.214	242.351–244.678	264.506–268.214
ALP	310.179–311.116	333.199–334.459	267.815–269.549	291.560–294.480
ALQ	292.544–293.387	314.083–315.421	250.220–253.428	273.827–277.154
BGP	278.870–279.791	300.006–301.265	238.761–240.923	260.076–263.402
BGQ	261.140–261.957	281.049–282.234	222.562–224.440	244.112–245.651
BJP	282.184-283.305	304.034–305.456	241.986–244.446	264.095–066.813
BJQ	264.446–265.209	285.328–286.239	225.365–227.130	246.183–249.370
BLP	291.514–292.302	231.219–314.555	250.510–252.145	272.239–275.964
BLQ	273.738–274.524	294.201–295.540	234.301–235.788	255.542–258.325
CGP	260.650–261.263	280.564–281.511	221.930–222.966	242.156–244.451
CGQ	242.817–243.305	261.518–262.355	205.615–206.434	225.979–226.375
CJP	263.832–264.774	284.502–285.700	224.737–226.764	245.775–248.698
CJQ	246.075–246.566	265.653–266.359	208.211–209.157	227.080–230.091
CLP	272.840–273.778	293.552–294.796	232.254–234.515	254.053–257.006
CLQ	255.427–255.928	274.804–275.611	217.025–217.992	235.972–238.626
DGP	239.219–239.740	257.407–258.261	202.018–203.124	220.095–222.574
DGQ	221.339–221.884	238.360–239.228	185.625–186.602	204.163–204.903
DJP	242.394–243.228	261.345–262.449	204.767–206.591	224.186–226.826
DJQ	224.846–225.025	242.582–243.233	188.403–189.222	205.232–209.091
DLP	251.717–282.264	270.695–271.548	213.240–214.395	232.617–235.723
DLQ	233.967–234.474	251.598–252.534	197.119–198.123	215.546–217.682
EGP	239.219–239.740	257.407–258.261	202.018–203.124	220.095–222.574
EGQ	221.339–221.884	238.360–239.228	185.625–186.602	204.163–204.903
EJP	260.183–261.166	280.322–281.546	221.061–223.253	241.788–244.788
EJQ	242.438–243.080	261.561–262.328	204.769–205.992	223.756–226.494
ELP	269.540–270.198	289.673–290.643	229.875–231.128	250.316–253.087
ELQ	251.747–252.437	270.626–271.630	213.484–215.035	232.623–235.451
FGP	274.688–275.515	295.390–296.369	234.055–236.282	255.795–258.201
FGQ	256.883–257.658	276.343–277.337	217.594–219.729	237.806–240.446
FJP	278.007–279.011	299.327–300.559	237.469–239.708	259.407–262.458
FJQ	260.232–260.884	280.301–281.288	221.082–222.534	243.105–244.183
FLP	287.340–288.006	308.702–309.656	246.104–247.404	267.744–270.756
FLQ	269.553–270.227	289.991–290.643	229.790–231.253	251.910–253.122

Table 4.7. Ranges of the parameters of the N14–H14····O10 IHB for all the compounds in which it is present.

The symbols α and β are used to indicate the presence of bifurcation.

Molecule	Bond length ranges (Å)		N····O distance range (Å)		$N\hat{H}O$ bond angle ranges (^{o})	
	DFT	HF	DFT	HF	DFT	HF
AGP α	2.054-2.056	2.086-2.088	2.866-2.869	2.858-2.861	135.34-135.44	132.92-132.94
β	1.990-1.993	2.026-2.031	2.827-2.829	2.818-2.823	137.87-137.95	134.93-134.96
AGQ	1.991-1.992	2.026-2.030	2.827-2.829	2.819-2.823	137.20-137.93	134.93-134.97
AJP	1.993-1.989	2.026-2.030	2.826-8.829	2.818-2.823	137.93-137.97	134.93-134.96
AJQ α	2.056-2.058	2.079-2.088	2.867-2.870	2.853-2.862	135.25-135.32	132.78-133.06
β	1.991-1.989	2.025-2.031	2.826-2.828	2.818-2.823	137.92-137.95	134.92-134.96
ALP	1.979-1.993	2.008-2.031	2.821-2.830	2.805-2.823	137.91-138.47	134.93-135.46
ALQ	1.990-1.993	2.026-2.030	2.827-2.829	2.818-2.823	137.90-137.92	134.93-137.97
BGP α	2.047	2.080-2.082	2.863	2.855-2.856	135.72	133.01-133.04
β	1.980	2.010-2.016	2.822	2.812-2.818	138.52-138.53	135.87-135.92
BGQ	1.979-1.982	2.011-2.016	2.821-2.24	2.813-2.818	138.50-138.51	135.86-135.93
BJP α	2.049	2.077-2.083	2.864-2.865	2.851-2.858	135.62-135.74	132.98-133.06
β	1.979-1.981	2.010-2.016	2.822-2.823	2.812-2.817	138.52-138.53	135.88-135.81
BJQ	2.049-2.051	2.077-2.084	2.864-2.867	2.851-2.857	135.62-135.75	132.97-133.07
BLP α	2.033-2.047	2.061-2.082	2.863-2.864	2.855-2.859	135.72-137.48	133.01-134.89
β	1.981	2.011-2.017	2.823	2.812-2.818	138.52-138.53	135.87-135.91
BLQ α	2.032-2.050	2.061-2.084	2.862-2.867	2.850-2.860	135.72-137.46	133.06-134.90
β	1.980	2.012-2.016	2.822	2.813-2.817	138.52	135.87-135.92
CGP	2.063-2.065	2.098-2.104	2.866-2.869	2.858-2.865	138.38-134.52	131.52-131.71
CGQ	2.063-2.067	2.098-2.105	2.866-2.871	2.858-2.866	134.41-134.49	131.55-131.71
CJP	2.064-2.066	2.099-2.104	2.867-2.870	2.858-2.865	134.36-134.48	131.48-131.64
CJQ	2.064-2.065	2.100-2.104	2.867-2.869	2.858-2.863	134.32-138.38	131.41-131.54
CLP	2.063-2.064	2.098-2.104	2.866-2.869	2.858-2.865	134.37-134.53	131.53-131.73
CLQ	2.063	2.099-2.104	2.866	2.858-2.864	138.38-134.39	131.51-131.60
DGP α	2.051	2.085-2.086	2.856	2.849-2.850	134.69-134.70	132.10-132.15
β	1.980-1.981	2.019-2.023	2.810-2.811	2.805-2.809	137.23-137.24	134.31-134.33
DGQ α	2.051	2.080	2.856	2.845	134.72	132.16
β	1.981	2.019-2.024	2.810-2.811	2.806-2.810	137.23-137.28	134.29-134.34
DJP α	2.052	2.081-2.088	2.857-2.858	2.845-2.852	134.66-134.76	132.10-132.14
β	1.980-1.982	2.018-2.025	2.810-2.811	2.804-2.810	137.22-137.25	134.28-134.32
DJQ α	2.053-2.054	2.079-2.088	2.857-2.859	2.844-2.853	134.61-134.67	132.06-132.13
β	1.979-1.980	2.019-2.023	2.809-2.810	2.805-2.809	137.26	134.30-134.33
DLP α	2.050-2.052	2.080-2.087	2.855-2.859	2.845-2.853	134.69-134.83	132.09-132.22
β	1.980-1.982	2.019-2.024	2.810-2.811	2.805-2.810	137.21-134.24	134.30-134.33
DLQ	2.05	2.080	2.857	2.845	134.69	132.16
EGP α	2.054	2.085-2.090	2.864	2.854-2.859	135.12-135.13	132.45
β	1.973-1.975	2.009-2.029	2.814	2.803-2.820	138.25-138.26	134.44-134.48
EGQ α	2.037-2.040	2.070-2.080	2.859-2.862	2.847-2.856	136.49-136.55	133.47-133.41
β	1.986-1.988	2.021-2.026	2.820-2.822	2.813-2.817	137.67-137.69	134.80-134.85

EJP α	2.055	2.085-2.092	2.865-2.866	2.853-2.860	135.13-135.28	132.38-132.47
β	1.974-1.975	2.028-2.033	2.814	1.816-2.821	138.25-138.26	134.42-134.46
EJQ α	2.055-2.056	2.086-2.090	2.864-2.867	2.854-2.861	135.04-135.20	132.35-132.43
β	1.987-1.988	2.021-2.026	2.821	2.812-2.817	137.65-137.66	134.79-134.83
ELP α	2.054-2.055	2.084-2.091	2.859-2.861	2.853-2.859	135.14-135.15	132.45
β	1.974-1.977	2.028-2.033	2.813-2.816	2.816-2.821	138.24-138.27	134.43-134.47
ELQ	1.987-1.988	2.022-2.026	2.821	2.813-2.816	137.65-137.67	134.81-134.85
FGP α	2.038-2.039	2.084-2.091	2.859-2.861	2.854-2.860	136.44-136.55	132.61-132.70
β	1.977	2.028-2.031	2.816	2.819-2.823	138.27-138.28	134.78-135.15
FGQ α	2.037	2.069	2.859	2.847	136.48	133.50
β	1.989	2.026	2.823	2.817	137.70	134.89
FJP α	2.039	2.085-2.091	2.860-2.861	2.855-2.861	136.41-136.42	132.55-132.64
β	1.975-1.977	2.028-2.032	2.815-2.816	2.819-2.823	138.28-138.29	134.71-134.75
FJQ α	2.038-2.043	2.070-2.093	2.859-2.864	2.854-2.863	136.42-136.47	131.58-133.45
β	1.986-1.988	2.021-2.026	2.820-2.821	2.813-2.817	137.70-137.70	134.87-134.93
FLP α	2.038	2.084-2.090	2.859	2.854-2.860	136.44	732.60-132.61
β	1.976-1.978	2.028-2.032	2.815-2.817	2.819-2.823	138.25-138.28	134.75-134.79
FLQ α	2.036-2.054	2.076-2.091	2.858-2.864	2.854-2.861	135.18-136.52	132.62-133.02
β	1.975-1.988	2.021-2.032	2.815-2.822	2.813-2.823		134.76-134.90

Table 4.8. Ranges of the parameters of the N14–H14····O9 IHB for all the compounds in which it is present.

The symbols α and β are used to indicate the presence of bifurcation.

Molecule	Bond length ranges (Å)		N····O distance range (Å)		NĤO bond angle ranges (º)	
	DFT	HF	DFT	HF	DFT	HF
AGP	2.040-2.055	2.070-2.088	2.864-2.869	2.853-2.861	135.32-136.86	132.87-132.94
AGQ	2.041-2.059	2.070-2.089	2.866-2.871	2.853-2.862	135.35-136.88	132.87-134.15
AJP	2.042-2.045	2.071-2.078	2.866-2.869	2.854-2.861	136.80-136.86	134.06-134.11
AJQ	2.042-2.057	2.070-2.088	2.866-2.868	2.853-2.860	132.26-136.84	132.78-134.10
ALP	2.041-2.055	2.071-2.089	2.866-2.870	2.853-2.862	135.33-137.02	132.85-134.14
ALQ	2.041-2.059	2.070-2.089	2.866-2.871	2.853-2.862	135.36-136.87	132.87-134.15
BGP	2.033-2.050	2.061-2.082	2.862-2.866	2.851-2.858	135.76-137.47	133.04-134.91
BGQ	2.031-2.051	2.060-2.084	2.861-2.867	2.850-2.859	135.73-137.48	133.08-134.90
BJP	2.034	2.062-2.068	2.864	2.852-2.859	137.35-137.43	134.80-134.86
BJQ	2.033-2.049	2.061-2.083	2.862-2.866	2.851-2.861	135.63-137.44	132.92-134.86
BLP	2.047-2.049	2.076-2.082	2.863-2.865	2.851-2.857	135.76-135.77	133.04-133.12
BLQ	2.046-2.049	2.075-2.083	2.863-2.866	2.850-2.858	135.82-135.83	133.06-133.14
CGP	2.025-2.033	2.059-2.065	2.852-2.859	2.844-2.852	136.80-137.15	134.29-134.42
CGQ	2.033-2.062	2.058-2.097	2.858-2.866	2.844-2.857	134.46-136.87	131.57-134.38
CJP	2.027-2.033	2.059.2.066	2.854-2.858	2.844-2.852	136.75-137.10	134.22-134.36
CJQ	2.030-2.068	2.060-2.106	2.858-2.871	2.844-2.866	134.34-136.78	131.43-134.27
CLP	2.025-2.034	2.058-2.065	2.853-2.858	2.844-2.852	136.80-137.14	134.29-134.41
CLQ	2.032-2.063	2.059-2.104	2.857-2.867	2.844-2.865	134.51-136.87	131.68-134.37
DGP	2.050-2.052	2.080-2.087	2.856-2.858	2.845-2.852	134.71-134.81	132.14-132.22
DGQ	2.050-2.052	2.079-2.088	2.856-2.859	2.845-2.853	134.76-134.82	132.08-132.23
DJP	2.052	2.076-2.087	2.857-2.858	2.842-2.852	134.66-134.76	132.17-132.27
DJQ	2.052-2.053	2.081-2.088	2.857-2.858	2.846-2.852	134.60-134.71	132.01-132.15
DLP	2.050-2.052	2.080-2.087	2.856-2.858	2.845-2.852	134.72-134.80	132.15-132.22
DLQ	2.049-2.053	2.079-2.087	2.855-2.859	2.845-2.853	134.72-134.84	132.16-132.26
EGP	2.052-2.054	2.079-2.090	2.863-2.866	2.850-2.860	135.17-135.32	132.44-132.87
EGQ	2.052-2.053	2.078-2.093	2.864-2.867	2.850-2.857	135.21-135.30	132.44-132.86
EJP	2.054-2.055	2.079-2.086	2.863-2.865	2.850-2.857	135.05-135.18	132.74-132.75
EJQ	2.052-2.057	2.079-2.092	2.862-2.867	2.850-2.860	135.06-135.19	132.35-132.75
ELP	2.052-2.054	2.079-2.090	2.862-2.865	2.853-2.860	135.17-135.35	132.43-132.87
ELQ	2.051-2.055	2.078-2.092	2.862-2.866	2.850-2.861	135.20-135.28	132.43-132.86
FGP	2.038-2.055	2.078-2.091	2.859-2.866	2.851-2.862	135.20-136.54	132.61-132.96
FGQ	2.037-2.055	2.077-2.085	2.858-2.866	2.850-2.857	135.20-136.49	132.62-132.95
FJP	2.054-2.055	2.084-2.085	2.863-2.865	2.855-2.856	135.14-135.23	132.83-132.90
FJQ	2.036-2.056	2.078-2.095	2.858-2.867	2.858-2.867	135.13-136.48	132.59-132.89
FLP	2.037-2.054	2.078-2.091	2.859-2.865	2.851-2.861	135.19-136.55	132.60-132.95
FLQ	2.036-2.055	2.084-2.093	2.858-2.866	2.850-2.864	135.19-136.53	132.62-132.94

Table 4.9. Ranges of the parameters of the N11–H11····O13 IHB for all the compounds in which it is present.

The symbols α and β are used to indicate the presence of bifurcation.

Molecule	Bond length ranges (Å)		N····O distance range (Å)		NĤO bond angle ranges (°)	
	DFT	HF	DFT	HF	DFT	HF
AGP α	2.386-2.390	2.354-2.364	2.277-2.279	2.235-2.236	71.33-71.57	70.39-70.83
β	2.347-2.348	2.313-2.314	2.276-2.277	2.235	73.40	72.93-72.95
AGQ α	2.386-2.390	2.358-2.364	2.276-2.279	2.325-2.326	71.34-71.54	70.40-70.83
β	2.347-2.348	2.313-2.314	2.276	2.325	73.40-73.41	72.93-72.95
AJP α	2.386-2.390	2.354-2.361	2.278-2.279	2.235-2.236	71.32-71.57	70.40-70.83
β	2.347	2.312-2.314	2.276	2.235	73.42-73.43	72.95-72.98
AJQ α	2.386-2.390	2.354-2.364	2.278-2.279	2.235-2.237	71.34-71.58	70.40-70.82
β	2.46-2.347	2.312-2.313	2.276	2.235	73.42-73.44	72.96-72.99
ALP α	2.386-2.390	2.355-2.364	2.278-2.279	2.235-2.236	71.33-71.45	70.40-70.77
β	2.344-2.348	2.308-2.314	2.275-2.277	2.234-2.235	73.34-73.53	72.93-73.14
ALQ α	2.386-2.390	2.354-2.364	2.278-2.279	2.235-2.236	71.34-71.57	70.39-70.82
β	2.347-2.348	2.313-2.314	2.276	2.235	73.40	72.93-72.95
BGP α	2.383-2.389	2.351-2.363	2.277-2.278	2.234-2.236	71.36-71.64	70.43-70.94
β	2.346	2.307-2.309	2.275	2.232-2.233	73.37-73.41	73.08-73.11
BGQ α	2.383-2.389	2.350-2.363	2.277-2.278	2.234-2.236	71.36-71.63	70.43-70.95
β	2.344-2.346	2.308-2.309	2.274-2.275	2.233	73.38-73.39	73.08-73.10
BJP α	2.386-2.389	2.351-2.363	2.277-2.278	2.234-2.236	71.35-71.65	70.42-70.94
β	2.345-2.346	2.307-2.308	2.274-2.275	2.232-2.233	73.40-73.41	73.11-73.13
BJQ	2.384-2.389	2.353-2.363	2.277-2.278	2.234-2.236	71.37-71.64	70.42-70.94
BLP α	2.384-2.389	2.350-2.363	2.277-2.278	2.234-2.236	71.37-71.65	70.43-70.96
β	2.346-2.347	2.307-2.308	2.275	2.232-2.233	73.37-73.39	73.11
BLQ α	2.383-2.389	2.351-2.363	2.277-2.278	2.234-2.236	71.36-73.20	70.43-70.94
β	2.346	2.308-2.309	2.275	2.233	73.38-73.39	73.08-73.10
CGP	2.384-2.399	2.352-2.370	2.277-2.282	2.234-2.237	70.85-71.73	70.08-70.92
CGQ	2.389-2.399	2.357-2.370	2.277-2.282	2.236-2.238	70.85-71.58	70.09-70.85
CJP	2.384-2.399	2.352-2.370	2.277-2.282	2.234-2.237	70.83-71.74	70.08-70.91
CJQ	2.389-2.399	2.357-2.370	2.277-2.282	2.236-2.238	70.85-71.59	70.09-70.84
CLP	2.384-2.399	2.352-2.371	2.277-2.282	2.234-2.238	70.85-71.73	70.04-70.92
CLQ	2.389-2.396	2.355-2.370	2.277-2.282	2.236-2.238	70.84-71.58	70.08-70.92
DGP α	2.397-2.399	2.365-2.370	2.280	2.237-2.238	71.01-71.11	70.20-70.38
β	2.358-2.359	2.319-2.321	2.280	2.237-2.238	73.05-73.08	72.73-72.76
DGQ α	2.397-2.399	2.365-2.370	2.280	2.237-2.238	71.02-71.10	70.21-70.37
β	2.358	2.320-2.321	2.280	2.237-2.238	73.07-73.08	72.73-72.75
DJP α	2.397-2.399	2.364-2.370	2.280	2.236-2.238	71.02-71.10	70.20-70.37
β	2.358	2.319-2.320	2.280	2.237-2.238	73.07.73.07	72.47-72.77
DJQ α	2.396-2.398	2.362-2.370	2.280	2.237-2.238	71.03-71.11	70.20-70.38
β	2.358	2.320	2.280	2.237-2.238	73.08	72.75
DLP α	2.396-2.399	2.365-2.370	2.280	2.237-2.238	71.01-71.11	70.20-70.38
β	2.358-2.359	2.319-2.321	2.280	2.237-2.238	73.05-73.08	72.73-72.76

DLQ α	2.397-2.398	2.366-2.370	2.280	2.237-2.238	71.03-71.10	70.19-70.37
β	2.358	2.320-2.321	2.280	2.237-2.238	73.05-73.07	72.73-72.74
EGP α	2.391-2.393	2.360-2.367	2.277-2.279	2.236-2.237	71.19-71.30	70.24-70.55
β	2.349	2.312-2.318	2.276	2.235-2.237	73.31-73.35	72.79-73.02
EGQ α	2.386-2.393	2.360-2.367	2.277-2.279	2.236-2.237	71.18-71.54	70.24-70.55
β	2.352	2.315-2.316	2.277-2.278	2.235-2.236	73.23-73.24	72.88-72.89
EJP α	2.391-2.393	2.360-2.367	2.277-2.279	2.236-2.237	71.17-71.32	70.24-70.56
β	2.348-2.349	2.317-2.318	2.276	2.236-2.237	73.33-73.35	72.81-72.84
EJQ α	2.391-2.393	2.360-2.367	2.277-2.279	2.236-2.237	71.17-71.29	70.25-70.56
β	2.351	2.314-2.315	2.277	2.235-2.236	73.27-73.29	72.91-72.93
ELP α	2.391-2.393	2.361-2.367	2.277-2.279	2.236-2.237	71.17-71-30	70.24-70.55
β	2.348-2.349	2.317-2.319	2.276	2.236-2.237	73.33-73.35	72.79-72.83
ELQ α	2.391-2.393	2.363-2.367	2.277-2.279	2.236-2.237	71.18-71.29	70.24-70.56
β	2.352	2.315-2.316	2.277-2.278	2.236	73.23-72.25	72.88-72.89
FGP α	2.387-2.393	2.360-2.366	2.278-2.279	2.236-2.237	71.24-71.53	70.27-70.58
β	2.349	2.314-2.316	2.277	2.235-2.236	73.34-73.37	72.86-72.95
FGQ α	2.387-2.393	2.659-2.366	2.278-2.279	2.236-2.237	71.25-71.51	70.28-70.67
β	2.352	2.315	2.278	2.236	73.27	72.90
FJP α	2.387-2.393	2.360-2.366	2.276-2.279	2.236-2.237	71.24-73.35	70.28-70.58
β	2.348-2.349	2.315-2.316	2.236	2.235-2.236	73.35-73.37	72.87-72.90
FJQ α	2.387-2.399	2.359-2.366	2.279-2.279	2.236-2.237	71.26-71.51	70.27-70.67
β	2.351	2.314-2.315	2.277	2.235-2.236	72.27-73.28	72.92-72.93
FLP α	2.387-2.393	2.360-2.366	2.278-2.279	2.236-2.237	71.25-71.53	70.28-70.58
β	2.348-2.349	2.315-2.316	2.276-2.277	2.235-2.236	73.34-73.37	72.86-72.90
FLQ α	2.397-2.393	2.360-2.367	2.278-2.279	2.236-2.237	71.25-71.51	70.25-70.58
β	2.349-2.352	2.314-2.316	2.276-2.278	2.235-2.236	73.26-73.34	72.86-72.91

Table 4.10. Ranges of the parameters of the N11–H11····O10 IHB for all the compounds in which it is present.

The symbols α and β are used to indicate the presence of bifurcation.

Molecule	Bond length ranges (Å)		N····O distance range (Å)		NĤO bond angle ranges (º)	
	DFT	HF	DFT	HF	DFT	HF
AGP	2.591-2.599	2.499-2.512	2.497-2.499	2.428-2.431	73.03-73.34	73.87-74.34
AGQ	2.590-2.598	2.499-2.512	2.497-2.498	2.428-2.431	73.07-73.40	73.86-74.37
AJP	2.592-2.598	2.499-2.511	2.498-2.499	2.429-2.431	73.10-73.34	73.88-74.35
AJQ	2.592-2.598	2.500-2.512	2.497-2.499	2.429-2.431	73.08-73.32	74.07-74.34
ALP	2.591-2.598	2.499-2.512	2.497-2.499	2.428-2.431	73.07-73.37	73.87-74.35
ALQ	2.590-2.598	2.504-2.512	2.497-2.499	2.428-2.431	73.09-73.39	73.87-74.37
BGP	2.594-2.600	2.502-2.513	2.498-2.500	2.429-2.431	73.03-73.25	73.83-74.25
BGQ	2.592-2.601	2.501-2.513	2.498-2.500	2.429-2.432	72.99-73.29	73.81-74.23
BJP	2.596-2.599	2.505-2.511	2.499-2.500	2.430-2.432	73.06-73.15	73.94-74.14
BJQ	2.595-2.601	2.502-2.513	2.498-2.500	2.429-2.432	73.00-73.21	73.83-74.25
BLP	2.594-2.598	2.502-2.509	2.498-2.499	2.429-2.431	73.09-73.23	73.98-74.25
BLQ	2.593-2.597	2.502-2.509	2.498-2.499	2.429-2.431	73.11-73.26	73.97-74.26
CGP	2.600-2.607	2.505-2.521	2.500-2.501	2.430-2.433	72.70-72.99	73.47-74.14
CGQ	2.587-2.607	2.498-2.521	2.497-2.501	2.428-2.433	72.72-73.53	73.46-74.40
CJP	2.600-2.607	2.505-2.521	2.500-2.501	2.430-2.433	72.71-73.01	73.47-74.14
CJQ	2.582-2.607	2.491-2.521	2.495-2.501	2.427-2.433	72.71-73.73	73.47-74.71
CLP	2.600-2.607	2.505-2.521	2.500-2.501	2.430-2.433	72.71-73.00	73.47-74.14
CLQ	2.584-2.608	2.491-2.523	2.496-2.501	2.427-2.433	72.70-73.64	73.39-74.68
DGP	2.599	2.509-2.511	2.499	2.431	73.03	73.89-74.00
DGQ	2.594-2.598	2.502-2.511	2.498-2.499	2.429-2.431	73.07-73.20	73.88-74.21
DJP	2.595-2.598	2.503-2.513	2.498-2.499	2.429-2.431	73.08-73.17	73.81-74.19
DJQ	2.595-2.599	2.503.2.511	2.498-2.499	2.429-2.431	73.05-73.17	73.89-74.19
DLP	2.595-2.599	2.503-2.510	2.498-2.499	2.429-2.431	73.03-73.19	73.91-74.19
DLQ	2.595-2.599	2.503-2.511	2.498-2.499	2.429-2.431	73.03-73.20	73.90-74.22
EGP	2.592-2.597	2.498-2.508	2.497.2.499	2.428-4.431	73.14-73.30	73.93-74.39
EGQ	2.591-2.597	2.498-2.510	2.497-2.499	2.428-2.431	73.13-73.33	73.91-74.41
EJP	2.592-2.597	2.503-2.510	2.498-2.499	2.429-2.431	73.14-73.30	73.93-74.21
EJQ	2.591-2.595	2.499-2.510	2.497-2.499	2.428-2.431	73.15-73.33	73.93-74.37
ELP	2.591-2.597	2.498-2.510	2.497-2.499	2.428-2.431	73.14-73.32	73.93-74.39
ELQ	2.591-2.597	2.498-2.510	2.497-2.499	2.428-2.431	73.13-73.32	73.90-74.40
FGP	2.592-2.605	2.502-2.510	2.497-2.499	2.429-2.431	72.75-73.30	73.92-74.25
FGQ	2.592-2.605	2.497-2.511	2.498-2.500	2.428-2.431	72.76-73.30	73.90-74.44
FJP	2.592-5.596	2.503-2.510	2.498-2.499	2.429-2.431	73.15-73.30	73.92-74.21
FJQ	2.592-2.605	2.498-511	2.498-2.500	2.428-2.431	72.74-72.89	73.90-74.19
FLP	2.593-2.605	2.498-2.510	2.498-2.499	2.428-2.431	72.74-73.26	73.93-74.41
FLQ	2.592-2.599	2.495-2.510	2.498-2.499	2.427-2.499	72.97-73.30	73.90-74.52

Table 4.11. Ranges of the parameters of the N11–H11····O9 IHB for all the compounds in which it is present.

The symbols α and β are used to indicate the presence of bifurcation.

Molecule	Bond length ranges (Å)		N····O distance range (Å)		NĤO bond angle ranges (º)	
	DFT	HF	DFT	HF	DFT	HF
AGP α	2.591.2.596	2.499-2.505	2.497-2.499	2.428-2.430	73.17-73.34	74.17-74.36
β	2.440-2.443	2.939-2.394	2.464	2.404-2.405	79.27-79.38	78.63-78.67
AGQ	2.440-2.443	2.390-2.392	2.464	2.404-2.405	79.28-79.38	78.63-78-68
AJQ	2.594-2.595	2.500-2.511	2.498-2.499	2.429-2.431	73.21-73.33	73.86-74.35
BGP α	2.598	2.507	2.499	2.431	73.09	74.07-74.09
β	2.436-2.439	2.391-2.392	2.464	2.404-2.405	79.46-79.61	78.71-78.75
BJP	2.594-2.598	2.502-2.509	2.498-2.499	2.429-2.431	73.11-73.25	73.98-74.25
BJQ	2.593-2.598	2.502-2.509	2.498-2.499	2.429-2.431	73.12-73.26	73.99-74.26
BLP	2.597-2.600	2.505-2.513	2.499-2.500	2.430-2.432	73.04-73.13	73.81-74.14
BLQ	2.592-2.598	2.501-2.513	2.498-2.500	2.429-2.432	73.02-73.29	73.82-74.28
CGP α	2.583-2.587	2.491-2.498	2.496-2.497	2.427-2.428	73.51-73.67	74.40-74.69
β	2.435-2.438	2.386-2.389	2.470	2.406	79.8179.95	78.99-79.10
CGQ	2.582-2.587	2.491-2.498	2.495-2.497	2.427-2.428	73.53-73.72	74.42-74.70
CJP	2.582-2.587	2.489-2.496	2.495-2.497	2.427-2.249	73.53-73.73	74.40-74.68
CJQ	2.583-2.587	2.496-2.499	2.496-2.497	2.429	73.54-73.67	74.37-74.41
CLP	2.583-2.587	2.490-2.498	2.496-2.497	2.426-2.428	73.51-73.67	74.41-74.73
CLQ	2.587	2.496-2.498	2.497	2.428	73.51	74.42-74.54
DGP α	2.599	2.508-2.511	2.499	2.431	73.03	73.88-74.02
β	2.445-2.446	2.395-2.396	2.464-2.465	2.405	79.13-79.19	73.52-78.56
DGQ α	2.598	2.511	2.499	2.431	73.06	73.90
β	2.445-2.446	2.395-2.396	2.465	2.405	79.13-79.20	78.51-78.56
DJP	2.595-2.598	2.504-2.511	2.498-2.499	2.429-2.431	73.08-73.18	73.91-74.17
DJQ	2.595-2.598	2.503-2.511	2.498-2.499	2.429-2.431	73.0773.19	73.88-74.20
DLP	2.594-2.600	2.503-2.511	2.498-2.499	2.429-2.431	73.01-73.20	73.89-74.20
DLQ	2.598	2.510	2.499	2.431	73.07	73.90
EGP α	2.595	2.503.2.505	2.498	2.430	73.17-73.18	74.12-74.23
β	2.244-2.446	2.395-2.396	2.464-2.465	2.405	79.14-79.20	78.53-78.57
EGQ α	2.600-2.605	2.506-2.515	2.499-2.493	2.429-2.432	72.73-72.91	73.69-74.05
β	2.444-2.446	2.395-2.396	2.464-2.465	2.405	79.14-79.20	78.53-78.58
EJP	2.591-2.594	2.499-2.506	2.497-2.498	2.497-2.498	73.22-73.33	74.10-74.38
EJQ	2.591-2.595	2.504-2.506	2.497-2.498	2.430	73.17-73.33	74.10-74.21
ELP	2.594	2.503-2.506	2.498	2.430	73.20	74.09-74.23
FGP α	2.600-2.605	2.498-2.505	2.498-2.499	2.428-2.430	72.76-72.91	74.13-74.42
β	2.445-2.443	2.394-2.396	2.464-2.465	2.404-2.405	79.18-79.24	78.55-78.59
FGQ α	2.605	2.516	2.500	2.432	72.76	73.66
β	2.444-2.445	2.394-2.396	2.464-2.465	2.404-2.405	79.19-79.23	78.55-78.60
FJP	2.598-2.604	2.498-2.505	2.499-2.607	2.428-2.430	68.72-72.79	74.14-74.41
FJQ	2.599-2.604	2.497-2.516	2.498-2.500	2.428-2.432	72.78-72.98	73.66-74.46
FLP	2.605	2.502-2.505	2.499	2.430	72.75	74.14-74.27

FLQ	2.596-2.600	2.498-2.509	2.498-2.500	2.428-2.430	72.76-73.16	73.95-74.41

Table 4.12. Energy difference between lowest energy conformer without any IHB and the highest energy conformer with at least one IHB for the calculated conformers of the considered compounds.

Compounds	Energy difference (kcal/mol)	
	DFT	HF
AGP	5.581	6.435
AGQ	5.586	6.450
AJP	16.152	15.263
AJQ	6.696	5.637
ALP	8.760	8.083
ALQ	8.480	7.836
BGP	5.607	7.229
BGQ	8.768	8.249
BJP	16.446	15.760
BJQ	8.128	4.983
BLP	7.535	7.758
BLQ	7.353	6.693
CGP	5.319	6.024
CGQ	9.647	8.653
CJP	14.815	13.190
CJQ	7.463	6.403
CLP	7.312	5.282
CLQ	9.618	8.603
DGP	5.590	6.425
DGQ	5.603	6.442
DJP	16.796	13.279
DJQ	0.522	0.048
DLP	9.053	5.721
DLQ	7.741	6.890
EGP	5.579	6.428
EGQ	5.592	6.444
EJP	16.886	13.146
EJQ	7.033	6.071
ELP	8.856	5.223
ELQ	9.129	8.271
FGP	5.580	6.431
FGQ	5.590	6.447
FJP	17.035	13.125
FJQ	9.029	8.246
FLP	8.895	5.202
FLQ	9.267	7.899

Table 4.13. Ranges of the dipole moments for each of the molecules considered.

Molecule	Dipole moments ranges (Debye)	
	DFT	HF
AGP	5.3973–9.7881	5.3625–10.0639
AGQ	5.5198–9.8865	5.5540–10.2168
AJP	4.4163–8.1508	4.0082–8.4151
AJQ	3.7197–9.5732	3.6429–9.9673
ALP	5.6355–9.6009	5.0445–9.8593
ALQ	6.1064–9.7569	6.1217–10.0688
BGP	5.2828–9.9492	5.3039–10.1800
BGQ	6.3620–10.0437	6.3568–10.3030
BJP	4.5103–8.2516	4.0658–8.4950
BJQ	3.8621–9.7088	3.3352–10.0634
BLP	6.0489–9.7683	5.3142–9.9915
BLQ	6.3974–9.6951	5.8227–10.1763
CGP	5.3526–9.9031	5.5723–10.1733
CGQ	6.6208–9.9946	6.3982–10.2990
CJP	4.6196–8.1671	4.0945.8.4467
CJQ	4.0729–9.6308	3.8585–10.0419
CLP	6.1990–9.9657	5.4210–10.2186
CLQ	5.5314–9.0720	4.9051–9.3851
DGP	5.2093–10.0722	5.1915–10.2986
DGQ	5.3279–10.1681	5.4160–10.4330
DJP	4.6408–8.3605	4.1473–8.5981
DJQ	3.9729–8.7584	3.4082–9.0396
DLP	6.1499–9.8573	5.4098–10.0933
DLQ	6.4780–10.0361	6.3602–10.3085
EGP	5.4058–10.0076	5.3329–10.2601
EGQ	5.5091–10.1133	5.5456–10.3893
EJP	4.5201–8.3318	4.0380–8.5786
EJQ	4.0324–9.7683	3.7890–10.1501
ELP	5.9929–9.8160	5.4065–10.0562
ELQ	6.3959–10.0201	6.2967–10.3603
FGP	5.5460–10.0423	5.4192–10.2785
FGQ	5.6310–10.1372	5.6311–10.4033
FJP	4.3584–8.3566	3.9488–8.6026
FJQ	5.8391–9.9058	5.9340–10.3731
FLP	5.9160–9.8431	5.4829–10.0755
FLQ	6.1762–10.0225	6.0928–10.3684

Table 4.14. Ranges of dipole moments for each conformer type in each of the compounds considered.

Molecules	Conformer type	Dipole moments ranges (Debye)	
		DFT	HF
AGP	m	6.2094–7.1485	5.7648–7.0273
	p	6.1758–7.1539	5.8802–6.9837
	k	5.9887–6.8125	5.9565–6.7316
	g	5.3973–6.5944	5.3625–6.9499
	j	9.3860–9.7881	7.9106–10.0639
AGQ	m	6.3812–7.1274	6.3442–6.9493
	k	6.1490–6.7902	6.1884–6.7155
	g	5.5198–6.5046	5.5540–6.7883
	j	9.4825–9.8865	9.7609–10.2168
AJP	m	4.4163–5.8197	4.0082–5.6497
	k	4.3272–5.3519	4.2145–5.2782
	j	7.8330–8.1508	7.7998–8.1305
AJQ	m	4.9202–6.2182	4.0775–6.1856
	p	3.8264–5.1049	3.6625–4.9481
	k	3.7197–4.7512	3.6429–4.6444
	j	8.7689–9.5732	9.0824–9.9673
ALP	m	5.8707–6.3711	5.0445–6.1044
	k	5.6355–6.6809	5.4478–6.6236
	j	9.3083–9.6009	7.6413–9.8593
ALQ	m	6.3329–6.9510	6.2829–6.8002
	k	6.1064–6.6381	6.1219–6.5639
	j	9.4618–9.7569	9.1294–10.0688
BGP	m	6.3073–7.1291	5.7919–6.9927
	p	6.2528–6.2533	5.4640–5.8287
	k	6.2109–6.9481	5.7070–6.8235
	g	5.2828–6.5638	5.3039–6.9663
	j	9.5200–9.9492	8.0190–10.1800
BGQ	m	6.4424–7.1450	6.3568–6.9420
	k	6.3620–6.9358	6.3242–6.8197
	j	9.6228–10.0437	9.8651–10.3030
BJP	m	4.6160–5.6943	4.0516–5.5240
	p	4.5102–5.7824	4.0658–5.6077
	k	4.5610–5.4554	4.3269–5.3389
	j	7.9502–8.2516	7.8660–8.2140
BJQ	m	3.8620–6.2479	3.3352–6.1893
	p	4.9244–5.9974	3.6951–5.9499
	j	8.9230–9.7088	9.1869–10.0634
BLP	m	6.0907–7.0266	5.8932–6.8995
	p	6.0489–7.0048	5.3142–6.8329
	k	6.0954–6.8532	5.6731–6.7793
	j	9.5050–9.7683	7.7789–9.9915
BLQ	m	6.5790–7.1674	6.3465–6.9648

	p	6.3974–7.1683	5.8227–6.8021
	k	6.4103–6.7045	6.3351–6.5986
	j	9.6923–9.9151	9.9063–10.1763
CGP	m	6.3633–7.1340	5.8395–6.9585
	p	6.4380–7.2370	5.5858–7.0506
	g	5.3526–6.7464	5.5723–7.3460
	j	9.4778–9.9031	8.0340–10.1733
CGQ	m	6.4906–7.1576	6.3982–6.9791
	p	6.6208–7.2367	6.5220–7.0402
	j	9.5669–9.9946	9.8442–10.2290
CJP	m	4.5690–5.7338	4.1094–5.5368
	p	4.7012–5.8300	4.1254–5.6555
	j	7.8621–8.1671	7.8072–8.1758
CJQ	m	4.9229–6.3519	4.0938–6.2980
	p	4.0729–5.2175	3.8462–4.8212
	j	8.8641–9.6308	9.1706–10.0419
CLP	m	6.1511–7.0316	5.6514–6.9207
	p	6.2373–7.1236	5.4261–6.9555
	j	9.2238–9.9657	7.9328–10.2186
CLQ	m	5.5314–6.5640	5.3199–6.3706
	p	5.6566	4.9731–5.4503
	j	9.0272–9.0720	7.4177–9.3851
DGP	m	6.4319–7.1882	5.8713–7.0240
	p	6.3647–6.3649	5.8325–6.1666
	k	6.3231–7.0475	5.8271–6.9188
	g	5.2093–6.5873	5.1915–6.9199
	j	9.6673–10.0722	8.1770–10.2986
DGQ	m	6.6176–7.2176	6.4448–6.9951
	p	6.5488	6.4240
	k	6.4646–7.0454	6.4206–6.9168
	g	5.3279–6.4706	5.4160–6.7369
	j	9.7579–10.1681	10.0064–10.4330
DJP	m	4.6410–5.8197	4.4624–5.6271
	p	4.6408–5.8197	4.1473–5.6279
	k	4.6849–5.5527	4.4388–5.4269
	j	8.0528–8.3605	7.9514–8.3241
DJQ	m	3.9727–6.4008	3.4082–6.2425
	p	4.0262–5.1710	3.7847–4.9724
	k	5.9002–6.2918	5.8825–6.2394
	j	8.4357–8.7584	8.8201–9.0396
DLP	m	6.2201–7.0876	5.6831–6.9872
	p	6.1648–7.1232	5.4098–6.9233
	k	6.1499–6.9135	5.7085–6.8028
	j	9.5719–9.8573	9.7872–10.0933
DLQ	m	6.5061–7.2407	6.3602–7.0092
	p	6.5523	6.4197
	k	6.4780–6.9493	6.4212–6.8213
	j	9.8169–10.0361	10.0673–10.3085
EGP	m	6.2746–7.2621	5.7703–7.1062

	p	6.3666–6.3675	5.5593–6.1859
	k	6.1658–6.8686	5.6640–6.8092
	g	5.4058–6.7092	5.3329–7.0159
	j	9.5883–10.0076	8.1125–10.2601
EGQ	m	6.4572–7.2718	6.3629–7.0531
	p	6.6145–7.2855	6.4777–7.0336
	k	6.4264–7.0188	6.4090–69001
	g	5.5091–6.6296	5.5456–6.8402
	j	9.6750–10.1133	9.9404–10.3893
EJP	m	4.4781–5.7258	4.0380–5.5667
	p	4.6275–5.9186	4.1570–5.7170
	k	4.5201–5.3749	4.3056–5.3008
	j	8.0117–8.3318	7.9454–8.5756
EJQ	m	5.0760–6.1891	4.1858–5.9219
	p	4.0324–5.2480	3.7890–5.0376
	k	4.8574–4.9889	4.6893–4.8452
	j	8.9685–9.7683	9.2669–10.1501
ELP	m	6.0605–7.1687	5.5782–7.0136
	p	6.1632–6.1637	5.4065–5.9741
	k	5.9929–6.7318	5.5519–6.6613
	j	9.3328–9.8160	8.4049–10.0562
ELQ	m	6.3959–7.1218	6.2967–6.9042
	k	6.4670–6.7946	6.4121–6.6889
	j	9.1213–10.0201	7.5112–10.3603
FGP	m	6.1572–7.3633	6.0198–7.1690
	p	6.5199–7.3754	5.5995–7.1438
	k	6.0882–6.7550	5.9353–6.6975
	g	5.5460–6.8802	5.4192–7.0978
	j	9.5095–10.0423	8.1102–10.2785
FGQ	m	6.3364–7.3684	6.2743–7.1118
	k	7.0580	6.9282
	g	5.6310–6.7434	5.6311–6.9241
	j	9.6351–9.9410	10.4047
FJP	m	4.3584–5.6388	3.9488–5.4980
	p	4.7762–5.2520	4.2076–5.7888
	k	4.4441–5.2519	4.2580–5.226
	j	8.0422–8.3566	7.9805–8.6026
FJQ	m	5.8391–6.4866	5.9340–6.3594
	p	6.3011–6.4050	6.1336–6.3542
	k	6.0053–6.0962	6.1045–6.1088
	j	8.7672–9.9058	9.1057–10.3731
FLP	m	5.9419–7.2493	5.4892–7.0785
	p	6.3142–6.3145	5.4458–5.9985
	k	5.9160–6.6205	5.4829–6.5841
	j	9.3586–9.8431	7.8391–10.0755
FLQ	m	6.2737–7.2279	6.2101–6.9681
	p	6.2510–7.1957	6.2299–6.9699
	k	6.1762–6.8330	6.0928–6.7233
	j	9.6246–10.0225	9.8165–10.3684

Table 4.15. Ranges of dipole moments of molecules for each of the conformer type.

Molecules are arranged in order of increasing DFT dipole moments.

Conformer type	Molecules	Dipole moments ranges Debye)	
		DFT	HF
m	BJQ	3.8620–6.2479	3.3352–6.1893
	DJQ	3.9727–6.4008	3.4082–6.2425
	FJP	4.3584–5.6388	3.9488–5.4980
	AJP	4.4163–5.8197	4.0082–5.6497
	EJP	4.4781–5.7258	4.0380–5.5667
	CJP	4.5690–5.7338	4.1094–5.5368
	BJP	4.6160–5.6943	4.0516–5.5240
	DJP	4.6410–5.8197	4.4624–5.6271
	AJQ	4.9202–6.2182	4.0775–6.1856
	CJQ	4.9229–6.3519	4.0938–6.2980
	EJQ	5.0760–6.1891	4.1858–5.9219
	CLQ	5.5314–6.5640	5.3199–6.3706
	FJQ	5.8391–6.4866	5.9340–6.3594
	ALP	5.8707–6.3711	5.0445–6.1044
	FLP	5.9419–7.2493	5.4892–7.0785
	ELP	6.0605–7.1687	5.5782–7.0136
	BLP	6.0907–7.0266	5.8932–6.8995
	CLP	6.1511–7.0316	5.6514–6.9207
	FGP	6.1572–7.3633	6.0198–7.1690
	AGP	6.2094–7.1485	5.7648–7.0273
	DLP	6.2201–7.0876	5.6831–6.9872
	FLQ	6.2737–7.2279	6.2101–6.9681
	EGP	6.2746–7.2621	5.7703–7.1062
	BGP	6.3073–7.1291	5.7919–6.9927
	ALQ	6.3329–6.9510	6.2829–6.8002
	FGQ	6.3364–7.3684	6.2743–7.1118
	CGP	6.3633–7.1340	5.8395–7.0181
	AGQ	6.3812–7.1274	6.3442–6.9493
	ELQ	6.3959–7.1218	6.2967–6.9042
	DGP	6.4319–7.1882	5.8713–7.0240
	BGQ	6.4424–7.1450	6.3568–6.9420
	EGQ	6.4572–7.2718	6.3629–7.0531
	CGQ	6.4906–7.1576	6.3982–6.9791
	DLQ	6.5061–7.2407	6.3602–7.0092
	BLQ	6.5790–7.1674	6.3465–6.9648
	DGQ	6.6176–7.2176	6.4448–6.9951
p	AJQ	3.8264–5.1049	3.6625–4.9481
	DJQ	4.0262–5.1710	3.7847–4.9724
	EJQ	4.0324–5.2480	3.7890–5.0376
	CJQ	4.0729–5.2175	3.8462–4.8212
	BJP	4.5102–5.7824	4.0658–5.6077
	EJP	4.6275–5.9186	4.1570–5.7170

	DJP	4.6408–5.8197	4.1473–5.6279
	CJP	4.7012–5.8300	4.1254–5.6555
	FJP	4.7762–5.2520	4.2076–5.7888
	BJQ	4.9244–5.9974	3.6951–5.9499
	CLQ	5.6566	4.9731–5.4503
	ELP	6.1632–6.1637	5.4065–5.9741
	DLP	6.1648–7.1232	5.4098–6.9233
	AGP	6.1758–7.1539	5.8802–6.9837
	CLP	6.2373–7.1236	5.4261–6.9555
	FLQ	6.2510–7.1957	6.2299–6.9699
	BGP	6.2528–6.2533	5.4640–5.8287
	FJQ	6.3011–6.4050	6.1336–6.3542
	FLP	6.3142–6.3145	5.4458–5.9985
	DGP	6.3647–6.3649	5.8325–6.1666
	EGP	6.3666–6.3675	5.5593–6.1859
	BLQ	6.3974–7.1683	5.8227–6.8021
	CGP	6.4380–7.2370	5.5858–7.0506
	DGQ	6.5488	6.4240
	DLQ	6.5523	6.4197
	FGP	6.5199–7.3754	5.5995–7.1438
	EGQ	6.6145–7.2855	6.4777–7.0336
	CGQ	6.6208–7.2367	6.5220–7.0402
k	AJQ	3.7197–4.7512	3.6429–4.6444
	AJP	4.3272–5.3519	4.2145–5.2782
	FJP	4.4441–5.2519	4.2580–5.226
	EJP	4.5201–5.3749	4.3056–5.3008
	BJP	4.5610–5.4554	4.3269–5.3389
	DJP	4.6849–5.5527	4.4388–5.4269
	EJQ	4.8574–4.9889	4.6893–4.8452
	ALP	5.6355–6.6809	5.4478–6.6236
	DJQ	5.9002–6.2918	5.8825–6.2394
	FLP	5.9160–6.6205	5.4829–6.5841
	AGP	5.9887–6.8125	5.9565–6.7316
	ELP	5.9929–6.7318	5.5519–6.6613
	FJQ	6.0053–6.0962	6.1045–6.1088
	FGP	6.0882–6.7550	5.9353–6.6975
	BLP	6.0954–6.8532	5.6731–6.7793
	ALQ	6.1064–6.6381	6.1219–6.5639
	AGQ	6.1490–6.7902	6.1884–6.7155
	DLP	6.1499–6.9135	5.7085–6.8028
	EGP	6.1658–6.8686	5.6640–6.8092
	FLQ	6.1762–6.8330	6.0928–6.7233
	BGP	6.2109–6.9481	5.7070–6.8235
	DGP	6.3231–7.0475	5.8271–6.9188
	BGQ	6.3620–6.9358	6.3242–6.8197
	BLQ	6.4103–6.7045	6.3351–6.5986
	EGQ	6.4264–7.0188	6.4090–69001
	DGQ	6.4646–7.0454	6.4206–6.9168

	ELQ	6.4670–6.7946	6.4121–6.6889
	DLQ	6.4780–6.9493	6.4212–6.8213
	FGQ	7.0580	6.9282
g	DGP	5.2093–6.5873	5.1915–6.9199
	BGP	5.2828–6.5638	5.3039–6.9663
	DGQ	5.3279–6.4706	5.4160–6.7369
	CGP	5.3526–6.7464	5.5723–7.3460
	AGP	5.3973–6.5944	5.3625–6.9499
	EGP	5.4058–6.7092	5.3329–7.0159
	EGQ	5.5091–6.6296	5.5456–6.8402
	AGQ	5.5198–6.5046	5.5540–6.7883
	FGP	5.5460–6.8802	5.4192–7.0978
	FGQ	5.6310–6.7434	5.6311–6.9241
j	AJP	7.8330–8.1508	7.7998–8.1305
	CJP	7.8621–8.1671	7.8072–8.1758
	BJP	7.9502–8.2516	7.8660–8.2140
	EJP	8.0117–8.3318	7.9454–8.5756
	FJP	8.0422–8.3566	7.9805–8.6026
	DJP	8.0528–8.3605	7.9514–8.3241
	DJQ	8.4357–8.7584	8.8201–9.0396
	FJQ	8.7672–9.9058	9.1057–10.3731
	AJQ	8.7689–9.5732	9.0824–9.9673
	CJQ	8.8641–9.6308	9.1706–10.0419
	BJQ	8.9230–9.7088	9.1869–10.0634
	EJQ	8.9685–9.7683	9.2669–10.1501
	CLQ	9.0272–9.0720	7.4177–9.3851
	ELQ	9.1213–10.0201	7.5112–10.3603
	CLP	9.2238–9.9657	7.9328–10.2186
	ALP	9.3083–9.6009	7.6413–9.8593
	ELP	9.3328–9.8160	8.4049–10.0562
	FLP	9.3586–9.8431	7.8391–10.0755
	AGP	9.3860–9.7881	7.9106–10.0639
	ALQ	9.4618–9.7569	9.1294–10.0688
	AGQ	9.4825–9.8865	9.7609–10.2168
	CGP	9.4778–9.9031	8.0340–10.1733
	BLP	9.5050–9.7683	7.7789–9.9915
	FGP	9.5095–10.0423	8.1102–10.2785
	BGP	9.5200–9.9492	8.0190–10.1800
	CGQ	9.5669–9.9946	9.8442–10.2290
	DLP	9.5719–9.8573	9.7872–10.0933
	EGP	9.5883–10.0076	8.1125–10.2601
	BGQ	9.6228–10.0437	9.8651–10.3030
	FLQ	9.6246–10.0225	9.8165–10.3684
	FGQ	9.6351–9.9410	10.4047
	DGP	9.6673–10.0722	8.1770–10.2986
	EGQ	9.6750–10.1133	9.9404–10.3893
	BLQ	9.6923–9.9151	9.9063–10.1763

	DGQ	9.7579–10.1681	10.0064–10.4330
	DLQ	9.8169–10.0361	10.0673–10.3085

Table 4.16: Ranges of the HOMO–LUMO energy gaps for each of the compounds considered.

Molecule	HOMO–LUMO energy gap ranges			
	DFT	HF	Width of the ranges	
			DFT	HF
AGP	111.552–118.392	278.890–285.542	6.840	6.652
AGQ	115.207–121.232	278.903–286.263	6.025	7.360
AJP	108.973–111.452	277.779–282.448	2.479	4.669
AJQ	107.034–117.940	276.267–282.348	10.906	6.081
ALP	106.068–112.456	276.593–282.166	6.388	5.573
ALQ	108.421–116.372	278.426–282.122	7.951	3.696
BGP	113.239–118.085	278.250–283.371	4.846	5.121
BGQ	114.891–119.057	278.255–286.207	4.166	7.952
BJP	108.685–111.232	278.488–282.404	2.547	3.916
BJQ	108.101–117.664	276.995–282.304	9.563	5.309
BLP	108.954–114.213	278.997–283.207	5.259	4.210
BLQ	105.597–117.225	272.301–284.870	11.628	12.569
CGP	112.104–117.576	278.727–285.096	5.472	6.369
CGQ	115.675–118.787	278.702–286.119	3.112	7.417
CJP	108.904–111.000	277.353–282.341	2.096	4.988
CJQ	107.555–117.432	278.947–282.235	9.877	3.288
CLP	108.779–111.264	278.432–282.153	2.485	3.803
CLQ	109.519–112.619	278.921–282.210	3.100	3.289
DGP	111.201–117.765	278.256–285.109	6.564	6.853
DGQ	114.872–120.639	278.244–286.138	5.767	7.894
DJP	108.471–111.025	277.365–282.354	2.554	4.989
DJQ	107.812–122.163	275.953–282.323	14.351	6.370
DLP	107.812–111.966	277.786–282.072	4.154	4.286
DLQ	105.233–117.526	278.256–284.748	12.293	6.492
EGP	111.377–118.078	278.099–285.316	6.701	7.217
EGQ	114.972–121.003	278.294–286.213	6.031	7.919
EJP	108.716–111.377	277.572–282.404	2.661	4.832
EJQ	107.850–117.727	275.866–282.310	9.877	6.444
ELP	107.982–112.722	277.943–282.115	4.740	4.172
ELQ	112.010–116.083	278.325–282.285	4.073	3.960
FGP	111.395–118.179	278.413–285.435	6.784	7.110
FGQ	115.035–121.122	278.281–286.238	6.087	7.957
FJP	108.816–111.314	277.679–282.423	2.489	4.744
FJQ	113.661–117.765	278.551–285.454	4.104	6.903
FLP	108.026–112.305	278.407–282.247	4.279	3.840
FLQ	112.054–116.177	278.232–282.134	4.123	3.811

Chapter 5

Discussion and conclusions

This chapter presents the discussion and the conclusions based on all the observations noted during the analysis of the results, as reported in chapter 4, and considerations for future studies on the molecules considered.

5.1. Overall discussions and inferences

The computational studies of the sulfonylureas molecules reported in this work have all been done in *vacuo*. Only new sulfonylureas, which are yet to be synthesized, were studied. The objective was to provide information about these compounds, which could be relevant to researchers working on them experimentally. Different R and R′ were considered, so that this study covers a broad variety of sulfonylureas molecules with groups that can be of interest in view of medically related properties.

Both DFT and HF methods were used in this study because of the advantages of obtaining results from two different methods. The HF/6-31G(d,p) is the cheapest option that can give reasonable results; it was considered interesting to evaluate its performance for these molecules in view of the possibility that it can be used for fast screening of a large number of molecules. The DFT/B3LYP results were used as reference in organizing the materials considered in the analysis; it appears reasonable to consider the DFT results as benchmarks because DFT takes into account also part of the electron correlation.

The most stable conformers of each of the compounds considered were successfully identified. The results show how different factors can influence the molecular properties. They show the importance of the intramolecular hydrogen bonds (IHBs) as a stabilizing factor influencing the energy of the conformers. The presence, the number, and the type of IHBs all have significant influence on the relative energy of individual conformers. The greater the number of IHBs, the lower the relative energies of the conformers. The importance of the IHBs is also made evident by the fact that the highest energy conformers are characterized by the absence of IHBs, and the energy difference between the highest energy conformer with at least one IHB and the lowest energy conformer without any IHBs is at least 5 kcal/mol (often greater).

Five different conformer types were identified across all the compounds considered and were denoted by m/p, k, g and j. They differ by the number and type of IHBs present and by some relevant geometrical features. The different conformer types have different relative energy ranges across conformers. The number of individual conformers and the conformer types differ for different compounds.

The m/p conformers (conformers with three IHBs) are the conformers with the lowest relative energies in most of the compounds considered. The k conformers (conformers with two IHBs) are also amongst the lowest energy conformers and they are also the ones with shortest IHBs, both for the H14····O10 and the H11····O13 IHBs. The g conformers (with only the H11····O9 IHB) were found to have higher relative energy than the m/p and k conformers. The j conformers (conformers without IHBs) are always the conformers with the highest relative energies in all the compounds.

Given their importance in stabilizing the molecules, the IHBs were given specific attention. The m/p conformers differ from the other conformer types because of the presence of two IHBs with the same proton donor and two different proton acceptors (the proton acceptors are the sp^2 hybridized oxygen atoms O13 and O10). These are known as bifurcated hydrogen bonds; the bifurcation is on the hydrogen atom H11. This bifurcation plays an important role in the stabilization of the conformers because it allows the presence of three simultaneous IHBs, while when there is no bifurcation, only two IHBs may be present. It may happen that, in some cases, the combined effects of these two IHBs can have comparable or greater stabilizing effect than the three IHBs of the m/p conformers, but in the majority of cases, the three simultaneous IHBs have an overall greater stabilizing effect. The bifurcation affects the parameters of the IHBs (H11····O9/H11····O13 and H11····O10/H11····O13) because the bond length in the case of bifurcation is longer than when the same IHB (H11····O9 or H11····O13) is present alone in a conformer. The presence of the bifurcated IHBs also causes a slight increase in the length of the H14····O10 and H14····O9 IHBs in comparison to the cases where one of these IHBs is present in a conformer when there are no bifurcated IHBs.

It is also interesting to note that R′ has some influence on the type of IHB formed. Comparisons of molecules with different R′ shows that R′ = pyrrolidine allows the possibility of conformers with only one IHB, namely H11····O9 (while the N14–H14 bond does not form any IHB in those conformers). The nature of R has also some influence on the IHBs; for instance, it was found that R = cyclopropyl (group C) prevents the formation of non-bifurcated IHBs; this is typical of cyclopropyl and not of the other cyclic R considered. It has to be recalled also that the number of IHBs depends on the geometry of the thiourea group; therefore, this geometry has influence on the relative energies of the individual conformers across the compounds. The length of the chain between O7 and N18 also has some effect on conformational preferences. It was observed that the energy difference between the lowest energy conformer without any IHB and the highest energy conformer with at least one IHB is greatest in JP compounds (J means R′ = morpholine and P means that there are three carbon atoms in the chain between O7 and N18).

The IR vibrational frequencies (harmonic approximations) are analyzed for the N11–H11 and N14–H14 bonds because they can form IHBs and the formation of the IHBs may affect the vibrational frequencies of the donor.

Red shifts (decrease of the vibrational frequency of the donor) are observed for N14–H14 when it forms H14····O9 or H14····O10, and the red shifts is greater for IHBs with shorter bond length (stronger IHBs). The most interesting thing – because it does not occur often – is the presence of blue shifts in the vibrational frequencies of the N11–H11 bond when it forms IHBs. In the DFT results, this blue shift is greater when N11–H11 forms a single IHB (H11····O9 or H11····013) than when it forms the bifurcated ones. The blue shifts are greater when the bond lengths of the IHBs formed by N11–H11 are longer (when the IHBs are weaker). This observation will require further investigation in future, through the consideration of additional sulfonylurea molecules. It is interesting to note that the situation discussed for these molecules is similar to the case where the amino N–H bond forms an IHB with a possibility of bifurcation. This also suggests the importance of further investigation of the blue shifts in sulfonylureas.

The study considered also the energy corrected for ZPE and the Gibbs free energy. The trends of these energies, and of the uncorrected ones, are very similar for some of the compounds considered. Where there are some reversals in the relative energy sequences for some conformers, their differences are often marginal. The values of the ZPE corrected energy are often smaller than those of the uncorrected energy. The values of the Gibbs free energies can be higher or lower than the values of the other quantities.

Besides the number and types of IHBs, other factors have some influence on the relative energies of the conformers. The influence by the nature of R and R′ mainly concerns the IHBs that can be formed, as already discussed. Conformers may also differ by the orientation of the R groups (except when R=methyl); however, these different orientations of R do not have much influence on the energy of the conformers (different orientation has been denoted with different lower-case letters combined with numbers in the naming of the conformers to facilitate comparisons). The relative energy of the individual conformers is also influenced by the orientation of the chain between O7 and N18. It was found that the more stable orientations are parallel to the plane of the benzene ring (denoted by q/r) or perpendicular to the plane of the benzene ring (denoted by s/t). The influence of this orientation is however limited.

The dipole moments are influenced by the nature of R′ and also by the IHBs present. For all the conformers, the dipole moments are lower in the J compounds (R′=morpholine) than in the G (R′=pyrrolidine) and L (R′=diethylamine) compounds. The IHBs do not have a significant influence on the dipole moments of the conformers with two or three IHBs (k and m/p conformers respectively). The m/p and k conformers have very close dipole moments, while the dipole moment is lowest in the conformers with one IHB (g conformers in G compounds) and highest in the conformers without any IHB (j conformers).

The HOMO–LUMO energy gaps show some dependence on the nature of R′. Considering the ranges of all the energy gaps of all the compounds considered, it can be established that R′ determines whether the range of the energy gaps is broad or narrow. The ranges of the HOMO–LUMO energy gaps of the P and Q compounds (compounds with three or two carbon atoms in the chain between O7 and N18, respectively) are not much different when R′=pyrrolidine (G compounds) and R′=diethylamine (L compounds), with some exceptions; the range width is slightly greater when R′=morpholine (J compounds). The distribution of the electron density for the HOMO and the LUMO depends on the conformer types and not significantly on the nature of R and R′. Similar distributions were observed in corresponding conformers across compounds, regardless of their R and R′. The electron density distribution is more on the benzene ring for most conformers; the HOMO shows some distribution on O7 and N18, while for some conformers, the HOMO is distributed only on the R′ group.

The DFT and the HF results show a large number of similarities. There are some differences in the optimization results: in some cases, different inputs optimized to the same conformer with DFT and to different conformers with HF. This also means that the HF method gave more individual conformers than the DFT method for most of the compounds considered. The relative energies of the q/r conformers are very similar with both DFT and HF, while the s/t conformers have higher relative energies in the HF results than in the DFT results. While the HOMO–LUMO energy–gap values are very different with DFT and HF, the width of the gap ranges for each compound do not differ much and are very close for the P and Q compounds.

DFT and HF differ also concerning the effects of the formation of the IHBs on the vibrational frequencies of the donor (N–H). When both N11–H11 and N14–H14 form IHBs, their simultaneous presence may influence the changes in their vibrational frequencies (the presence of each of the IHBs influences the vibrational frequency change of the donor of the other IHB). When N11–H11 forms bifurcated IHBs and N14–H14 also forms an IHB, the vibrational frequency of N11–H11 shows a blue shift with both DFT and HF, and the vibrational frequency of N14–H14 shows a red shift with DFT and may have either a red shift or a blue shift with HF, depending on the conformers. When N11–H11 forms H11····O13 IHB and N14–H14 forms H14····O10 IHB, the vibrational frequency of the N11–H11 bond shows a small blue shift with DFT and a small red shift with HF, and the vibrational frequency of N14–H14 show the greatest red shifts observed for these compounds with DFT and either a red shift or a blue shift with HF. When N11–H11 forms H11····O9 and N14–H14 does not form any IHB, the vibrational frequency of N11–H11 has comparatively great blue shifts with both DFT and HF.

5.2. Way forward

The study presented here is the first type of study that is performed on molecules, i.e., the conformational study in *vacuo*. The results are interesting, and so they suggest that it is very important to find additional information that is considered relevant to the study of biologically active molecules. Additional studies of these molecules in *vacuo* will involve the use of MP2, because MP2 takes into account both correlation energy and dispersion contributions. It may also be interesting to try DFT calculations with another functional that can be considered suitable for these molecules and has different properties than B3LYP. Also details that have not been taken into account in the present study will be added, for example, the different geometries of the R′ moiety when it can take significantly different geometries, like in the case of R ′= morpholine, which may exhibit both the chair and the boat conformations.

Since these molecules are biologically active, it is important to study them in solution because the biological activity is exerted in solution; therefore, it is important to investigate how different solvents with different polarities affect the molecular properties. Solvents with different polarities will be considered because molecules in the organisms can be present in media with different polarities. The solvents will include water because water is the main component of the body.

The study will also expand to include other molecules, namely, molecules that are already in use in the treatment of diabetes, to enable comparisons of the molecular properties of the new sulfonylureas considered here and those that are being used. This will also be useful to search for pattern and similarities that will be suitable to understand the activities of these molecules, also in view of the fact that the activities of the compounds that are already in use are known. After enough information is collected, it will be possible to do Quantitative Structure–Activity Relationship (QSAR) analysis, trying to identify the new compounds that can be more active.

In addition, there will be studies investigating the interaction between all the molecules considered and proteins that are considered suitable targets in the treatment of diabetes.

Chapter 6

Tables and figures

This chapter presents the tables and figures showing the results for all the calculated conformers of each of the compounds considered. The compounds and their conformers are denoted with acronyms using the symbols shown in tables 4.2 and 4.4.

6.1. Tables

This section presents the tables reporting the values of the relevant quantities from the results obtained. The table for each set of related property are grouped in individual sections. For each property, individual tables are devoted to individual compounds. Each table reports the results from the DFT/B3LYP/6-31+G(d,p) and HF/6-31G(d,p) calculations in *vacuo*, respectively denoted as DFT and HF in the columns' headings (in the cases where different inputs optimized to the same geometry with the DFT results, the DFT energy values are repeated). All the calculations for conformational studies were done with totally relaxed geometry (full optimization). The conformers are listed in order of increasing DFT relative energies in all the tables.

6.1.1. Relative energies, HOMO–LUMO energy gaps and dipole moments of the conformers of each of the compounds considered.

This section presents the tables reporting the relative energies, HOMO–LUMO energy differences and dipole moments of the conformers of the compounds considered. Considering these quantities together helps investigate possible relationships between the relative energies and the other quantities. For instance, if two conformers have the same relative energies, dipole moments can be used to confirm whether the concerned conformers have the same or different geometry.

Table 6.1. Relative energies, HOMO-LUMO energy gaps and dipole moments of the calculated conformers of compound AGP

The absolute energy of the lowest energy conformer (AGP-m-r-u1) is -1604.8614678/DFT and -1596.6844934/HF.

Conformers	Relative energy (kcal/mol)		HOMO-LUMO energy difference (kcal/mol)		Dipole moment (Debye)	
	DFT	HF	DFT	HF	DFT	HF
AGP-m-r-u1	0.000	0.000	112.870	278.959	6.2095	6.0556
AGP-m-s-u1	0.000	2.428	112.864	283.584	6.2094	5.7648
AGP-p-t-u3	0.003	2.450	112.851	283.647	6.1758	5.8802
AGP-m-q-u1	0.036	0.031	113.115	279.160	7.1485	7.0273
AGP-p-r-u3	0.037	0.030	113.134	279.179	7.1539	6.9837
AGP-k-q-u1	1.154	1.440	112.381	280.001	5.9887	5.9565
AGP-k-r-u1	1.379	1.679	111.552	278.407	6.8125	6.7316
AGP-m-r-u2	1.763	1.806	112.669	278.890	6.3459	6.1787
AGP-g-r-u3	4.532	2.880	118.392	280.358	5.3973	5.3625
AGP-g-q-u3	4.664	3.119	118.380	280.283	6.5944	6.9499
AGP-j-q-u3	10.245	9.554	115.838	282.172	9.7881	10.0639
AGP-j-r-u3	10.351	9.659	115.305	281.162	9.3860	9.6275
AGP-j-s-u3	10.351	11.782	115.311	285.542	9.3863	7.9106

Table 6.2. Relative energies, HOMO-LUMO energy gaps and dipole moments of the calculated conformers of compound AGQ

The absolute energy of the lowest energy conformer (AGQ-m-r-u1) is -1565.5437451/DFT and -1557.6472956/HF.

Conformers	Relative energy (kcal/mol)		HOMO-LUMO energy difference (kcal/mol)		Dipole moment (Debye)	
	DFT	HF	DFT	HF	DFT	HF
AGQ-m-r-u1	0.000	0.000	116.336	278.903	6.3812	6.3442
AGQ-m-q-u1	0.015	0.004	116.738	279.135	7.1274	6.9493
AGQ-k-q-u1	1.156	1.441	115.972	279.919	6.1490	6.1884
AGQ-k-r-u1	1.366	1.660	115.207	278.382	6.7902	6.7155
AGQ-m-r-u2	1.761	1.799	116.161	278.846	6.5371	6.4193
AGQ-m-q-u2	1.774	1.811	116.449	278.991	7.0916	6.9330
AGQ-g-r-u3	4.496	2.917	121.232	280.346	5.5234	5.5540
AGQ-g-t-u3	4.496	5.438	121.238	284.563	5.5198	6.7032
AGQ-g-q-u3	4.662	3.114	121.307	280.246	6.5046	6.7883
AGQ-j-q-u3	10.248	9.564	119.330	282.090	9.8865	10.1960
AGQ-j-r-u3	10.279	9.635	118.803	281.130	9.4825	9.7609
AGQ-j-t-u3	10.279	12.269	118.803	286.263	9.4823	10.2168

Table 6.3. Relative energies, HOMO-LUMO energy gaps and dipole moments of the calculated conformers of compound AJP

The absolute energy of the lowest energy conformer (AJP-m-r-u1) is -1680.0729544/DFT and -1671.5328934/HF.

Conformers	Relative energy (kcal/mol)		HOMO-LUMO energy difference (kcal/mol)		Dipole moment (Debye)	
	DFT	HF	DFT	HF	DFT	HF
AJP-m-r-u1	0.000	0.000	111.414	279.223	4.4163	4.3183
AJP-m-s-u1	0.000	2.406	111.414	280.503	4.4168	4.0242
AJP-m-q-u1	0.092	0.034	111.653	279.430	5.8197	5.6497
AJP-k-q-u1	1.171	1.458	110.962	280.277	4.3272	4.2957
AJP-k-r-u1	1.392	1.703	110.065	278.658	5.3509	5.2782
AJP-k-s-u1	1.392	4.025	110.065	279.016	5.3519	4.2145
AJP-m-r-u2	1.770	1.810	111.207	279.154	4.5815	4.4517
AJP-m-s-u2	1.770	4.220	111.207	280.170	4.5805	4.0082
AJP-m-q-u2	1.842	1.834	111.452	279.323	5.7133	5.5146
AJP-j-q-u3	17.994	17.097	109.488	282.448	7.8330	8.1305
AJP-j-r-u3	18.137	17.257	108.973	281.400	8.1497	8.4151
AJP-j-s-u3	18.137	19.349	108.973	277.779	8.1508	7.7998

Table 6.4. Relative energies, HOMO-LUMO energy gaps and dipole moments of the calculated conformers of compound AJQ

The absolute energy of the lowest energy conformer is -1640.7423255/DFT (AJQ-p-q-u5) and -1632.4828216/HF (AJQ-p-q-u3).

Conformers	Relative energy (kcal/mol)		HOMO-LUMO energy difference (kcal/mol)		Dipole moment (Debye)	
	DFT	HF	DFT	HF	DFT	HF
AJQ-p-q-u5	0.000	0.464	108.873	279.304	3.8264	3.7717
AJQ-m-q-u1	0.052	0.045	109.212	279.555	5.0595	4.9281
AJQ-m-q-u2	0.465	0.456	115.010	279.233	6.0186	6.0565
AJQ-m-r-u2	0.470	0.455	114.784	279.097	6.2182	6.1856
AJQ-p-q-u3	0.583	0.000	104.399	279.354	4.9145	3.6625
AJQ-m-r-u1	0.583	0.689	108.151	279.398	4.9202	4.7034
AJQ-p-q-u5	0.583	1.156	108.176	279.336	4.9096	4.8046
AJQ-m-s-u1	0.583	3.109	108.139	276.267	4.9211	4.0775
AJQ-p-r-u3	0.615	0.707	108.578	279.599	5.1049	4.9481
AJQ-p-s-u3	0.615	3.115	108.572	276.066	5.1034	4.1154
AJQ-m-q-u1	0.617	0.713	108.528	279.580	5.0958	4.9294
AJQ-k-q-u1	1.175	1.466	108.496	280.396	3.7197	3.6429
AJQ-k-q-u1′	1.770	2.162	107.781	280.421	4.6112	4.4892
AJQ-k-r-u1	1.974	2.390	107.034	278.827	4.7512	4.6444
AJQ-j-q-u1	8.670	8.027	117.940	282.348	8.7689	9.0824
AJQ-j-r-u1	8.838	8.271	117.526	281.312	9.5732	9.9673

Table 6.5. Relative energies, HOMO-LUMO energy gaps and dipole moments of the calculated conformers of compound ALP

The absolute energy of the lowest energy conformer (ALP-m-r-u1) is -1606.0689394/DFT and -1597.8459495/HF.

Conformers	Relative energy (kcal/mol)		HOMO-LUMO energy difference (kcal/mol)		Dipole moment (Debye)	
	DFT	HF	DFT	HF	DFT	HF
ALP-m-r-u1	0.000	0.000	107.354	279.047	5.8707	5.6320
ALP-m-s-u1	0.000	2.431	107.348	276.939	5.8711	5.0445
ALP-m-q-u1	0.029	0.017	107.662	279.260	6.3711	6.1044
ALP-k-q-u1	1.156	1.443	106.915	280.107	5.6355	5.4879
ALP-k-r-u1	1.367	1.681	106.068	278.501	6.0059	5.8268
ALP-k-q-u1′	1.448	1.788	109.030	279.995	5.8060	5.7733
ALP-k-r-u1′	1.667	2.029	108.176	278.394	6.6809	6.6236
ALP-k-s-u1	1.667	4.384	108.176	278.087	6.6806	5.4478
ALP-k-r-u3	1.679	2.123	108.277	278.112	6.6274	6.5627
ALP-m-r-u2	1.768	1.806	107.153	278.978	5.9602	5.6921
ALP-m-s-u2	1.768	4.242	107.147	276.593	5.9598	5.0486
ALP-m-q-u2	1.780	1.816	107.430	279.154	6.3619	6.0676
ALP-j-q-u3	10.540	9.899	112.456	282.166	9.6009	9.8593
ALP-j-r-u3	10.647	10.012	111.973	281.162	9.3083	9.5564
ALP-j-s-u3	10.647	12.129	111.973	281.651	9.3083	7.6413

Table 6.6. Relative energies, HOMO-LUMO energy gaps and dipole moments of the calculated conformers of compound ALQ

The absolute energy of the lowest energy conformer (ALQ-m-r-u1) is -1566.7512114/DFT and -1558.8085966/HF.

Conformers	Relative energy (kcal/mol)		HOMO-LUMO energy difference (kcal/mol)		Dipole moment (Debye)	
	DFT	HF	DFT	HF	DFT	HF
ALQ-m-r-u1	0.000	0.000	113.385	278.934	6.3329	6.2829
ALQ-m-q-u1	0.011	0.001	113.792	279.172	6.9790	6.8002
ALQ-k-q-u1	1.159	1.444	113.021	279.957	6.1064	6.1219
ALQ-k-r-u1	1.365	1.661	112.243	278.426	6.6381	6.5639
ALQ-m-r-u2	1.764	1.801	113.196	278.878	6.4747	6.3495
ALQ-m-q-u2	1.775	1.807	113.510	279.028	6.9510	6.7866
ALQ-j-q-u3	10.255	9.564	116.372	282.122	9.7569	10.0688
ALQ-j-r-u3	10.341	9.643	115.826	281.162	9.4618	9.1294
ALQ-j-q-u3	11.692	10.764	108.779	281.996	9.6311	9.8698
ALQ-j-r-u3	11.778	10.907	108.421	281.024	9.6957	10.0134

Table 6.7. Relative energies, HOMO-LUMO energy gaps and dipole moments of the calculated conformers of compound BGP

The absolute energy of the lowest energy conformer is -1565.517238/DFT (BGP-p-s-v3) and -1557.6175979/HF (BGP-m-r-v1).

Conformers	Relative energy (kcal/mol)		HOMO-LUMO energy difference (kcal/mol)		Dipole moment (Debye)	
	DFT	HF	DFT	HF	DFT	HF
BGP-p-s-v3	0.000	2.428	112.481	283.283	6.2528	5.4640
BGP-p-t-v3	0.000	2.454	112.475	283.371	6.2533	5.8287
BGP-m-r-v1	0.001	0.000	112.506	278.928	6.3073	6.1008
BGP-m-s-v1	0.001	2.440	112.506	283.364	6.3074	5.7975
BGP-m-q-v1	0.031	0.031	112.682	279.053	7.1291	6.9927
BGP-k-q-v3	1.079	1.366	112.061	279.875	6.2109	6.1013
BGP-k-r-v3	1.300	1.607	111.239	278.250	6.9474	6.8235
BGP-k-s-v3	1.300	3.962	111.239	281.808	6.9481	5.7070
BGP-m-r-v2	1.548	1.395	112.337	278.827	6.3999	6.2056
BGP-m-s-v2	1.548	3.834	112.337	283.057	6.3993	5.7919
BGP-m-q-v2	1.569	1.416	112.487	278.997	7.0962	6.9574
BGP-g-r-v1	4.572	2.940	118.085	280.321	5.2828	5.3039
BGP-g-q-v1	4.712	3.183	118.097	280.220	6.5638	6.9663
BGP-j-q-v5	10.319	10.412	115.524	282.134	9.9492	10.1800
BGP-j-r-v5	10.423	10.511	115.016	281.130	9.5209	9.6946
BGP-j-s-v5	10.423	12.642	115.016	285.385	9.5200	8.0190

Table 6.8. Relative energies, HOMO-LUMO energy gaps and dipole moments of the calculated conformers of compound BGQ

The absolute energy of the lowest energy conformer (BGQ-m-r-v1) is -1526.1995171/DFT and.-1518.5804025/HF.

Conformers	Relative energy (kcal/mol)		HOMO-LUMO energy difference (kcal/mol)		Dipole moment (Debye)	
	DFT	HF	DFT	HF	DFT	HF
BGQ-m-r-v1	0.000	0.000	115.989	278.865	6.4424	6.3568
BGQ-m-q-v1	0.016	0.008	116.321	279.041	7.1450	6.9432
BGQ-k-q-v1	1.083	1.368	115.694	279.781	6.3620	6.3242
BGQ-k-r-v1	1.289	1.590	114.891	278.255	6.9358	6.8197
BGQ-m-r-v2	1.546	1.389	115.882	278.777	6.5702	6.4453
BGQ-m-q-v2	1.558	1.400	116.064	278.928	7.0798	6.9420
BGQ-j-q-v3	10.327	9.649	119.057	282.046	10.0437	10.3030
BGQ-j-r-v3	10.353	9.719	118.530	281.086	9.6234	9.8651
BGQ-j-t-v3	10.353	12.362	118.530	286.207	9.6228	10.2961

Table 6.9. Relative energies, HOMO-LUMO energy gaps and dipole moments of the calculated conformers of compound BJP

The absolute energy of the lowest energy conformer (BJP-p-q-v3) is -1640.7287187/DFT and -1632.4659954/HF.

Conformers	Relative energy (kcal/mol)		HOMO-LUMO energy difference (kcal/mol)		Dipole moment (Debye)	
	DFT	HF	DFT	HF	DFT	HF
BJP-p-q-v3	0.000	0.000	111.057	279.191	4.5102	4.3543
BJP-p-s-v3	0.000	2.418	111.057	280.289	4.5103	4.0658
BJP-p-r-v3	0.087	0.034	111.232	279.336	5.7824	5.6077
BJP-k-q-v1	1.095	1.384	110.649	280.139	4.5610	4.4538
BJP-k-r-v1	1.312	1.631	109.776	278.488	5.4554	5.3389
BJP-k-s-v1	1.312	3.959	109.783	278.815	5.4554	4.3269
BJP-m-r-v2	1.548	1.399	110.887	279.091	4.6160	4.4735
BJP-m-s-v2	1.548	3.817	110.887	280.001	4.6160	4.0516
BJP-m-q-v2	1.621	1.422	111.038	279.260	5.6943	5.5240
BJP-j-r-v3	18.067	17.182	109.199	282.404	7.9502	8.2140
BJP-j-s-v3	18.210	17.341	108.685	281.356	8.2516	8.4950
BJP-j-q-v3	18.210	19.437	108.678	277.597	8.2513	7.8660

Table 6.10. Relative energies, HOMO-LUMO energy gaps and dipole moments of the calculated conformers of compound BJQ

The absolute energy of the lowest energy conformer (BJQ-p-r-v3) is -1601.4005076/DFT and -1593.4182525/HF.

Conformers	Relative energy (kcal/mol)		HOMO-LUMO energy difference (kcal/mol)		Dipole moment (Debye)	
	DFT	HF	DFT	HF	DFT	HF
BJQ-p-r-v3	0.000	0.000	114.972	279.242	5.9974	5.9499
BJQ-m-s-v1	1.518	3.877	108.534	277.033	3.8621	3.3352
BJQ-m-t-v1	1.518	3.897	108.540	276.995	3.8620	3.5966
BJQ-m-q-v2	1.540	1.380	114.878	279.223	6.0914	5.9757
BJQ-m-r-v2	1.552	1.400	114.545	279.003	6.2479	6.1893
BJQ-m-q-v1	1.570	1.508	108.791	279.461	5.0277	4.8881
BJQ-p-q-v3	2.101	1.463	107.806	279.329	4.9283	3.6951
BJQ-p-q-v3′	2.101	2.154	107.800	279.361	4.9244	4.6979
BJQ-p-r-v3	2.133	2.171	108.101	279.505	5.0970	4.9278
BJQ-p-s-v3	2.133	4.589	108.107	275.878	5.0986	4.0987
BJQ-j-q-v3	10.261	9.572	117.664	282.304	8.9230	9.1869
BJQ-j-q-v3	10.427	9.816	117.263	281.268	9.7088	10.0634

Table 6.11. Relative energies, HOMO-LUMO energy gaps and dipole moments of the calculated conformers of compound BLP

The absolute energy of the lowest energy conformer is -1566.7244485/DFT (BLP-k-q-v1) and -1558.7785037/HF (BLP-m-r-v1).

Conformers	Relative energy (kcal/mol)		HOMO-LUMO energy difference (kcal/mol)		Dipole moment (Debye)	
	DFT	HF	DFT	HF	DFT	HF
BLP-k-q-v1	0.000	0.132	110.743	279.850	6.0954	6.0017
BLP-p-s-v3	0.131	2.438	109.130	279.518	6.0490	5.3142
BLP-p-t-v3	0.131	2.463	109.136	279.480	6.0489	5.6394
BLP-m-r-v1	0.133	0.000	109.174	278.928	6.0907	5.8932
BLP-m-s-v1	0.133	2.448	109.180	279.480	6.0909	5.6049
BLP-m-r-v1′	0.168	0.034	109.306	279.066	7.0266	6.8995
BLP-k-r-v1	0.219	0.377	109.902	278.225	6.8532	6.7793
BLP-k-s-v1	0.219	2.755	109.902	279.624	6.8531	5.6731
BLP-p-q-v4	1.679	1.419	108.954	278.997	6.1678	6.8329
BLP-p-s-v4	1.679	3.834	108.954	279.210	6.1674	5.3573
BLP-p-t-v4	1.679	3.860	108.954	279.141	6.1676	5.6614
BLP-p-r-v4	1.708	1.419	109.130	278.997	7.0048	6.8329
BLP-j-q-v5	9.243	9.177	114.213	282.109	9.7683	9.9915
BLP-j-r-v5	9.351	9.289	113.698	281.118	9.5052	9.7163
BLP-j-s-v5	9.351	11.425	113.698	283.207	9.5050	7.7789

Table 6.12. Relative energies, HOMO-LUMO energy gaps and dipole moments of the calculated conformers of compound BLQ

The absolute energy of the lowest energy conformer (BLQ-p-q-v3) is -1527.4069852/DFT and -1519.7417033/HF.

Conformers	Relative energy (kcal/mol)		HOMO-LUMO energy difference (kcal/mol)		Dipole moment (Debye)	
	DFT	HF	DFT	HF	DFT	HF
BLQ-p-q-v3	0.000	0.000	113.039	278.903	6.3974	6.2938
BLQ-p-r-v3	0.015	0.005	113.378	279.078	6.9990	6.7943
BLQ-p-r-v3	0.017	0.011	113.347	279.047	6.9595	6.8021
BLQ-k-q-v1	1.081	1.358	112.745	279.831	6.4103	6.3351
BLQ-k-r-v1	1.290	1.597	111.966	278.256	6.7045	6.5986
BLQ-m-r-v1	1.465	1.225	105.597	278.758	6.5790	6.3465
BLQ-m-q-v1	1.479	1.236	105.854	278.896	7.1674	6.9648
BLQ-m-s-v1	1.479	3.833	105.848	272.301	7.1683	5.8227
BLQ-p-q-v4	1.551	1.394	112.883	278.796	6.4812	6.3717
BLQ-p-r-v4	1.560	1.392	113.234	279.003	6.9778	6.7886
BLQ-j-q-v3	8.913	8.085	117.714	282.053	9.9151	10.1763
BLQ-j-q-v5	8.913	8.859	117.721	282.053	9.9135	10.1750
BLQ-j-r-v3	8.947	8.174	117.225	281.093	9.6951	9.9317
BLQ-j-r-v5	8.947	8.945	117.225	281.099	9.6923	9.9063
BLQ-j-t-v3	8.947	10.835	117.225	284.864	9.6923	10.1682

BLQ-j-t-v5	8.947	11.605	117.225	284.870	9.6930	10.1536

Table 6.13. Relative energies, HOMO-LUMO energy gaps and dipole moments of the calculated conformers of compound CGP

The absolute energy of the lowest energy conformer (CGP-p-q-w5) is -1526.192343/DFT and -1518.5726605/HF.

Conformers	Relative energy (kcal/mol)		HOMO-LUMO energy difference (kcal/mol)		Dipole moment (Debye)	
	DFT	HF	DFT	HF	DFT	HF
CGP-p-q-w5	0.000	0.000	112.111	278.752	6.4382	6.2715
CGP-p-s-w5	0.000	2.415	112.104	282.963	6.4380	5.5858
CGP-p-r-w5	0.029	0.011	112.450	279.154	7.2370	7.0506
CGP-m-r-w1	0.233	0.668	112.236	278.846	6.3640	6.1579
CGP-m-s-w1	0.233	3.107	112.243	283.076	6.3633	5.8418
CGP-m-q-w1	0.270	0.693	112.387	279.047	7.1340	7.0181
CGP-m-r-w2	2.758	3.651	112.211	278.727	6.4096	6.2190
CGP-m-s-w2	2.758	6.101	112.205	282.837	6.4098	5.8395
CGP-m-q-w2	2.782	3.664	112.299	278.878	7.1168	6.9585
CGP-g-r-w5	4.417	3.004	117.576	280.528	5.3526	5.5723
CGP-g-q-w5	4.580	3.288	117.507	280.214	6.7464	7.3460
CGP-j-q-w5	9.899	9.312	115.236	282.059	9.9031	10.1733
CGP-j-r-w5	9.994	9.411	114.734	281.055	9.4799	9.6989
CGP-j-s-w5	9.994	11.552	114.734	285.096	9.4778	8.0340

Table 6.14. Relative energies, HOMO-LUMO energy gaps and dipole moments of the calculated conformers of compound CGQ

The absolute energy of the lowest energy conformer is -1486.8746263/DFT (CGQ-p-q-w5) and -1479.5354864/HF (CGQ-p-r-w5).

Conformers	Relative energy (kcal/mol)		HOMO-LUMO energy difference (kcal/mol)		Dipole moment (Debye)	
	DFT	HF	DFT	HF	DFT	HF
CGQ-p-q-w5	0.000	0.012	115.675	278.702	6.6208	6.5220
CGQ-m-q-w3	0.002	0.008	115.700	278.718	6.6642	6.5151
CGQ-p-r-w5	0.014	0.000	116.114	279.116	7.2367	7.0402
CGQ-m-r-w1	0.234	0.679	115.744	278.783	6.4906	6.3982
CGQ-m-q-w1	0.255	0.683	116.077	279.016	7.1576	6.9791
CGQ-j-q-w5	9.902	9.336	118.787	281.977	9.9946	10.2990
CGQ-j-r-w5	9.926	9.402	118.254	281.017	9.5676	9.8442
CGQ-j-t-w5	9.926	12.052	118.260	286.119	9.5669	10.2478

Table 6.15. Relative energies, HOMO-LUMO energy gaps and dipole moments of the calculated conformers of compound CJP

The absolute energy of the lowest energy conformer (CJP-p-q-w3) is -1601.4038186/DFT and -1593.4210477/HF.

Conformers	Relative energy (kcal/mol)		HOMO-LUMO energy difference (kcal/mol)		Dipole moment (Debye)	
	DFT	HF	DFT	HF	DFT	HF
CJP-p-q-w3	0.000	0.000	110.705	279.022	4.7017	4.5357
CJP-p-s-w3	0.000	2.405	110.705	279.957	4.7012	4.1254
CJP-p- r-w3	0.036	0.016	111.000	279.411	5.8300	5.6555
CJP-m-r-w1	0.229	0.664	110.812	279.110	4.5690	4.4093
CJP-m-r-w2	2.754	3.649	110.755	278.991	4.6203	4.4791
CJP-m-s-w2	2.754	6.078	110.755	279.800	4.6196	4.1094
CJP-m-t-w2	2.754	6.087	110.755	279.794	4.6196	4.0945
CJP-m-q-w2	2.830	3.663	110.843	279.147	5.7338	5.5368
CJP-j-q-w1	17.645	16.853	108.904	282.341	7.8621	8.1758
CJP-j-r-w1	17.786	17.007	108.390	281.300	8.1643	8.4467
CJP-j-s-w1	17.786	19.117	108.390	277.353	8.1671	7.8072

Table 6.16. Relative energies, HOMO-LUMO energy gaps and dipole moments of the calculated conformers of compound CJQ

The absolute energy of the lowest energy conformer (CJQ-m-q-w6) is -1562.0756132/DFT and -1554.3733544/HF.

Conformers	Relative energy (kcal/mol)		HOMO-LUMO energy difference (kcal/mol)		Dipole moment (Debye)	
	DFT	HF	DFT	HF	DFT	HF
CJQ-m-q-w6	0.000	0.000	114.834	279.361	6.1986	6.0656
CJQ-m-r-w6	0.006	0.032	114.382	278.947	6.3519	6.2980
CJQ-p-q-w5	1.529	1.496	108.214	279.160	4.0729	3.8585
CJQ-m-q-w1	1.811	2.201	108.559	279.455	5.0135	4.8992
CJQ-p-q-w5	2.117	1.499	107.486	279.204	5.0551	3.8462
CJQ-p-q-w5′	2.117	2.189	107.486	279.191	5.0538	4.8212
CJQ-p-s-w5	2.145	4.163	107.919	275.545	5.2175	4.1971
CJQ-m-r-w1	2.343	2.849	107.555	279.285	4.9229	4.7228
CJQ-m-s-w1	2.343	5.282	107.555	275.878	4.9242	4.0938
CJQ-m-q-w1′	2.378	2.869	107.837	279.461	5.1213	4.9545
CJQ-j-q-w5	9.841	9.272	117.432	282.235	8.8641	9.1706
CJQ-j-r-w5	10.002	9.512	116.987	281.206	9.6308	10.0419

Table 6.17. Relative energies, HOMO-LUMO energy gaps and dipole moments of the calculated conformers of compound CLP

The absolute energy of the lowest energy conformer (CLP-p-q-w5) is -1527.3993433/DFT and -1519.7335655/HF.

Conformers	Relative energy (kcal/mol)		HOMO-LUMO energy difference (kcal/mol)		Dipole moment (Debye)	
	DFT	HF	DFT	HF	DFT	HF
CLP-p-q-w5	0.000	0.000	108.779	278.758	6.2373	6.0700
CLP-p-s-w5	0.000	2.425	108.779	279.179	6.2374	5.4261
CLP-p-r-w5	0.033	0.015	109.080	279.154	7.1235	6.9532
CLP-p-r-w5′	0.033	0.016	109.080	279.185	7.1236	6.9555
CLP-m-r-w1	0.231	0.667	108.879	278.840	6.1511	5.9515
CLP-m-s-w1	0.231	3.116	108.892	279.191	6.1513	5.6514
CLP-m-q-w1	0.271	0.696	109.017	279.034	7.0316	6.9207
CLP-m-q-w2	2.757	3.652	108.867	279.727	6.1990	6.0219
CLP-m-s-w2	2.757	6.109	108.860	278.953	6.1990	5.6538
CLP-m-q-w2	2.789	3.666	108.936	278.871	7.0104	6.8566
CLP-j-q-w5	9.590	8.948	109.751	282.153	9.2238	9.3833
CLP-j-r-w5	9.716	9.097	109.249	281.130	9.2679	9.4951
CLP-j-s-w5	9.716	11.239	109.256	278.432	9.2712	8.2964
CLP-j-q-w6	10.774	10.395	112.023	282.159	9.9657	10.2186
CLP-j-r-w6	10.841	10.483	111.251	281.187	9.4207	9.7448
CLP-j-s-w6	10.841	12.611	111.264	281.463	9.4225	7.9328

Table 6.18. Relative energies, HOMO-LUMO energy gaps and dipole moments of the calculated conformers of compound CLQ

The absolute energy of the lowest energy conformer (CLQ-p-q-w5) is -1488.081854/DFT and -1480.6963878/HF.

Conformers	Relative energy (kcal/mol)		HOMO-LUMO energy difference (kcal/mol)		Dipole moment (Debye)	
	DFT	HF	DFT	HF	DFT	HF
CLQ-p-q-w5	0.000	0.000	109.525	278.921	5.6566	5.4503
CLQ-p-s-w5	0.000	2.471	109.519	278.093	5.6566	4.9731
CLQ-m-q-w1	0.033	0.014	109.864	279.304	6.5641	6.3706
CLQ-m-r-w1′	0.237	0.666	109.626	279.003	5.5315	5.3276
CLQ-m-r-w1	0.237	0.667	109.626	279.009	5.5315	5.3199
CLQ-m-s-w1	0.237	3.149	109.626	278.219	5.5314	4.9051
CLQ-m-q-w1′	0.275	0.694	109.864	279.204	6.5095	6.3231
CLQ-j-q-w5	9.893	9.297	112.619	282.210	9.0272	9.2227
CLQ-j-r-w5	9.967	9.442	112.092	281.224	9.0685	9.3851
CLQ-j-s-w6	9.967	11.601	112.098	280.057	9.0720	7.4177

Table 6.19. Relative energies, HOMO-LUMO energy gaps and dipole moments of the calculated conformers of compound DGP

The absolute energy of the lowest energy conformer is -1448.8035537/DFT (DGP-m-r) and -1441.7002616/HF (DGP-p-q).

Conformers	Relative energy (kcal/mol)		HOMO-LUMO energy difference (kcal/mol)		Dipole moment (Debye)	
	DFT	HF	DFT	HF	DFT	HF
DGP-m-r	0.000	0.001	112.312	278.878	6.4326	6.1914
DGP-m-s	0.000	2.445	112.312	283.151	6.4319	5.8713
DGP-p-q	0.002	0.000	112.286	278.878	6.3649	6.1666
DGP-p-s	0.002	2.434	112.286	283.088	6.3649	5.5591
DGP-p-t	0.002	2.460	112.286	283.220	6.3647	5.8325
DGP-m-q	0.044	0.029	112.475	279.047	7.1882	7.0240
DGP-k-q	1.090	1.346	112.035	279.882	6.3231	6.1995
DGP-k-r	1.310	1.587	111.207	278.256	7.0475	6.9188
DGP-k-s	1.310	3.945	111.201	281.689	7.0472	5.8271
DGP-g-r	4.630	3.002	117.765	280.289	5.2093	5.1915
DGP-g-q	4.775	3.250	117.740	280.195	6.5873	6.9199
DGP-j-q	10.365	9.675	115.299	282.078	10.0722	10.2986
DGP-j-r	10.425	9.780	114.809	281.080	9.6699	9.8655
DGP-j-s	10.425	11.915	114.815	285.109	9.6673	8.1770

Table 6.20. Relative energies, HOMO-LUMO energy gaps and dipole moments of the calculated conformers of compound DGQ

The absolute energy of the lowest energy conformer (DGQ-m-r) is -1409.4858356/DFT and -1402.6630721/HF.

Conformers	Relative energy (kcal/mol)		HOMO-LUMO energy difference (kcal/mol)		Dipole moment (Debye)	
	DFT	HF	DFT	HF	DFT	HF
DGQ-m-r	0.000	0.000	115.832	278.834	6.6176	6.4448
DGQ-p-q	0.003	0.003	115.801	278.821	6.5488	6.4240
DGQ-m-q	0.027	0.009	116.114	279.022	7.2176	6.9951
DGQ-m-q′	0.031	0.016	116.070	278.978	7.1668	6.9931
DGQ-k-q	1.093	1.351	115.656	279.794	6.4646	6.4206
DGQ-k-r	1.299	1.573	114.872	278.244	7.0454	6.9168
DGQ-g-r	4.601	3.045	120.639	280.271	5.3279	5.4160
DGQ-g-t	4.601	5.580	120.632	284.011	5.3295	6.4632
DGQ-g-q	4.771	3.248	120.752	280.151	6.4706	6.7369
DGQ-j-q	10.374	9.690	118.863	281.996	10.1681	10.4330
DGQ-j-r	10.399	9.761	118.348	281.042	9.7598	10.0064
DGQ-j-t	10.399	12.411	118.348	286.138	9.7579	10.4038

Table 6.21. Relative energies, HOMO-LUMO energy gaps and dipole moments of the calculated conformers of compound DJP

The absolute energy of the lowest energy conformer is -1524.0150266/DFT (DJP-m-r) and -1516.5486541/HF (DJP-p-q).

Conformers	Relative energy (kcal/mol)		HOMO-LUMO energy difference (kcal/mol)		Dipole moment (Debye)	
	DFT	HF	DFT	HF	DFT	HF
DJP-m-r	0.000	0.003	110.831	279.141	4.6410	4.4624
DJP-p-s	0.000	2.424	110.843	280.076	4.6408	4.1473
DJP-p-q	0.041	0.000	111.025	279.147	5.8200	4.4456
DJP-m-q	0.041	0.031	111.025	279.311	5.8197	5.6271
DJP-p-r	0.041	0.032	111.025	279.311	5.8197	5.6279
DJP-k-q	1.108	1.363	110.592	280.145	4.6849	4.5655
DJP-k-r	1.320	1.609	109.745	278.514	5.5527	5.4269
DJP-k-r′	1.320	1.610	109.751	278.507	5.5527	5.4263
DJP-k-s	1.320	3.940	109.745	278.702	5.5519	4.4388
DJP-j-q	18.116	17.219	108.973	282.354	8.0528	8.3241
DJP-j-s	18.260	17.380	108.477	281.312	8.3574	8.5981
DJP-j-r	18.260	19.484	108.471	277.365	8.3605	7.9514

Table 6.22. Relative energies, HOMO-LUMO energy gaps and dipole moments of the calculated conformers of compound DJQ

The absolute energy of the lowest energy conformer (DJQ-m-q) is -1484.6868132/DFT and -1477.5009145/HF.

Conformers	Relative energy (kcal/mol)		HOMO-LUMO energy difference (kcal/mol)		Dipole moment (Debye)	
	DFT	HF	DFT	HF	DFT	HF
DJQ-m-q	0.000	0.000	114.552	279.085	6.4008	6.2425
DJQ-k-q	1.088	1.349	114.351	280.032	6.2918	6.2394
DJQ-k-r	1.291	1.584	113.592	278.457	5.9002	5.8825
DJQ-m-r	1.514	1.466	108.377	279.273	3.9733	3.7722
DJQ-m-s	1.514	3.886	108.383	276.844	3.9729	3.4082
DJQ-m-t	1.514	3.907	108.377	276.895	3.9727	3.5598
DJQ-m-s′	1.514	4.593	108.377	275.953	3.9731	4.1147
DJQ-m-q	1.576	1.508	108.609	279.442	5.0746	4.9100
DJQ-p-q	1.577	1.467	108.365	279.279	4.0262	3.7847
DJQ-m-r′	2.105	2.155	107.643	279.317	5.0239	4.7569
DJQ-p-q′	2.106	2.158	107.612	279.311	5.0335	4.7536
DJQ-p-r	2.139	2.172	107.900	279.486	5.1710	4.9724
DJQ-m-q	2.144	2.177	107.875	279.467	5.1708	4.9691
DJQ-j-q	2.666	2.129	122.163	282.323	8.7584	9.0396
DJQ-j-r	2.788	2.318	121.749	281.306	8.4357	8.8201

Table 6.23. Relative energies, HOMO-LUMO energy gaps and dipole moments of the calculated conformers of compound DLP

The absolute energy of the lowest energy conformer is -1450.0105569/DFT (DLP-m-r) and -1442.8611673/HF (DLP-p-q).

Conformers	Relative energy (kcal/mol)		HOMO-LUMO energy difference (kcal/mol)		Dipole moment (Debye)	
	DFT	HF	DFT	HF	DFT	HF
DLP-m-r	0.000	0.001	108.954	278.878	6.2205	5.9872
DLP-m-s	0.000	2.454	108.961	279.260	6.2201	5.6831
DLP-p-q	0.002	0.000	108.942	278.878	6.1650	5.9656
DLP-p-s	0.002	2.444	108.942	279.298	6.1648	5.4098
DLP-p-t	0.002	2.470	108.942	279.354	6.1652	5.6364
DLP-m-q	0.049	0.032	109.124	279.047	7.0876	6.9280
DLP-p-r	0.051	0.033	109.136	279.053	7.1232	6.9233
DLP-k-q	1.093	1.349	108.678	279.869	6.1499	6.0237
DLP-k-r	1.312	1.592	107.825	278.250	6.9135	6.8028
DLP-k-s	1.312	3.955	107.812	277.786	6.9124	5.7085
DLP-j-q	10.365	9.676	111.966	282.072	9.8573	10.0933
DLP-j-s	10.430	11.917	111.471	281.237	9.5719	7.9034
DLP-j-r	10.476	9.789	111.477	281.086	9.5728	9.7872

Table 6.24. Relative energies, HOMO-LUMO energy gaps and dipole moments of the calculated conformers of compound DLQ

The absolute energy of the lowest energy conformer (DLQ-p-q) is -1410.6955599/DFT and -1403.826859/HF.

Conformers	Relative energy (kcal/mol)		HOMO-LUMO energy difference (kcal/mol)		Dipole moment (Debye)	
	DFT	HF	DFT	HF	DFT	HF
DLQ-p-q	0.000	0.000	114.489	278.821	6.5523	6.4197
DLQ-k-q	1.090	1.348	114.338	279.806	6.4780	6.4212
DLQ-k-r	1.233	1.568	113.592	278.256	6.9493	6.8213
DLQ-m-r	1.419	1.563	112.826	278.852	6.5061	6.3602
DLQ-m-q	1.442	1.567	113.184	279.053	7.0718	6.8480
DLQ-m-r′	2.887	2.787	105.233	278.702	6.6874	6.4227
DLQ-m-q′	2.903	2.796	105.685	278.915	7.2407	7.0092
DLQ-j-q	10.374	9.686	117.526	281.996	10.0361	10.3085
DLQ-j-r	10.412	9.776	117.056	281.049	9.8189	10.0673
DLQ-j-t	10.412	12.444	117.062	294.634	9.8169	10.2785

Table 6.25. Relative energies, HOMO-LUMO energy gaps and dipole moments of the calculated conformers of compound EGP

The absolute energy of the lowest energy conformer (EGP-m-r-x4) is -1488.1239664/DFT and -1480.7412028/HF.

Conformers	Relative energy (kcal/mol)		HOMO-LUMO energy difference (kcal/mol)		Dipole moment (Debye)	
	DFT	HF	DFT	HF	DFT	HF
EGP-m-r-x4	0.000	0.000	112.494	278.896	6.2754	6.1077
EGP-m-s-x4	0.000	2.439	112.487	283.258	6.2746	5.7703
EGP-m-q-x4	0.036	0.024	112.707	279.085	7.0879	6.9664
EGP-m-r-x1	0.313	0.320	112.537	278.890	6.4241	6.1883
EGP-m-s-x1	0.313	2.754	112.531	283.383	6.4242	5.8931
EGP-p-q-x3	0.316	0.322	112.512	278.871	6.3675	6.1859
EGP-p-s-x3	0.316	2.741	112.519	283.283	6.3666	5.5593
EGP-m-q-x1	0.359	0.350	112.807	279.147	7.2621	7.1062
EGP-k-q-x1	1.159	1.716	112.217	279.988	6.1658	6.0164
EGP-k-r-x2	1.374	1.662	111.395	278.099	6.8686	6.8092
EGP-k-q-x1′	1.374	1.954	111.377	278.388	6.8668	6.7741
EGP-k-s-x1	1.374	4.311	111.383	281.846	6.8669	5.6640
EGP-g-r-x1	4.794	2.232	118.078	280.340	5.4058	5.3329
EGP-g-q-x1	4.948	3.480	118.060	280.258	6.7092	7.0159
EGP-j-q-x3	10.527	9.908	115.581	282.128	10.0076	10.2601
EGP-j-r-x3	10.628	10.012	115.060	281.124	9.5886	9.7996
EGP-j-s-x3	10.628	12.141	115.066	285.316	9.5883	8.1125

Table 6.26. Relative energies, HOMO-LUMO energy gaps and dipole moments of the calculated conformers of compound EGQ

The absolute energy of the lowest energy conformer (EGQ-m-r-x4) is -1448.8062434/DFT and -1441.7040137/HF.

Conformers	Relative energy (kcal/mol)		HOMO-LUMO energy difference (kcal/mol)		Dipole moment (Debye)	
	DFT	HF	DFT	HF	DFT	HF
EGQ-m-r-x4	0.000	0.000	115.995	278.852	6.4572	6.3629
EGQ-m-q-x4	0.021	0.013	116.271	279.022	7.0516	6.9328
EGQ-m-r-x1	0.312	0.325	116.033	278.840	6.5640	6.4488
EGQ-m-q-x1	0.339	0.327	116.459	279.116	7.2718	7.0531
EGQ-p-q-x3	0.358	0.378	115.913	278.796	6.6145	6.4777
EGQ-p-r-x3	0.375	0.379	116.284	279.066	7.2855	7.0336
EGQ-k-q-x4	1.152	1.361	115.744	279.838	6.4264	6.4090
EGQ-k-r-x4	1.358	1.581	114.972	278.294	7.0188	6.9001
EGQ-g-r-x1	4.764	3.276	120.927	280.327	5.5139	5.5456
EGQ-g-t-x1	4.764	5.806	120.927	284.356	5.5091	6.6557
EGQ-g-q-x1	4.939	3.479	121.003	280.214	6.6296	6.8402
EGQ-j-q-x3	10.531	9.923	119.076	282.046	10.1133	10.3893
EGQ-j-r-x3	10.556	9.993	118.562	281.086	9.6779	9.9404

EGQ-j-t-x3	10.556	12.636	118.562	286.213	9.6750	10.3791

Table 6.27. Relative energies, HOMO-LUMO energy gaps and dipole moments of the calculated conformers of compound EJP

The absolute energy of the lowest energy conformer (EJP-m-s-x4) is -1563.3354469/DFT and -1555.5895988/HF.

Conformers	Relative energy (kcal/mol)		HOMO-LUMO energy difference (kcal/mol)		Dipole moment (Debye)	
	DFT	HF	DFT	HF	DFT	HF
EJP-m-s-x4	0.000	0.000	111.038	279.166	4.4790	4.3679
EJP-m-r-x4	0.000	2.419	111.038	280.183	4.4781	4.0380
EJP-m-q-x4	0.083	0.028	111.239	279.348	5.7258	5.5667
EJP-p-s-x4	0.083	2.733	111.239	280.296	5.7256	4.1570
EJP-p-q-x4	0.315	0.321	111.094	279.160	4.6275	4.4439
EJP-p-r-x4	0.361	0.353	111.377	279.411	5.9186	5.7170
EJP-k-q-x1	1.177	1.733	110.780	280.258	4.5201	4.3801
EJP-k-r-x1	1.389	1.976	109.921	278.645	5.3747	5.3008
EJP-k-r-x1′	1.389	1.977	109.914	278.645	5.3749	5.2994
EJP-k-s-x1	1.389	4.306	109.914	278.852	5.3746	4.3056
EJP-j-q-x3	18.275	17.452	109.212	282.404	8.0117	8.2985
EJP-j-r-x3	18.423	17.611	108.722	281.356	8.3318	8.5756
EJP-j-s-x3	18.423	19.709	108.716	277.572	8.3296	7.9454

Table 6.28. Relative energies, HOMO-LUMO energy gaps and dipole moments of the calculated conformers of compound EJQ

The absolute energy of the lowest energy conformer (EJQ-m-q-x4) is -1224.0072361/DFT and -1516.5418831/HF.

Conformers	Relative energy (kcal/mol)		HOMO-LUMO energy difference (kcal/mol)		Dipole moment (Debye)	
	DFT	HF	DFT	HF	DFT	HF
EJQ-m-q-x4	0.000	0.000	115.048	279.304	6.0126	5.9215
EJQ-m-r-x4	0.003	0.019	114.677	279.311	6.1891	5.9219
EJQ-p-q-x4	1.833	1.801	108.578	279.292	4.0324	3.7890
EJQ-p-q-x4′	2.425	2.493	107.850	279.329	5.0586	4.8035
EJQ-m-r-x1	2.426	2.490	107.894	279.239	5.0773	4.8037
EJQ-m-s-x1	2.426	4.916	107.894	276.192	5.0760	4.1858
EJQ-p-r-x4	2.457	2.507	108.270	279.580	5.2444	5.0376
EJQ-p-s-x4	2.457	4.922	108.270	275.866	5.2480	4.2043
EJQ-m-q-x1	2.461	2.513	108.258	279.568	5.2544	5.0297
EJQ-k-q-x4	3.286	3.558	107.542	280.340	4.8574	4.6893
EJQ-k-r-x4	3.435	3.788	106.783	278.733	4.9889	4.8452
EJQ-j-q-x3	10.468	9.859	117.727	282.310	8.9685	9.2669
EJQ-j-r-x3	10.634	10.102	117.300	281.275	9.7683	10.1501

Table 6.29. Relative energies, HOMO-LUMO energy gaps and dipole moments of the calculated conformers of compound ELP

The absolute energy of the lowest energy conformer (ELP-m-s-x4) is -1489.3309682/DFT and -1481.9021084/HF.

Conformers	Relative energy (kcal/mol)		HOMO-LUMO energy difference (kcal/mol)		Dipole moment (Debye)	
	DFT	HF	DFT	HF	DFT	HF
ELP-m-s-x4	0.000	0.000	109.136	278.890	6.0605	5.9044
ELP-m-q-x4	0.000	2.448	109.143	279.367	6.0607	5.5782
ELP-m-q-x4	0.040	0.027	109.350	279.078	6.9808	6.8699
ELP-m-r-x1	0.314	0.320	109.180	278.890	6.2101	5.9802
ELP-m-s-x1	0.314	2.762	109.180	279.493	6.2097	5.6978
ELP-p-s-x4	0.315	0.321	109.180	278.890	6.1637	5.9741
ELP-p-s-x4′	0.315	2.751	109.174	279.536	6.1632	5.4065
ELP-m-q-x1	0.361	0.353	109.450	279.141	7.1687	7.0136
ELP-k-q-x1	1.160	1.719	108.873	279.982	5.9929	5.8393
ELP-k-r-x1	1.377	1.958	107.982	278.382	6.7317	6.6613
ELP-k-s-x1	1.377	4.321	107.982	277.943	6.7318	5.5519
ELP-j-q-x3	10.223	9.544	110.096	282.222	9.3328	9.4793
ELP-j-r-x3	10.355	9.698	109.582	281.199	9.3993	9.6064
ELP-j-s-x3	10.355	11.828	109.588	278.652	9.3993	8.4049
ELP-j-q-x3′	10.527	9.908	112.199	282.115	9.8160	10.0562
ELP-j-r-x3′	10.630	10.020	111.722	281.130	9.4973	9.7237
ELP-j-s-x3′	10.630	12.142	111.722	281.444	9.4949	7.8380

Table 6.30. Relative energies, HOMO-LUMO energy gaps and dipole moments of the calculated conformers of compound ELQ

The absolute energy of the lowest energy conformer (ELQ-m-r-x4) is -1450.0137157/DFT and -1442.8653131/HF.

Conformers	Relative energy (kcal/mol)		HOMO-LUMO energy difference (kcal/mol)		Dipole moment (Debye)	
	DFT	HF	DFT	HF	DFT	HF
ELQ-m-r-x4	0.000	0.000	113.065	278.884	6.3959	6.2967
ELQ-m-q-x4	0.021	0.007	113.341	279.060	6.9128	6.7826
ELQ-m-r-x1	0.322	0.324	113.065	278.878	6.5289	6.3880
ELQ-m-q-x1	0.343	0.323	113.535	279.154	7.1218	6.9042
ELQ-k-q-x4	1.147	1.349	112.788	279.875	6.4670	6.4121
ELQ-k-r-x4	1.359	1.589	112.010	278.325	6.7946	6.6889
ELQ-j-q-x3	10.488	9.860	116.083	282.109	9.6101	9.8082
ELQ-j-r-x3	10.622	10.068	115.656	281.099	10.0201	10.3603
ELQ-j-q-x3′	10.672	10.133	112.889	282.285	9.1213	9.3177
ELQ-j-r-x3′	10.755	10.281	112.437	281.275	9.2248	9.4981
ELQ-j-s-x3	10.755	12.428	112.437	280.239	9.2245	7.5112

Table 6.31. Relative energies, HOMO-LUMO energy gaps and dipole moments of the calculated conformers of compound FGP

The absolute energy of the lowest energy conformer (FGP-m-r-x4) is -1527.441576/DFT and -1519.7791999/HF.

Conformers	Relative energy (kcal/mol)		HOMO-LUMO energy difference (kcal/mol)		Dipole moment (Debye)	
	DFT	HF	DFT	HF	DFT	HF
FGP-m-r-x4	0.000	0.000	112.537	278.903	6.1577	6.0198
FGP-m-s-x4	0.000	2.437	112.537	283.320	6.1572	5.6820
FGP-m-q-x4	0.031	0.023	112.776	279.091	6.9880	6.8933
FGP-m-r-x1	0.334	0.426	112.494	278.903	6.5638	6.2161
FGP-m-s-x1	0.334	2.856	112.494	283.483	6.5636	5.9453
FGP-p-q-x4	0.337	0.427	112.475	278.909	6.5199	6.2082
FGP-p-s-x4	0.337	2.843	112.468	283.371	6.5200	5.5995
FGP-m-q-x1	0.372	0.458	112.788	279.166	7.3633	7.1690
FGP-p-r-x4	0.374	0.457	112.776	279.166	7.3754	7.1438
FGP-k-q-x1	1.163	1.837	112.243	280.013	6.0882	5.9353
FGP-k-r-x1	1.375	2.073	111.395	278.413	6.7550	6.6975
FGP-k-r-x1	1.375	2.075	111.395	278.419	6.7549	6.6794
FGP-g-r-x1	4.949	3.327	118.179	280.365	5.5461	5.4203
FGP-g-r-x1′	4.949	3.328	118.179	280.365	5.5460	5.4192
FGP-g-q-x1	5.099	3.575	118.135	280.277	6.8802	7.0978
FGP-j-q-x3	10.679	10.006	115.675	282.147	10.0423	10.2785
FGP-j-r-x3	10.776	10.109	115.167	281.143	9.5781	9.7997
FGP-j-s-x3	10.855	12.235	115.123	285.435	9.5095	8.1102

Table 6.32. Relative energies, HOMO-LUMO energy gaps and dipole moments of the calculated conformers of compound FGQ

The absolute energy of the lowest energy conformer (FGQ-m-r-x4) is -1488.1238524/DFT and -1480.7420108/HF.

Conformers	Relative energy (kcal/mol)		HOMO-LUMO energy difference (kcal/mol)		Dipole moment (Debye)	
	DFT	HF	DFT	HF	DFT	HF
FGQ-m-r-x4	0.000	0.000	116.070	278.865	6.3364	6.2743
FGQ-m-q-x4	0.013	0.011	116.334	279.028	6.9571	6.8562
FGQ-p-q-x4	0.336	0.364	116.001	278.281	6.7064	6.5429
FGQ-m-r-x1	0.336	0.432	116.001	278.852	6.7062	6.4860
FGQ-m-q-x1	0.350	0.434	116.409	279.141	7.3684	7.1118
FGQ-k-r-x4	1.362	1.580	115.035	278.300	7.0580	6.9282
FGQ-g-r-x1	4.917	3.371	121.028	280.346	5.6335	5.6311
FGQ-g-t-x1	4.917	5.898	121.034	284.418	5.6310	6.7648
FGQ-g-q-x1	5.094	3.574	121.122	280.239	6.7434	6.9241
FGQ-j-q-x3	10.684	10.021	119.164	282.072	10.1372	10.4047
FGQ-j-r-x3	10.704	10.091	118.637	281.105	9.6720	9.9410
FGQ-j-t-x3	10.783	12.730	118.618	286.238	9.6351	10.4033

Table 6.33. Relative energies, HOMO-LUMO energy gaps and dipole moments of the calculated conformers of compound FJP

The absolute energy of the lowest energy conformer (FJP-m-r-x4) is -1602.6530627/DFT and -1594.6275975/HF.

Conformers	Relative energy (kcal/mol)		HOMO-LUMO energy difference (kcal/mol)		Dipole moment (Debye)	
	DFT	HF	DFT	HF	DFT	HF
FJP-m-r-x4	0.000	0.000	111.100	279.179	4.3602	4.2807
FJP-m-s-x4	0.000	2.416	111.094	280.246	4.3584	3.9488
FJP-m-q-x4	0.081	0.026	111.314	279.361	5.6388	5.4980
FJP-p-q-x4	0.342	0.427	111.044	279.179	4.7764	4.4693
FJP-p-s-x4	0.342	2.835	111.050	280.409	4.7762	4.2076
FJP-k-q-x1	1.184	1.853	110.818	280.283	4.4441	4.3029
FJP-p-r-x1	1.394	0.461	109.946	279.423	5.2520	5.7888
FJP-k-r-x1	1.394	2.095	109.946	278.670	5.2513	5.2266
FJP-k-s-x1	1.394	4.424	109.940	278.947	5.2519	4.2580
FJP-j-q-x3	18.429	17.549	109.331	282.423	8.0422	8.3237
FJP-j-r-x3	18.573	17.708	108.816	281.381	8.3565	8.6026
FJP-j-s-x3	18.573	19.802	108.823	277.679	8.3566	7.9805

Table 6.34. Relative energies, HOMO-LUMO energy gaps and dipole moments of the calculated conformers of compound FJQ

The absolute energy of the lowest energy conformer (FJQ-m-q-x4) is -1563.3245053/DFT and -1555.579682/HF.

Conformers	Relative energy (kcal/mol)		HOMO-LUMO energy difference (kcal/mol)		Dipole moment (Debye)	
	DFT	HF	DFT	HF	DFT	HF
FJQ-m-q-x4	0.000	0.000	114.978	279.267	5.8391	5.9340
FJQ-m-r-x4	0.008	0.002	114.690	279.110	6.0847	6.0984
FJQ-p-r-x4	0.338	0.412	115.066	279.398	6.3011	6.1336
FJQ-p-q-x4	0.347	0.372	114.615	279.060	6.4047	6.3476
FJQ-p-q-x4′	0.347	0.438	114.615	279.097	6.4050	6.3542
FJQ-m-q-x1	0.349	0.435	114.953	279.329	6.2180	6.1646
FJQ-m-r-x1	0.350	0.432	114.684	279.122	6.4866	6.3594
FJQ-k-q-x4	1.175	1.383	114.395	280.082	6.0053	6.1088
FJQ-k-r-x4	1.378	1.585	113.661	278.551	6.0962	6.1045
FJQ-j-q-x3	10.406	9.831	117.834	282.329	8.9799	9.2697
FJQ-j-r-x3	10.570	10.075	117.382	281.287	9.7943	10.1693
FJQ-j-r-x3′	10.688	10.067	117.250	281.325	8.7688	9.1057
FJQ-j-t-x3	10.688	12.687	117.250	285.454	8.7672	9.1141
FJQ-j-q-x3′	10.717	10.062	117.765	282.304	9.9058	10.3731

Table 6.35. Relative energies, HOMO-LUMO energy gaps and dipole moments of the calculated conformers of compound FLP

The absolute energy of the lowest energy conformer (FLP-m-r-x4) is -1528.6485771/DFT and -1520.9401057/HF.

Conformers	Relative energy (kcal/mol)		HOMO-LUMO energy difference (kcal/mol)		Dipole moment (Debye)	
	DFT	HF	DFT	HF	DFT	HF
FLP-m-r-x4	0.000	0.000	109.193	278.903	5.9419	5.8158
FLP-m-q-x4	0.034	0.026	109.412	279.097	6.8814	6.7975
FLP-m-r-x1	0.334	0.426	109.143	278.903	6.3503	6.0055
FLP-m-s-x4	0.334	2.446	109.143	279.436	6.3508	5.4892
FLP-m-s-x1	0.334	2.865	109.149	279.605	6.3503	5.7484
FLP-p-q-x4	0.337	0.427	109.143	278.903	6.3142	5.9985
FLP-p-s-x4	0.337	2.853	109.136	279.649	6.3145	5.4458
FLP-m-q-x1	0.378	0.461	109.406	279.160	7.2493	7.0785
FLP-k-q-x1	1.165	1.839	108.898	280.001	5.9160	5.7587
FLP-k-r-x1	1.379	2.077	108.026	278.407	6.6205	6.5841
FLP-k-s-x1	1.379	4.439	108.032	278.005	6.6202	5.4829
FLP-j-q-x3	10.374	9.641	110.172	282.247	9.3586	9.4948
FLP-j-r-x3	10.503	9.795	109.676	281.218	9.4018	9.6175
FLP-j-s-x3′	10.503	11.922	109.682	278.758	9.4018	8.4192
FLP-j-q-x3′	10.676	10.006	112.305	282.147	9.8431	10.0755
FLP-j-r-x3′	10.779	10.117	111.822	281.149	9.4841	9.7242
FLP-j-s-x3	10.779	12.236	111.816	281.551	9.4843	7.8391

Table 6.36. Relative energies, HOMO-LUMO energy gaps and dipole moments of the calculated conformers of compound FLQ

The absolute energy of the lowest energy conformer is -1489.3313178/DFT (FLQ-p-q-x2) and -1481.9033104/HF (FLQ-m-r-x4).

Conformers	Relative energy (kcal/mol)		HOMO-LUMO energy difference (kcal/mol)		Dipole moment (Debye)	
	DFT	HF	DFT	HF	DFT	HF
FLQ-p-q-x2	0.000	0.007	13.096	278.821	6.2510	6.2299
FLQ-m-r-x4	0.001	0.000	113.134	278.903	6.2737	6.2101
FLQ-m-q-x4	0.009	0.005	113.403	279.072	6.8155	6.7052
FLQ-p-q-x4	0.339	0.429	113.083	278.903	6.6941	6.4292
FLQ-m-r-x1	0.339	0.431	113.046	278.896	6.6588	6.4273
FLQ-m-q-x1	0.347	0.430	113.485	179.179	7.2279	6.9617
FLQ-m-q-x1′	0.347	0.432	113.485	279.172	7.2279	6.9681
FLQ-p-r-x4	0.353	0.370	113.441	279.034	7.1957	6.9498
FLQ-p-r-x4′	0.353	0.439	113.447	279.154	7.1955	6.9699
FLQ-k-q-x4	1.147	1.347	112.839	279.888	6.4851	6.4263
FLQ-k-q-x1	1.165	1.844	112.908	279.957	6.1762	6.0928
FLQ-k-r-x4	1.362	1.587	112.054	278.332	6.8330	6.7233
FLQ-k-r-x1	1.368	2.059	112.111	278.445	6.6126	6.5322

FLQ-j-q-x3	10.635	9.958	116.177	282.134	9.6246	9.8165
FLQ-j-r-x3	10.769	10.166	115.757	281.118	10.0225	10.3684

6.1.2. Uncorrected relative energies, relative energies corrected for ZPE and Gibbs free energies and corresponding corrections for each compound considered.

In this section, tables 6.37–6.72 reports the uncorrected relative energy, relative energy corrected for ZPE (sum of electronic and zero-point energies) and Gibbs free energies (sum of electronic and thermal free energies) for the calculated conformers of all the compounds considered. Tables 6.73–6.108 reports the ZPE corrections to the electronic energy and thermal corrections to the Gibbs free energies for each of the compound considered. All these results were obtained through frequency calculations (harmonic-approximation).

Table 6.37. Uncorrected relative energy (ΔE, kcal/mol), relative energy corrected for ZPE (ΔE$_{corrected}$, kcal/mol) and Gibbs free energy (ΔG$_{corrected}$, kcal/mol) of the calculated conformers of compound AGP.

The absolute values for the lowest energy conformers for E$_{corrected}$ are -1604.386243/DFT (AGP-p-t-u3) and -1596.173253/HF (AGP-m-r-u1); the absolute free energy of the lowest energy conformer is -1604.451283/DFT (AGP-p-t-u3) and -1596.236560/HF (AGP-m-r-u1).

Conformers	DFT			HF		
	ΔE (kcal/mol)	ΔE$_{corrected}$ (kcal/mol)	ΔG$_{corrected}$ (kcal/mol)	ΔE (kcal/mol)	ΔE$_{corrected}$ (kcal/mol)	ΔG$_{corrected}$ (kcal/mol)
AGP-m-r-u1	0,000	0,010	0,041	0.000	0.000	0.000
AGP-m-s-u1	0,000	0,010	0,040	2.428	2.070	0.850
AGP-p-t-u3	0,003	0,000	0,000	2.450	2.095	0.535
AGP-m-q-u1	0,036	0,028	0,023	0.031	0.018	0.032
AGP-p-r-u3	0,037	0,060	0,253	0.030	0.014	0.014
AGP-k-q-u1	1,154	1,099	0,653	1.440	1.364	1.035
AGP-k-r-u1	1,379	1,251	0,326	1.679	1.576	1.189
AGP-m-r-u2	1,763	2,014	2,820	1.806	2.143	2.951
AGP-g-r-u3	4,532	3,869	3,545	2.880	2.307	2.398
AGP-g-q-u3	4,664	4,020	3,797	3.119	2.548	2.653
AGP-j-q-u3	10,245	9,671	9,266	9.554	9.008	8.948
AGP-j-r-u3	10,351	9,746	9,445	9.659	9.091	8.991
AGP-j-s-u3	10,351	9,746	9,445	11.782	10.886	9.733

Table 6.38. Uncorrected relative energy (ΔE, kcal/mol), relative energy corrected for ZPE ($\Delta E_{corrected}$, kcal/mol) and Gibbs free energy ($\Delta G_{corrected}$, kcal/mol) of the calculated conformers of compound AGQ.

The absolute values for the lowest energy conformer for $E_{corrected}$ are -1565.096946/DFT (AGQ-m-r-u1) and -1557.166398/HF; the absolute free energy of the lowest energy conformer is (AGQ-m-r-u1) -1565.159933 / DFT and -1557.227671/HF.

Conformers	DFT			HF		
	ΔE (kcal/mol)	$\Delta E_{corrected}$ (kcal/mol)	$\Delta G_{corrected}$ (kcal/mol)	ΔE (kcal/mol)	$\Delta E_{corrected}$ (kcal/mol)	$\Delta G_{corrected}$ (kcal/mol)
AGQ-m-r-u1	0.000	0.000	0.000	0.000	0.008	0.000
AGQ-m-q-u1	0.015	0.037	0.210	0.004	0.000	0.010
AGQ-k-q-u1	1.156	1.082	0.459	1.441	1.373	1.038
AGQ-k-r-u1	1.366	1.239	0.454	1.660	1.567	1.176
AGQ-m-r-u2	1.761	2.004	2.780	1.799	2.145	2.953
AGQ-m-q-u2	1.774	2.016	2.852	1.811	2.147	2.971
AGQ-g-r-u3	4.496	3.872	3.724	2.917	2.350	2.439
AGQ-g-t-u3	4.496	3.870	3.715	5.438	4.539	3.192
AGQ-g-q-u3	4.662	4.012	3.772	3.114	2.552	2.649
AGQ-j-q-u3	10.248	9.689	9.544	9.564	9.024	8.950
AGQ-j-r-u3	10.279	9.680	9.236	9.635	9.078	8.975
AGQ-j-t-u3	10.279	9.679	9.237	12.269	11.365	12.163

Table 6.39. Uncorrected relative energy (ΔE, kcal/mol), relative energy corrected for ZPE ($\Delta E_{corrected}$, kcal/mol) and Gibbs free energy ($\Delta G_{corrected}$, kcal/mol) of the calculated conformers of compound AJP.

The absolute values for the lowest energy conformers for $E_{corrected}$ are -1679.592155/DFT (AJP-m-s-u1) and -1671.014974/HF (AJP-m-r-u1); the absolute free energy of the lowest energy conformer is -1679.657476/DFT (AJP-m-q-u1) and -1671.078163/HF (AJP-m-r-u1).

Conformers	DFT			HF		
	ΔE (kcal/mol)	$\Delta E_{corrected}$ (kcal/mol)	$\Delta G_{corrected}$ (kcal/mol)	ΔE (kcal/mol)	$\Delta E_{corrected}$ (kcal/mol)	$\Delta G_{corrected}$ (kcal/mol)
AJP-m-r-u1	0.000	0.001	0.100	0.000	0.000	0.000
AJP-m-s-u1	0.000	0.000	0.089	2.406	2.047	0.816
AJP-m-q-u1	0.092	0.071	0.000	0.034	0.019	0.020
AJP-k-q-u1	1.171	1.103	0.532	1.458	1.379	1.029
AJP-k-r-u1	1.392	1.272	0.639	1.703	1.596	1.185
AJP-k-s-u1	1.392	1.269	0.604	4.025	3.572	1.815
AJP-m-r-u2	1.770	2.018	2.838	1.810	2.147	2.951
AJP-m-s-u2	1.770	2.018	2.836	4.220	4.196	3.761
AJP-m-q-u2	1.842	2.058	2.635	1.834	2.158	2.975
AJP-j-q-u3	17.994	17.129	16.398	17.097	16.299	15.854
AJP-j-r-u3	18.137	17.238	16.545	17.257	16.435	15.949
AJP-j-s-u3	18.137	17.237	16.539	19.349	18.199	16.648

Table 6.40. Uncorrected relative energy (ΔE, kcal/mol), relative energy corrected for ZPE ($\Delta E_{corrected}$, kcal/mol) and Gibbs free energy ($\Delta G_{corrected}$, kcal/mol) of the calculated conformers of compound AJQ.

The absolute values for the lowest energy conformer for $E_{corrected}$ are -1640.290527/DFT (AJQ-p-q-u5) and -1631.995754/HF (AJQ-p-q- u3); the absolute free energy of the lowest energy conformers is -1640.354408/DFT (AJQ-p-q-u5) and -1632.057430/HF (AJQ-p-q- u3).

Conformers	DFT			HF		
	ΔE (kcal/mol)	$\Delta E_{corrected}$ (kcal/mol)	$\Delta G_{corrected}$ (kcal/mol)	ΔE (kcal/mol)	$\Delta E_{corrected}$ (kcal/mol)	$\Delta G_{corrected}$ (kcal/mol)
AJQ-p-q-u5	0.000	0.000	0.000	0.464	0.405	0.371
AJQ-m-q-u1	0.052	0.047	0.088	0.045	0.029	0.030
AJQ-m-q-u2	0.465	0.793	1.721	0.456	0.873	1.733
AJQ-m-r-u2	0.470	0.776	1.412	0.455	0.880	1.724
AJQ-p-q- u3	0.583	0.498	0.489	0.000	0.000	0.000
AJQ-m-r-u1	0.583	0.489	0.315	0.689	0.521	0.115
AJQ-p-q-u5	0.583	0.498	0.488	1.156	0.927	0.489
AJQ-m-s-u1	0.583	0.488	0.312	3.109	2.605	0.679
AJQ-p-r-u3	0.615	0.495	0.161	0.707	0.528	0.166
AJQ-p-s-u3	0.615	0.494	0.158	3.115	2.607	0.889
AJQ-m-q-u1	0.617	0.517	0.471	0.713	0.533	0.152
AJQ-k-q-u1	1.175	1.107	0.643	1.466	1.387	1.044
AJQ-k-q-u1	1.770	1.574	0.699	2.162	1.913	1.145
AJQ-k-r-u1	1.974	1.761	1.050	2.390	2.116	1.313
AJQ-j-q-u1	8.670	8.234	7.942	8.027	7.630	7.543
AJQ-j-r-u1	8.838	8.352	7.812	8.271	7.839	7.680

Table 6.41. Uncorrected relative energy (ΔE, kcal/mol), relative energy corrected for ZPE ($\Delta E_{corrected}$, kcal/mol) and Gibbs free energy ($\Delta G_{corrected}$, kcal/mol) of the calculated conformers of compound ALP.

The absolute values for the lowest energy conformers for $E_{corrected}$ are -1605.573575/DFT (ALP-m-q-u1) and -1597.313492/HF (ALP-m-r-u1); the absolute free energy of the lowest energy conformer is -1605.640892/DFT (ALP-m-q-u1) and -1597.378497/HF (ALP-m-r-u1).

Conformers	DFT			HF		
	ΔE (kcal/mol)	$\Delta E_{corrected}$ (kcal/mol)	$\Delta G_{corrected}$ (kcal/mol)	ΔE (kcal/mol)	$\Delta E_{corrected}$ (kcal/mol)	$\Delta G_{corrected}$ (kcal/mol)
ALP-m-r-u1	0.000	0.009	0.111	0.000	0.000	0.000
ALP-m-s-u1	0.000	0.008	0.107	2.431	2.073	0.799
ALP-m-q-u1	0.029	0.000	0.000	0.017	0.004	0.014
ALP-k-q-u1	1.156	1.110	0.777	1.443	1.366	1.027
ALP-k-r-u1	1.367	1.265	0.764	1.681	1.576	1.181
ALP-k-q-u1	1.448	1.295	1.073	1.788	1.685	1.686
ALP-k-r-u1′	1.667	1.453	1.102	2.029	1.898	1.849
ALP-k-s-u1	1.667	1.454	1.108	4.384	3.905	2.418
ALP-k-r-u3	1.679	1.457	0.892	2.123	1.972	1.513

ALP-m-r-u2	1.768	1.990	2.658	1.806	2.144	2.952
ALP-m-s-u2	1.768	1.990	2.656	4.242	4.219	3.747
ALP-m-q-u2	1.780	1.993	2.682	1.816	2.142	2.966
ALP-j-q-u3	10.540	9.856	9.708	9.899	9.325	9.595
ALP-j-r-u3	10.647	9.932	9.857	10.012	9.416	9.642
ALP-j-s-u3	10.647	9.931	9.852	12.129	11.206	10.358

Table 6.42. Uncorrected relative energy (ΔE, kcal/mol), relative energy corrected for ZPE (ΔE$_{\text{corrected}}$, kcal/mol) and Gibbs free energy (ΔG$_{\text{corrected}}$, kcal/mol) of the calculated conformers of compound ALQ.

The absolute values for the lowest energy conformer for E$_{\text{corrected}}$ are -1566.284348/DFT (ALQ-m-r-u1) and -1558.306498/HF (ALQ-m-q-u1); the absolute free energy of the lowest energy conformer is -1566.348909/DFT (ALQ-m-r-u1) and -1558.368761/HF (ALQ-m-q-u1).

Conformers	DFT			HF		
	ΔE (kcal/mol)	ΔE$_{\text{corrected}}$ (kcal/mol)	ΔG$_{\text{corrected}}$ (kcal/mol)	ΔE (kcal/mol)	ΔE$_{\text{corrected}}$ (kcal/mol)	ΔG$_{\text{corrected}}$ (kcal/mol)
ALQ-m-r-u1	0.000	0.000	0.000	0.000	0.011	0.003
ALQ-m-q-u1	0.011	0.025	0.195	0.001	0.000	0.000
ALQ-k-q-u1	1.159	1.062	0.377	1.444	1.377	1.028
ALQ-k-r-u1	1.365	1.227	0.484	1.661	1.570	1.167
ALQ-m-r-u2	1.764	1.992	2.743	1.801	2.150	2.948
ALQ-m-q-u2	1.775	1.974	2.621	1.807	2.146	2.959
ALQ-j-q-u3	10.255	9.681	9.519	9.564	9.028	8.950
ALQ-j-r-u3	10.341	9.732	9.326	9.643	9.089	8.971
ALQ-j-q-u3	11.692	10.905	10.286	10.764	9.796	8.632
ALQ-j-r-u3	11.778	10.971	9.551	10.907	9.918	8.733

Table 6.43. Uncorrected relative energy (ΔE, kcal/mol), relative energy corrected for ZPE (ΔE$_{\text{corrected}}$, kcal/mol) and Gibbs free energy (ΔG$_{\text{corrected}}$, kcal/mol) of the calculated conformers of compound BGP.

The absolute values for the lowest energy conformer for E$_{\text{corrected}}$ are -1565.071676/DFT (BGP-p-s-v3) and -1557.137916/HF (BGP-m-r-v1); the absolute free energy of the lowest energy conformer is -1565.134631/DFT (BGP-m-r-v1) and -1557.199181/HF (BGP-m-r-v1).

Conformers	DFT			HF		
	ΔE (kcal/mol)	ΔE$_{\text{corrected}}$ (kcal/mol)	ΔG$_{\text{corrected}}$ (kcal/mol)	ΔE (kcal/mol)	ΔE$_{\text{corrected}}$ (kcal/mol)	ΔG$_{\text{corrected}}$ (kcal/mol)
BGP-p-s-v3	0.000	0.000	0.080	2.428	2.070	0.782
BGP-p-t-v3	0.000	0.000	0.082	2.454	2.098	0.540
BGP-m-r-v1	0.001	0.007	0.000	0.000	0.000	0.000
BGP-m-s-v1	0.001	0.008	0.003	2.440	2.081	0.842
BGP-m-q-v1	0.031	0.036	0.291	0.031	0.019	0.031
BGP-k-q-v3	1.079	1.026	0.686	1.366	1.324	0.783

BGP-k-r-v3	1.300	1.209	0.819	1.607	1.539	0.951
BGP-k-s-v3	1.300	1.208	0.816	3.962	3.542	1.478
BGP-m-r-v2	1.548	1.745	2.381	1.395	1.655	2.236
BGP-m-s-v2	1.548	1.745	2.380	3.834	3.734	3.074
BGP-m-q-v2	1.569	1.744	2.469	1.416	1.665	2.262
BGP-g-r-v1	4.572	3.848	3.243	2.940	2.350	2.373
BGP-g-q-v1	4.712	4.000	3.620	3.183	2.595	2.631
BGP-j-q-v5	10.319	9.735	9.452	10.412	9.770	9.780
BGP-j-r-v5	10.423	9.805	9.582	10.511	9.844	9.814
BGP-j-s-v5	10.423	9.805	9.584	12.642	11.643	10.544

Table 6.44. Uncorrected relative energy (ΔE, kcal/mol), relative energy corrected for ZPE ($\Delta E_{corrected}$, kcal/mol) and Gibbs free energy ($\Delta G_{corrected}$, kcal/mol) of the calculated conformers of compound BGQ.

The absolute values for the lowest energy conformer for $E_{corrected}$ are -1525.782383/DFT (BGQ-m-r-v1) and -1518.131055/HF (BGQ-m-q-v1); the absolute free energy of the lowest energy conformer is (BGQ-m-r-v1) -1525.843109/DFT and -1518.190287/HF.

Conformers	DFT			HF		
	ΔE (kcal/mol)	$\Delta E_{corrected}$ (kcal/mol)	$\Delta G_{corrected}$ (kcal/mol)	ΔE (kcal/mol)	$\Delta E_{corrected}$ (kcal/mol)	$\Delta G_{corrected}$ (kcal/mol)
BGQ-m-r-v1	0.000	0.000	0.000	0.000	0.003	0.000
BGQ-m-q-v1	0.016	0.025	0.083	0.008	0.000	0.011
BGQ-k-q-v1	1.083	1.029	0.575	1.368	1.328	0.772
BGQ-k-r-v1	1.289	1.197	0.725	1.590	1.526	0.935
BGQ-m-r-v2	1.546	1.748	2.337	1.389	1.654	2.234
BGQ-m-q-v2	1.558	1.743	2.331	1.400	1.655	2.250
BGQ-j-q-v3	10.327	9.745	9.503	9.649	9.093	9.010
BGQ-j-r-v3	10.353	9.738	9.272	9.719	9.145	9.029
BGQ-j-t-v3	10.353	9.737	9.265	12.362	11.441	12.223

Table 6.45. Uncorrected relative energy (ΔE, kcal/mol), relative energy corrected for ZPE ($\Delta E_{corrected}$, kcal/mol) and Gibbs free energy ($\Delta G_{corrected}$, kcal/mol) of the calculated conformers of compound BJP.

The absolute values for the lowest energy conformer for $E_{corrected}$ are (BJP-p-q-v3) -1640.277586/DFT and -1631.979636/HF; the absolute free energy of the lowest energy conformer is (BJP-p-q-v3) -1640.340589/DFT and -1632.040791/HF.

Conformers	DFT			HF		
	ΔE (kcal/mol)	$\Delta E_{corrected}$ (kcal/mol)	$\Delta G_{corrected}$ (kcal/mol)	ΔE (kcal/mol)	$\Delta E_{corrected}$ (kcal/mol)	$\Delta G_{corrected}$ (kcal/mol)
BJP-p-q-v3	0.000	0.000	0.000	0.000	0.000	0.000
BJP-p-s-v3	0.000	0.000	0.002	2.418	2.059	0.813
BJP-p-r-v3	0.087	0.078	0.032	0.034	0.022	0.028

BJP-k-q-v1	1.095	1.040	0.482	1.384	1.341	0.778
BJP-k-r-v1	1.312	1.226	0.813	1.631	1.561	0.944
BJP-k-s-v1	1.312	1.226	0.808	3.959	3.538	1.483
BJP-m-r-v2	1.548	1.763	2.438	1.399	1.659	2.234
BJP-m-s-v2	1.548	1.763	2.439	3.817	3.717	3.047
BJP-m-q-v2	1.621	1.813	2.436	1.422	1.671	2.265
BJP-j-r-v3	18.067	17.201	16.498	17.182	16.374	15.923
BJP-j-s-v3	18.210	17.304	16.669	17.341	16.509	16.014
BJP-j-q-v3	18.210	17.304	16.669	19.437	18.277	16.712

Table 6.46. Uncorrected relative energy (ΔE, kcal/mol), relative energy corrected for ZPE ($\Delta E_{corrected}$, kcal/mol) and Gibbs free energy ($\Delta G_{corrected}$, kcal/mol) of the calculated conformers of compound BJQ.

The absolute values for the lowest energy conformer for $E_{corrected}$ are (BJQ-p-r-v3) -1600.978154/DFT and -1592.962532/HF; the absolute free energy of the lowest energy conformer is (BJQ-p-r-v3) -1601.039708/DFT and -1593.022214/HF.

Conformers	DFT			HF		
	ΔE (kcal/mol)	$\Delta E_{corrected}$ (kcal/mol)	$\Delta G_{corrected}$ (kcal/mol)	ΔE (kcal/mol)	$\Delta E_{corrected}$ (kcal/mol)	$\Delta G_{corrected}$ (kcal/mol)
BJQ-p-r-v3	0.000	0.000	0.000	0.001	0.000	0.000
BJQ-m-s-v1	1.518	1.364	1.183	3.877	3.411	2.223
BJQ-m-t-v1	1.518	1.364	1.185	3.897	3.435	1.834
BJQ-m-q-v2	1.540	1.717	2.265	1.380	1.640	2.231
BJQ-m-r-v2	1.552	1.724	2.113	1.400	1.669	2.242
BJQ-m-q-v1	1.570	1.426	1.370	1.508	1.361	1.394
BJQ-p-q-v3	2.101	1.868	1.715	1.463	1.330	1.360
BJQ-p-q-v3′	2.101	1.868	1.711	2.154	1.852	1.475
BJQ-p-r-v3	2.133	1.869	1.365	2.171	1.859	1.525
BJQ-p-s-v3	2.133	1.869	1.367	4.589	3.948	2.254
BJQ-j-q-v3	10.261	9.676	9.409	9.572	9.030	8.958
BJQ-j-r-v3	10.427	9.797	9.387	9.816	9.239	9.093

Table 6.47. Uncorrected relative energy (ΔE, kcal/mol), relative energy corrected for ZPE ($\Delta E_{corrected}$, kcal/mol) and Gibbs free energy ($\Delta G_{corrected}$, kcal/mol) of the calculated conformers of compound BLP.

The absolute values for the lowest energy conformer for $E_{corrected}$ are -1566.258990/DFT (BLP-k-q-v1) and -1558.277647/HF (BLP-m-r-v1); the absolute free energy of the lowest energy conformer is -1566.324531/DFT (BLP-k-s-v1) and -1558.341174/HF (BLP-k-q-v1).

Conformers	DFT			HF		
	ΔE (kcal/mol)	$\Delta E_{corrected}$ (kcal/mol)	$\Delta G_{corrected}$ (kcal/mol)	ΔE (kcal/mol)	$\Delta E_{corrected}$ (kcal/mol)	$\Delta G_{corrected}$ (kcal/mol)
BLP-k-q-v1	0.000	0.000	0.063	0.132	0.014	0.000
BLP-p-s-v3	0.131	0.154	0.547	2.438	2.079	1.417
BLP-p-t-v3	0.131	0.153	0.545	2.463	2.109	1.254
BLP-m-r-v1	0.133	0.166	0.511	0.000	0.000	0.688
BLP-m-s-v1	0.133	0.166	0.514	2.448	2.088	1.515
BLP-m-r-v1′	0.168	0.169	0.589	0.034	0.021	0.718
BLP-k-r-v1	0.219	0.174	0.007	0.377	0.231	0.170
BLP-k-s-v1	0.219	0.173	0.000	2.755	2.257	0.657
BLP-p-q-v4	1.679	1.901	2.868	1.419	1.657	2.930
BLP-p-s-v4	1.679	1.902	2.872	3.834	3.735	3.656
BLP-p-t-v4	1.679	1.901	2.864	3.860	3.765	3.464
BLP-p-r-v4	1.708	1.920	2.806	1.419	1.667	2.951
BLP-j-q-v5	9.243	8.707	8.865	9.177	8.458	8.997
BLP-j-r-v5	9.351	8.786	8.909	9.289	8.546	9.042
BLP-j-s-v5	9.351	8.786	8.909	11.425	10.351	9.758

Table 6.48. Uncorrected relative energy (ΔE, kcal/mol), relative energy corrected for ZPE ($\Delta E_{corrected}$, kcal/mol) and Gibbs free energy ($\Delta G_{corrected}$, kcal/mol) of the calculated conformers of compound BLQ.

The absolute values for the lowest energy conformer for $E_{corrected}$ are -1526.969799/DFT (BLQ-p-q-v3) and -1519.271152/HF (BLQ-p-r-v3); the absolute free energy of the lowest energy conformer is -1527.032344/DFT (BLQ-p-r-v3) and -1519.332520/HF (BLQ-m-r-v1).

Conformers	DFT			HF		
	ΔE (kcal/mol)	$\Delta E_{corrected}$ (kcal/mol)	$\Delta G_{corrected}$ (kcal/mol)	ΔE (kcal/mol)	$\Delta E_{corrected}$ (kcal/mol)	$\Delta G_{corrected}$ (kcal/mol)
BLQ-p-q-v3	0.000	0.000	0.107	0.000	0.004	0.712
BLQ-p-r-v3	0.015	0.005	0.076	0.005	0.000	0.719
BLQ-p-r-v3	0.017	0.003	0.000	0.011	0.005	0.722
BLQ-k-q-v1	1.081	0.992	0.576	1.358	1.320	1.486
BLQ-k-r-v1	1.290	1.194	0.892	1.597	1.534	1.646
BLQ-m-r-v1	1.465	1.288	1.118	1.225	0.757	0.000
BLQ-m-q-v1	1.479	1.259	0.688	1.236	0.766	0.124
BLQ-m-s-v1	1.479	1.258	0.665	3.833	3.020	3.554
BLQ-p-q-v4	1.551	1.737	2.430	1.394	1.659	2.947
BLQ-p-r-v4	1.560	1.717	2.258	1.392	1.647	2.951
BLQ-j-q-v3	8.913	8.309	7.943	8.085	7.454	7.930

BLQ-j-q-v5	8.913	8.309	7.941	8.859	8.143	8.704
BLQ-j-r-v3	8.947	8.346	8.162	8.174	7.524	7.962
BLQ-j-r-v5	8.947	8.346	8.158	8.945	8.208	8.734
BLQ-j-t-v5	8.947	8.346	8.159	11.605	10.531	12.031
BLQ-j-t-v3	8.947	8.346	8.157	10.835	9.847	11.280

Table 6.49. Uncorrected relative energy (ΔE, kcal/mol), relative energy corrected for ZPE ($\Delta E_{corrected}$, kcal/mol) and Gibbs free energy ($\Delta G_{corrected}$, kcal/mol) of the calculated conformers of compound CGP.

The absolute values for the lowest energy for $E_{corrected}$ conformer are -1525.776190/DFT (CGP-p-q-w5) and -1518.124245/HF (CGP-p-r-w5); the absolute free energy of the lowest energy conformer is -1525.837196/DFT (CGP-m-q-w1) and -1518.183609/HF (CGP-p-q-w5).

Conformers	DFT			HF		
	ΔE (kcal/mol)	$\Delta E_{corrected}$ (kcal/mol)	$\Delta G_{corrected}$ (kcal/mol)	ΔE (kcal/mol)	$\Delta E_{corrected}$ (kcal/mol)	$\Delta G_{corrected}$ (kcal/mol)
CGP-p-q-w5	0.000	0.000	0.109	0.000	0.004	0.000
CGP-p-s-w5	0.000	0.000	0.105	2.415	2.059	0.732
CGP-p-r-w5	0.029	0.039	0.114	0.011	0.000	0.008
CGP-m-r-w1	0.233	0.222	0.144	0.668	0.610	0.397
CGP-m-s-w1	0.233	0.222	0.142	3.107	2.690	1.256
CGP-m-q-w1	0.270	0.234	0.000	0.693	0.626	0.434
CGP-m-r-w2	2.758	2.882	3.090	3.651	3.777	3.960
CGP-m-s-w2	2.758	2.881	3.085	6.101	5.865	4.784
CGP-m-q-w2	2.782	2.884	3.185	3.664	3.780	3.981
CGP-g-r-w5	4.417	3.941	4.041	3.004	2.483	2.625
CGP-g-q-w5	4.580	4.110	4.217	3.288	2.760	2.907
CGP-j-q-w5	9.899	9.413	8.971	9.312	8.843	8.788
CGP-j-r-w5	9.994	9.504	9.365	9.411	8.922	8.837
CGP-j-s-w5	9.994	9.505	9.365	11.552	10.732	9.575

Table 6.50. Uncorrected relative energy (ΔE, kcal/mol), relative energy corrected for ZPE ($\Delta E_{corrected}$, kcal/mol) and Gibbs free energy ($\Delta G_{corrected}$, kcal/mol) of the calculated conformers of compound CGQ.

The absolute values for the lowest energy conformers for $E_{corrected}$ are -1486.486895/DFT (CGQ-p-q-w5) and -1479.117415/HF (CGQ-p-r-w5); the absolute free energy of the lowest energy conformer is -1486.545713/DFT (CGQ-p-q-w5) and -1479.174734/HF (CGQ-p-r-w5).

Conformers	DFT			HF		
	ΔE (kcal/mol)	$\Delta E_{corrected}$ (kcal/mol)	$\Delta G_{corrected}$ (kcal/mol)	ΔE (kcal/mol)	$\Delta E_{corrected}$ (kcal/mol)	$\Delta G_{corrected}$ (kcal/mol)
CGQ-p-q-w5	0.000	0.000	0.000	0.012	0.023	0.008
CGQ-m-q-w3	0.002	0.001	0.003	0.008	0.019	0.004
CGQ-p-r-w5	0.014	0.006	0.051	0.000	0.000	0.000
CGQ-m-r-w1	0.234	0.206	0.054	0.679	0.631	0.405
CGQ-m-q-w1	0.255	0.227	0.071	0.683	0.626	0.423
CGQ-j-q-w5	9.902	9.440	9.275	9.336	8.875	8.806
CGQ-j-r-w5	9.926	9.439	9.146	9.402	8.924	8.823
CGQ-j-t-w5	9.926	9.439	9.149	12.052	11.226	12.004

Table 6.51. Uncorrected relative energy (ΔE, kcal/mol), relative energy corrected for ZPE ($\Delta E_{corrected}$, kcal/mol) and Gibbs free energy ($\Delta G_{corrected}$, kcal/mol) of the calculated conformers of compound CJP.

The absolute values for the lowest energy conformer for $E_{corrected}$ are (CJP-p-q-w3) -1600.982066/DFT and -1592.965951/HF; the absolute free energy of the lowest energy conformer is -1601.043433/DFT (CJP-p-r-w3) and -1593.025216/HF (CJP-p-q-w3).

Conformers	DFT			HF		
	ΔE (kcal/mol)	$\Delta E_{corrected}$ (kcal/mol)	$\Delta G_{corrected}$ (kcal/mol)	ΔE (kcal/mol)	$\Delta E_{corrected}$ (kcal/mol)	$\Delta G_{corrected}$ (kcal/mol)
CJP-p-q-w3	0.000	0.000	0.371	0.000	0.000	0.000
CJP-p-s-w3	0.000	0.001	0.371	2.405	2.046	0.798
CJP-p- r-w3	0.036	0.005	0.000	0.016	0.003	0.012
CJP-m-r-w1	0.229	0.208	0.388	0.664	0.604	0.395
CJP-m-r-w2	2.754	2.874	3.325	3.649	3.771	3.959
CJP-m-s-w2	2.754	2.874	3.320	6.078	5.840	4.763
CJP-m-t-w2	2.754	2.874	3.323	6.087	5.853	4.295
CJP-m-q-w2	2.830	2.931	3.452	3.663	3.778	3.982
CJP-j-q-w1	17.645	16.867	16.334	16.853	16.131	15.708
CJP-j-r-w1	17.786	16.965	16.378	17.007	16.262	15.801
CJP-j-s-w1	17.786	16.965	16.384	19.117	18.041	16.504

Table 6.52. Uncorrected relative energy (ΔE, kcal/mol), relative energy corrected for ZPE ($\Delta E_{corrected}$, kcal/mol) and Gibbs free energy ($\Delta G_{corrected}$, kcal/mol) of the calculated conformers of compound CJQ.

The absolute values for the lowest energy conformer for $E_{corrected}$ are (CJQ-m-q-w6) -1561.682692/DFT and -1553.948900/HF; the absolute free energy of the lowest energy conformer is -1554.006636/DFT (CJQ-m-r-w6) and -1554.006681/HF (CJQ-m-q-w6).

Conformers	DFT			HF		
	ΔE (kcal/mol)	$\Delta E_{corrected}$ (kcal/mol)	$\Delta G_{corrected}$ (kcal/mol)	ΔE (kcal/mol)	$\Delta E_{corrected}$ (kcal/mol)	$\Delta G_{corrected}$ (kcal/mol)
CJQ-m-q-w6	0.000	0.000	0.010	0.000	0.000	0.000
CJQ-m-r-w6	0.006	0.010	0.000	0.032	0.042	0.028
CJQ-p-q-w5	1.529	1.389	1.173	1.496	1.365	1.389
CJQ-m-q-w1	1.811	1.649	1.502	2.201	1.995	1.795
CJQ-p-q-w5	2.117	1.888	1.660	1.499	1.373	1.409
CJQ-p-q-w5′	2.117	1.888	1.657	2.189	1.888	1.512
CJQ-p-s-w5	2.145	1.874	1.209	4.163	3.970	2.256
CJQ-m-r-w1	2.343	2.080	1.590	2.849	2.487	1.891
CJQ-m-s-w1	2.343	2.080	1.589	5.282	4.585	2.270
CJQ-m-q-w1′	2.378	2.100	1.682	2.869	2.503	1.972
CJQ-j-q-w5	9.841	9.390	9.167	9.272	8.819	8.772
CJQ-j-r-w5	10.002	9.515	9.159	9.512	9.024	8.902

Table 6.53. Uncorrected relative energy (ΔE, kcal/mol), relative energy corrected for ZPE ($\Delta E_{corrected}$, kcal/mol) and Gibbs free energy ($\Delta G_{corrected}$, kcal/mol) of the calculated conformers of compound CLP.

The absolute values for the lowest energy conformer for $E_{corrected}$ are -1526.963275/DFT (CLP-p-s-w5) and -1519.263978/HF (CLP-p-r-w5′); the absolute free energy of the lowest energy conformer is -1527.026328/DFT (CLP-p-s-w5) and -1519.324508/HF (CLP-p-q-w5).

Conformers	DFT			HF		
	ΔE (kcal/mol)	$\Delta E_{corrected}$ (kcal/mol)	$\Delta G_{corrected}$ (kcal/mol)	ΔE (kcal/mol)	$\Delta E_{corrected}$ (kcal/mol)	$\Delta G_{corrected}$ (kcal/mol)
CLP-p-q-w5	0.000	0.001	0.003	0.000	0.003	0.000
CLP-p-s-w5	0.000	0.000	0.000	2.425	2.070	0.678
CLP-p-r-w5	0.033	0.046	0.044	0.015	0.004	0.013
CLP-p-r-w5′	0.033	0.046	0.044	0.016	0.000	0.007
CLP-m-r-w1	0.231	0.229	0.150	0.667	0.611	0.398
CLP-m-s-w1	0.231	0.229	0.149	3.116	2.700	1.237
CLP-m-q-w1	0.271	0.254	0.115	0.696	0.629	0.430
CLP-m-q-w2	2.757	2.898	3.202	3.652	3.778	3.954
CLP-m-s-w2	2.757	2.897	3.191	6.109	5.875	4.772
CLP-m-q-w2	2.789	2.877	3.058	3.666	3.784	3.985
CLP-j-q-w5	9.590	9.258	8.980	8.948	8.508	8.121
CLP-j-r-w5	9.716	9.372	9.207	9.097	8.634	8.202
CLP-j-s-w5	9.716	9.371	9.204	11.239	10.445	8.918

CLP-j-q-w6	10.774	9.994	9.212	10.395	9.622	9.212
CLP-j-r-w6	10.841	10.047	9.051	10.483	9.668	9.172
CLP-j-s-w6	10.841	10.044	9.025	12.611	11.493	9.977

Table 6.54. Uncorrected relative energy (ΔE, kcal/mol), relative energy corrected for ZPE ($\Delta E_{corrected}$, kcal/mol) and Gibbs free energy ($\Delta G_{corrected}$, kcal/mol) of the calculated conformers of compound CLQ.

The absolute values for the lowest energy conformer for $E_{corrected}$ are (CLQ-p-q-w5) -1487.674007/DFT and -1480.257172/HF); the absolute free energy of the lowest energy conformer is -1487.734990/DFT (CLQ-p-q-w5) and -1480.316111/HF (CLQ-m-r-w1).

Conformers	DFT			HF		
	ΔE (kcal/mol)	$\Delta E_{corrected}$ (kcal/mol)	$\Delta G_{corrected}$ (kcal/mol)	ΔE (kcal/mol)	$\Delta E_{corrected}$ (kcal/mol)	$\Delta G_{corrected}$ (kcal/mol)
CLQ-p-q-w5	0.000	0.000	0.000	0.000	0.000	0.332
CLQ-p-s-w5	0.000	2.127	0.783	2.471	0.001	0.331
CLQ-m-q-w1	0.033	0.001	0.013	0.014	0.020	0.296
CLQ-m-q-w1′	0.275	0.623	0.430	0.694	0.218	0.225
CLQ-m-r-w1	0.237	0.607	0.400	0.666	0.167	0.000
CLQ-m-r-w1′	0.237	0.616	0.421	0.667	0.167	0.005
CLQ-m-s-w1	0.237	2.745	0.494	3.149	0.167	0.001
CLQ-j-q-w5	9.893	8.828	8.779	9.297	9.396	9.258
CLQ-j-r-w5	9.967	8.950	8.862	9.442	9.467	9.402
CLQ-j-s-w6	9.967	10.794	9.557	11.601	9.467	9.399

Table 6.55. Uncorrected relative energy (ΔE, kcal/mol), relative energy corrected for ZPE ($\Delta E_{corrected}$, kcal/mol) and Gibbs free energy ($\Delta G_{corrected}$, kcal/mol) of the calculated conformers of compound DGP.

The absolute values for the lowest energy conformer for $E_{corrected}$ are -1448.421533/DFT (DGP-p-s) and -1441.288696/HF (DGP-m-r); the absolute free energy of the lowest energy conformer is -1448.480010/DFT (DGP-p-s) and -1441.345575/HF (DGP-m-r).

Conformers	HF			DFT		
	$\Delta E_{not\ corrected\ for\ ZPE}$	$\Delta_{for\ ZPE}$	ΔG	$\Delta E_{not\ corrected\ for\ ZPE}$	$\Delta E_{corrected\ for\ ZPE}$	ΔG
DGP-m-r	0.000	0.018	0.097	0.001	0.000	0.000
DGP-m-s	0.000	0.019	0.095	2.445	2.082	0.847
DGP-p-q	0.002	0.000	0.005	0.000	0.000	0.002
DGP-p-s	0.002	0.000	0.000	2.434	2.071	0.754
DGP-p-a-t	0.002	0.000	0.002	2.460	2.100	0.404
DGP-m-q	0.044	0.047	0.105	0.029	0.016	0.033
DGP-k-q	1.090	0.949	0.258	1.346	1.210	0.774
DGP-k-r	1.310	1.121	0.334	1.587	1.424	0.937
DGP-k-s	1.310	1.118	0.301	3.945	3.424	1.471

DGP-g-r	4.630	4.068	3.948	3.002	2.472	2.620
DGP-g-q	4.775	4.215	4.090	3.250	2.721	2.875
DGP-j-q	10.365	9.885	9.748	9.675	9.174	9.134
DGP-j-r	10.425	9.922	9.704	9.780	9.258	9.188
DGP-j-s	10.425	9.923	9.710	11.915	11.061	9.913

Table 6.56. Uncorrected relative energy (ΔE, kcal/mol), relative energy corrected for ZPE ($\Delta E_{\text{corrected}}$, kcal/mol) and Gibbs free energy ($\Delta G_{\text{corrected}}$, kcal/mol) of the calculated conformers of compound DGQ.

The absolute values for the lowest energy conformer for $E_{\text{corrected}}$ are -1409.132250/DFT (DGQ-p-q) and -1402.281841/HF (DGQ-m-q); the absolute free energy of the lowest energy conformer is -1409.188812/DFT (DGQ-m-q′) and -1402.336692/HF (DGQ-p-q).

Conformers	DFT			HF		
	ΔE (kcal/mol)	$\Delta E_{\text{corrected}}$ (kcal/mol)	$\Delta G_{\text{corrected}}$ (kcal/mol)	ΔE (kcal/mol)	$\Delta E_{\text{corrected}}$ (kcal/mol)	$\Delta G_{\text{corrected}}$ (kcal/mol)
DGQ-m-r	0.000	0.029	0.216	0.000	0.003	0.008
DGQ-p-q	0.003	0.000	0.041	0.003	0.004	0.000
DGQ-m-q	0.027	0.033	0.178	0.009	0.000	0.019
DGQ-m-q′	0.031	0.024	0.000	0.016	0.008	0.023
DGQ-k-q	1.093	0.961	0.452	1.351	1.218	0.781
DGQ-k-r	1.299	1.126	0.539	1.573	1.415	0.934
DGQ-g-r	4.601	4.062	4.087	3.045	2.516	2.661
DGQ-g-t	4.601	4.064	4.093	5.580	4.714	5.736
DGQ-g-q	4.771	4.236	4.327	3.248	2.724	2.875
DGQ-j-q	10.374	9.898	9.862	9.690	9.191	9.146
DGQ-j-r	10.399	9.909	9.850	9.761	9.244	9.175
DGQ-j-t	10.399	9.910	9.849	12.411	11.545	12.319

Table 6.57. Uncorrected relative energy (ΔE, kcal/mol), relative energy corrected for ZPE ($\Delta E_{\text{corrected}}$, kcal/mol) and Gibbs free energy ($\Delta G_{\text{corrected}}$, kcal/mol) of the calculated conformers of compound DJP.

The absolute values for the lowest energy conformer for $E_{\text{corrected}}$ are (DJP-m-r) -1523.627438/DFT and -1516.130416/HF; the absolute free energy of the lowest energy conformer is (DJP-m-r) -1523.686275/DFT and -1516.187251/ HF.

Conformers	DFT			HF		
	ΔE (kcal/mol)	$\Delta E_{\text{corrected}}$ (kcal/mol)	$\Delta G_{\text{corrected}}$ (kcal/mol)	ΔE (kcal/mol)	$\Delta E_{\text{corrected}}$ (kcal/mol)	$\Delta G_{\text{corrected}}$ (kcal/mol)
DJP-m-r	0.000	0.000	0.000	0.003	0.000	0.000
DJP-p-s	0.000	0.000	0.003	2.424	2.065	0.856
DJP-p-q	0.041	0.053	0.337	0.000	0.001	0.040
DJP-m-q	0.041	0.053	0.338	0.031	0.021	0.074
DJP-p-r	0.041	0.053	0.337	0.032	0.023	0.073

DJP-k-q	1.108	0.939	0.114	1.363	1.226	0.808
DJP-k-r	1.320	1.135	0.475	1.609	1.448	0.990
DJP-k-r′	1.320	1.134	0.477	1.610	1.451	1.002
DJP-k-s	1.320	1.135	0.478	3.940	3.420	1.518
DJP-j-q	18.116	17.309	16.588	17.219	16.471	16.096
DJP-j-s	18.260	17.440	16.733	17.380	18.380	16.887
DJP-j-r	18.260	17.438	16.726	19.484	16.609	16.199

Table 6.58. Uncorrected relative energy (ΔE, kcal/mol), relative energy corrected for ZPE ($\Delta E_{corrected}$, kcal/mol) and Gibbs free energy ($\Delta G_{corrected}$, kcal/mol) of the calculated conformers of compound DJQ.

The absolute values for the lowest energy conformer for $E_{corrected}$ are (DJQ-m-q) 1484.328009/DFT and -1477.113298/HF; the absolute free energy of the lowest energy conformer is (DJQ-m-q) -1484.385269/DFT and -1477.168605/HF.

Conformers	DFT			HF		
	ΔE (kcal/mol)	$\Delta E_{corrected}$ (kcal/mol)	$\Delta G_{corrected}$ (kcal/mol)	ΔE (kcal/mol)	$\Delta E_{corrected}$ (kcal/mol)	$\Delta G_{corrected}$ (kcal/mol)
DJQ-m-q	0.000	0.000	0.000	0.000	0.000	0.000
DJQ-k-q	1.088	0.949	0.416	1.349	1.212	0.769
DJQ-k-r	1.291	1.111	0.473	1.584	1.422	0.918
DJQ-m-r	1.514	1.386	1.471	1.466	1.323	1.357
DJQ-m-s	1.514	1.386	1.469	3.886	3.408	2.211
DJQ-m-t	1.514	1.873	1.424	3.907	3.430	4.471
DJQ-m-s′	1.514	1.386	1.467	4.593	3.942	1.298
DJQ-m-q	1.576	1.424	1.378	1.508	1.353	1.396
DJQ-p-q-	1.577	1.384	1.443	1.467	1.324	1.357
DJQ-m-r′	2.105	1.861	1.570	2.155	1.846	1.493
DJQ-p-q′	2.106	1.854	1.563	2.158	1.848	1.486
DJQ-p-r	2.139	1.879	1.589	2.172	1.852	1.522
DJQ-m-q	2.144	1.873	1.424	2.177	1.857	1.530
DJQ-j-q	2.666	2.386	2.530	2.129	1.787	2.062
DJQ-j-r	2.788	2.481	2.571	2.318	1.948	2.177

Table 6.59. Uncorrected relative energy (ΔE, kcal/mol), relative energy corrected for ZPE ($\Delta E_{\mathrm{corrected}}$, kcal/mol) and Gibbs free energy ($\Delta G_{\mathrm{corrected}}$, kcal/mol) of the calculated conformers of compound DLP.

The absolute values for the lowest energy conformer for $E_{\mathrm{corrected}}$ are -1449.608590/DFT (DLP-p-q) and -1442.428429/HF (DLP-m-r); the absolute free energy of the lowest energy conformer is -1449.669152/DFT (DLP-p-r) and -1442.486476/HF (DLP-m-r).

Conformers	DFT			HF		
	ΔE (kcal/mol)	$\Delta E_{\mathrm{corrected}}$ (kcal/mol)	$\Delta G_{\mathrm{corrected}}$ (kcal/mol)	ΔE (kcal/mol)	$\Delta E_{\mathrm{corrected}}$ (kcal/mol)	$\Delta G_{\mathrm{corrected}}$ (kcal/mol)
DLP-m-r	0.000	0.026	0.158	0.001	0.000	0.000
DLP-m-s	0.000	0.026	0.160	2.454	2.092	0.824
DLP-p-q	0.002	0.000	0.034	0.000	0.001	0.006
DLP-p-s	0.002	0.000	0.033	2.444	2.083	0.713
CLP-p-t	0.002	0.000	0.033	2.470	2.109	3.070
DLP-m-q	0.049	0.024	0.018	0.032	0.019	0.034
DLP-p-r	0.051	0.030	0.000	0.033	0.019	0.035
DLP-k-q	1.093	0.963	0.365	1.349	1.212	0.773
DLP-k-r	1.312	1.113	0.318	1.592	1.431	0.954
DLP-k-s	1.312	1.118	0.372	3.955	3.436	1.450
DLP-j-q	10.365	9.886	9.806	9.676	9.176	9.138
DLP-j-s	10.430	9.920	9.763	11.917	11.065	9.901
DLP-j-r	10.476	9.955	9.810	9.789	9.267	9.191

Table 6.60. Uncorrected relative energy (ΔE, kcal/mol), relative energy corrected for ZPE ($\Delta E_{\mathrm{corrected}}$, kcal/mol) and Gibbs free energy ($\Delta G_{\mathrm{corrected}}$, kcal/mol) of the calculated conformers of compound DLQ.

The absolute values for the lowest energy conformer for $E_{\mathrm{corrected}}$ are (DLQ-p-q) -1410.321937/DFT and -1403.424542/HF; the absolute free energy of the lowest energy conformer is (DLQ-p-q) -1410.380072/DFT and -1403.480638/HF.

Conformers	DFT			HF		
	ΔE (kcal/mol)	$\Delta E_{\mathrm{corrected}}$ (kcal/mol)	$\Delta G_{\mathrm{corrected}}$ (kcal/mol)	ΔE (kcal/mol)	$\Delta E_{\mathrm{corrected}}$ (kcal/mol)	$\Delta G_{\mathrm{corrected}}$ (kcal/mol)
DLQ-p-q	0.000	0.000	0.000	0.000	0.000	0.000
DLQ-k-q	1.090	0.968	0.378	1.348	1.213	0.777
DLQ-k-r	1.233	1.076	0.380	1.568	1.409	0.918
DLQ-m-r	1.419	1.442	1.571	1.563	1.640	1.790
DLQ-m-q	1.442	1.433	1.410	1.567	1.632	1.798
DLQ-m-r′	2.887	2.659	2.149	2.787	2.391	1.076
DLQ-m-q′	2.903	2.703	2.343	2.796	2.366	3.221
DLQ-j-q	10.374	9.899	9.728	9.686	9.186	9.142
DLQ-j-r	10.412	9.927	9.821	9.776	9.258	9.179
DLQ-j-t	10.412	9.927	9.819	12.444	11.584	12.437

Table 6.61. Uncorrected relative energy (ΔE, kcal/mol), relative energy corrected for ZPE ($\Delta E_{corrected}$, kcal/mol) and Gibbs free energy ($\Delta G_{corrected}$, kcal/mol) of the calculated conformers of compound EGP.

The absolute values for the lowest energy conformer for $E_{corrected}$ are -1487.713325/DFT (EGP-m-s-x4) and -1480.299208/HF (EGP-m-r-x4); the absolute free energy of the lowest energy conformer is (EGP-p-q-x3) -1487.774143/DFT and -1480.358035/HF.

Conformers	DFT			HF		
	ΔE (kcal/mol)	$\Delta E_{corrected}$ (kcal/mol)	$\Delta G_{corrected}$ (kcal/mol)	ΔE (kcal/mol)	$\Delta E_{corrected}$ (kcal/mol)	$\Delta G_{corrected}$ (kcal/mol)
EGP-m-r-x4	0.000	0.001	0.363	0.000	0.000	0.084
EGP-m-s-x4	0.000	0.000	0.360	2.439	2.078	0.926
EGP-m-q-x4	0.036	0.011	0.362	0.024	0.013	0.114
EGP-m-r-x1	0.313	0.200	0.100	0.320	0.204	0.008
EGP-m-s-x1	0.313	0.200	0.101	2.754	2.278	0.858
EGP-p-q-x3	0.316	0.179	0.000	0.322	0.205	0.000
EGP-p-s-x3	0.316	0.179	0.006	2.741	2.267	0.778
EGP-m-q-x1	0.359	0.223	0.068	0.350	0.222	0.052
EGP-k-q-x1	1.159	1.047	0.747	1.716	1.507	0.914
EGP-k-r-x2	1.374	1.224	0.902	1.662	1.542	1.010
EGP-k-q-x1′	1.374	1.225	0.911	1.954	1.717	1.067
EGP-k-s-x1	1.374	1.224	0.906	4.311	3.722	1.662
EGP-g-r-x1	4.794	4.116	4.078	2.232	2.598	2.583
EGP-g-q-x1	4.948	4.241	4.074	3.480	2.846	2.836
EGP-j-q-x3	10.527	9.900	9.799	9.908	9.288	9.089
EGP-j-r-x3	10.628	9.963	9.839	10.012	9.372	9.140
EGP-j-s-x3	10.628	9.963	9.837	12.141	11.170	9.869

Table 6.62. Uncorrected relative energy (ΔE, kcal/mol), relative energy corrected for ZPE ($\Delta E_{corrected}$, kcal/mol) and Gibbs free energy ($\Delta G_{corrected}$, kcal/mol) of the calculated conformers of compound EGQ.

The absolute values for the lowest energy conformer for $E_{corrected}$ are (EGQ-m-r-x4) -1448.424059/DF and -1441.292348/HF; the absolute free energy of the lowest energy conformer is -1448.483098/DFT (EGQ-p-q-x3) and -1441.349124/HF (EGQ-m-r-x4)).

Conformers	DFT			HF		
	ΔE (kcal/mol)	$\Delta E_{corrected}$ (kcal/mol)	$\Delta G_{corrected}$ (kcal/mol)	ΔE (kcal/mol)	$\Delta E_{corrected}$ (kcal/mol)	$\Delta G_{corrected}$ (kcal/mol)
EGQ-m-r-x4	0.000	0.000	0.507	0.000	0.000	0.073
EGQ-m-q-x4	0.021	0.003	0.381	0.013	0.004	0.093
EGQ-m-r-x1	0.312	0.203	0.177	0.325	0.208	0.000
EGQ-m-q-x1	0.339	0.219	0.209	0.327	0.201	0.017
EGQ-p-q-x3	0.358	0.276	0.000	0.378	0.317	0.236
EGQ-p-r-x3	0.375	0.294	0.189	0.379	0.307	0.260
EGQ-k-q-x4	1.152	1.064	1.177	1.361	1.292	1.103
EGQ-k-r-x4	1.358	1.225	1.269	1.581	1.487	1.245

EGQ-g-r-x1	4.764	4.110	4.302	3.276	2.639	2.605
EGQ-g-t-x1	4.764	4.109	4.300	5.806	4.834	3.166
EGQ-g-q-x1	4.939	4.266	4.379	3.479	2.846	2.819
EGQ-j-q-x3	10.531	9.904	9.826	9.923	9.303	9.084
EGQ-j-r-x3	10.556	9.920	9.920	9.993	9.355	9.104
EGQ-j-t-x3	10.556	9.920	9.915	12.636	11.649	12.277

Table 6.63. Uncorrected relative energy (ΔE, kcal/mol), relative energy corrected for ZPE ($\Delta E_{corrected}$, kcal/mol) and Gibbs free energy ($\Delta G_{corrected}$, kcal/mol) of the calculated conformers of compound EJP.

The absolute values for the lowest energy conformer for $E_{corrected}$ are (EJP-m-s-x4) -1562.919252/DFT and -1555.140926/HF; the absolute free energy of the lowest energy conformer is (EJP-p-q-x4) -1562.980183/DFT and -1555.199635/HF.

Conformers	DFT			HF		
	ΔE (kcal/mol)	$\Delta E_{corrected}$ (kcal/mol)	$\Delta G_{corrected}$ (kcal/mol)	ΔE (kcal/mol)	$\Delta E_{corrected}$ (kcal/mol)	$\Delta G_{corrected}$ (kcal/mol)
EJP-m-s-x4	0.000	0.000	0.168	0.000	0.000	0.077
EJP-m-r-x4	0.000	0.000	0.167	2.419	2.058	0.892
EJP-m-q-x4	0.083	0.065	0.403	0.028	0.016	0.110
EJP-p-s-x4	0.083	0.065	0.401	2.733	2.258	0.809
EJP-p-q-x4	0.315	0.205	0.000	0.321	0.204	0.000
EJP-p-r-x4	0.361	0.248	0.039	0.353	0.225	0.053
EJP-k-q-x1	1.177	1.055	0.601	1.733	1.520	0.912
EJP-k-r-x1	1.389	1.244	0.722	1.976	1.738	1.080
EJP-k-r-x1′	1.389	1.244	0.718	1.977	1.739	1.076
EJP-k-s-x1	1.389	1.244	0.717	4.306	3.715	1.674
EJP-j-q-x3	18.275	17.363	16.740	17.452	16.581	16.000
EJP-j-r-x3	18.423	17.440	16.560	17.611	16.717	16.094
EJP-j-s-x3	18.423	17.440	16.552	19.709	18.485	16.791

Table 6.64. Uncorrected relative energy (ΔE, kcal/mol), relative energy corrected for ZPE ($\Delta E_{corrected}$, kcal/mol) and Gibbs free energy ($\Delta G_{corrected}$, kcal/mol) of the calculated conformers of compound EJQ.

The absolute values for the lowest energy conformer for $E_{corrected}$ are (EJQ-m-q-x4) -1523.619869/DFT and -1516.123850/HF; the absolute free energy of the lowest energy conformer is -1523.678970/DFT (EJQ-m-r-x4) and -1516.180941/HF (EJQ-m-q-x4).

Conformers	HF			DFT		
	ΔE (kcal/mol)	$\Delta E_{corrected}$ (kcal/mol)	$\Delta G_{corrected}$ (kcal/mol)	ΔE (kcal/mol)	$\Delta E_{corrected}$ (kcal/mol)	$\Delta G_{corrected}$ (kcal/mol)
EJQ-m-q-x4	0.000	0.000	0.002	0.000	0.000	0.000
EJQ-m-r-x4	0.003	0.012	0.000	0.019	0.028	0.007
EJQ-p-q-x4	1.833	1.606	1.142	1.801	1.551	1.285
EJQ-p-q-x4′	2.425	2.070	1.221	2.493	2.076	1.420
EJQ-m-r-x1	2.426	2.062	1.205	2.490	2.074	1.420
EJQ-m-s-x1	2.426	2.062	1.201	4.916	4.160	4.506
EJQ-p-r-x4	2.457	2.106	1.417	2.507	2.081	1.478
EJQ-p-s-x4	2.457	2.106	1.415	4.922	4.164	2.184
EJQ-m-q-x1	2.461	2.112	1.417	2.513	2.086	1.468
EJQ-k-q-x4	3.286	2.957	2.198	3.558	3.182	2.501
EJQ-k-r-x4	3.435	3.106	2.402	3.788	3.389	2.691
EJQ-j-q-x3	10.468	9.866	9.367	9.859	9.256	8.964
EJQ-j-r-x3	10.634	9.996	9.433	10.102	9.465	9.103

Table 6.65. Uncorrected relative energy (ΔE, kcal/mol), relative energy corrected for ZPE ($\Delta E_{corrected}$, kcal/mol) and Gibbs free energy ($\Delta G_{corrected}$, kcal/mol) of the calculated conformers of compound ELP.

The absolute values for the lowest energy conformer for $E_{corrected}$ are -1488.900396/DFT (ELP-m-q-x4) and -1481.438940/HF (ELP-m-s-x4); the absolute free energy of the lowest energy conformer is -1488.963379/DFT (ELP-p-s-x4) and -1481.498921/HF (ELP-m-r-x1).

Conformers	DFT			HF		
	ΔE (kcal/mol)	$\Delta E_{corrected}$ (kcal/mol)	$\Delta G_{corrected}$ (kcal/mol)	ΔE (kcal/mol)	$\Delta E_{corrected}$ (kcal/mol)	$\Delta G_{corrected}$ (kcal/mol)
ELP-m-s-x4	0.000	0.010	0.462	0.000	0.000	0.076
ELP-m-q-x4	0.000	0.009	0.461	2.448	2.088	0.905
ELP-m-q-x4	0.040	0.000	0.254	0.027	0.016	0.110
ELP-m-r-x1	0.314	0.206	0.210	0.320	0.204	0.000
ELP-m-s-x1	0.314	0.206	0.213	2.762	2.287	0.831
ELP-p-s-x4	0.315	0.177	0.000	0.321	0.205	0.001
ELP-p-s-x4′	0.315	0.178	0.004	2.751	2.277	0.709
ELP-m-q-x1	0.361	0.236	0.265	0.353	0.226	0.048
ELP-k-q-x1	1.160	1.064	0.879	1.719	1.509	0.911
ELP-k-r-x1	1.377	1.220	0.889	1.958	1.723	1.072
ELP-k-s-x1	1.377	1.219	0.890	4.321	3.732	1.633
ELP-j-q-x3	10.223	9.711	9.566	9.544	8.953	8.411
ELP-j-r-x3	10.355	9.807	9.564	9.698	9.081	8.496

ELP-j-s-x3	10.355	9.807	9.568	11.828	10.882	9.204
ELP-j-q-x3′	10.527	9.893	9.788	9.908	9.289	9.083
ELP-j-r-x3′	10.630	9.982	9.928	10.020	9.379	9.132
ELP-j-s-x3′	10.630	9.982	9.921	12.142	11.172	9.846

Table 6.66. Uncorrected relative energy (ΔE, kcal/mol), relative energy corrected for ZPE ($\Delta E_{corrected}$, kcal/mol) and Gibbs free energy ($\Delta G_{corrected}$, kcal/mol) of the calculated conformers of compound ELQ.

The absolute values for the lowest energy conformer for $E_{corrected}$ are (ELQ-m-q-x4) -1449.611480/DFT and -1442.432445/HF; the absolute free energy of the lowest energy conformer is (ELQ-m-r-x1) -1449.671977/DFT and -1442.490225/HF.

Conformers	DFT			HF		
	ΔE (kcal/mol)	$\Delta E_{corrected}$ (kcal/mol)	$\Delta G_{corrected}$ (kcal/mol)	ΔE (kcal/mol)	$\Delta E_{corrected}$ (kcal/mol)	$\Delta G_{corrected}$ (kcal/mol)
ELQ-m-r-x4	0.000	0.031	0.591	0.000	0.002	0.073
ELQ-m-q-x4	0.021	0.000	0.341	0.007	0.000	0.087
ELQ-m-r-x1	0.322	0.185	0.000	0.324	0.210	0.000
ELQ-m-q-x1	0.343	0.213	0.051	0.323	0.200	0.011
ELQ-k-q-x4	1.147	1.076	1.169	1.349	1.283	1.096
ELQ-k-r-x4	1.359	1.233	1.252	1.589	1.495	1.247
ELQ-j-q-x3	10.488	9.866	9.719	9.860	9.246	9.029
ELQ-j-r-x3	10.622	9.962	9.710	10.068	9.426	9.166
ELQ-j-q-x3′	10.672	10.054	9.721	10.133	9.470	8.887
ELQ-j-r-x3′	10.755	10.132	9.799	10.281	9.593	8.965
ELQ-j-s-x3	10.755	10.132	9.795	12.428	11.425	9.680

Table 6.67. Uncorrected relative energy (ΔE, kcal/mol), relative energy corrected for ZPE ($\Delta E_{corrected}$, kcal/mol) and Gibbs free energy ($\Delta G_{corrected}$, kcal/mol) of the calculated conformers of compound FGP.

The absolute values for the lowest energy conformer for $E_{corrected}$ are -1527.002518/DFT (FGP-m-q-x4) and -1519.306906/HF (FGP-m-r-x4); the absolute free energy of the lowest energy conformer is -1527.065430/DFT (FGP-m-s-x1) and -1519.367799/HF (FGP-m-r-x1).

Conformers	DFT			HF		
	ΔE (kcal/mol)	$\Delta E_{corrected}$ (kcal/mol)	$\Delta G_{corrected}$ (kcal/mol)	ΔE (kcal/mol)	$\Delta E_{corrected}$ (kcal/mol)	$\Delta G_{corrected}$ (kcal/mol)
FGP-m-r-x4	0.000	0.003	0.247	0.000	0.000	0.037
FGP-m-s-x4	0.000	0.003	0.246	2.437	2.078	0.882
FGP-m-q-x4	0.031	0.000	0.137	0.023	0.012	0.066
FGP-m-r-x1	0.334	0.254	0.002	0.426	0.309	0.000
FGP-m-s-x1	0.334	0.254	0.000	2.856	2.381	0.855
FGP-p-q-x4	0.337	0.248	0.003	0.427	0.311	0.004
FGP-p-s-x4	0.337	0.248	0.002	2.843	2.369	0.763

FGP-m-q-x1	0.372	0.293	0.224	0.458	0.329	0.047
FGP-p-r-x4	0.374	0.300	0.131	0.457	0.329	0.045
FGP-k-q-x1	1.163	1.059	0.774	1.837	1.640	0.742
FGP-k-r-x1	1.375	1.239	0.988	2.073	1.849	0.904
FGP-k-r-x1	1.375	1.239	0.990	2.075	1.865	2.623
FGP-g-r-x1	4.949	4.227	3.823	3.327	2.684	2.562
FGP-g-r-x1	4.949	4.227	3.824	3.328	2.682	2.550
FGP-g-q-x1	5.099	4.379	3.998	3.575	2.933	2.818
FGP-j-q-x3	10.679	10.020	9.607	10.006	9.378	9.086
FGP-j-r-x3	10.776	10.090	9.657	10.109	9.461	9.135
FGP-j-s-x3	10.855	10.031	8.875	12.235	11.257	9.871

Table 6.68. Uncorrected relative energy (ΔE, kcal/mol), relative energy corrected for ZPE ($\Delta E_{corrected}$, kcal/mol) and Gibbs free energy ($\Delta G_{corrected}$, kcal/mol) of the calculated conformers of compound FGQ.

The absolute values for the lowest energy conformer for $E_{corrected}$ are (FGQ-m-r-x4) -1487.713259/DFT and -1480.300046/HF; the absolute free energy of the lowest energy conformer is -1487.774004/DFT (FGQ-p-q-x4) and-1480.358905/HF (FGQ-m-r-x1).

Conformers	DFT			HF		
	ΔE (kcal/mol)	$\Delta E_{corrected}$ (kcal/mol)	$\Delta G_{corrected}$ (kcal/mol)	ΔE (kcal/mol)	$\Delta E_{corrected}$ (kcal/mol)	$\Delta G_{corrected}$ (kcal/mol)
FGQ-m-r-x4	0.000	0.000	0.195	0.000	0.000	0.036
FGQ-m-q-x4	0.013	0.019	0.199	0.011	0.003	0.055
FGQ-p-q-x4	0.336	0.270	0.000	0.364	0.299	0.163
FGQ-m-r-x1	0.336	0.270	0.002	0.432	0.314	0.000
FGQ-m-q-x1	0.350	0.280	0.054	0.434	0.307	0.019
FGQ-k-r-x4	1.362	1.245	1.009	1.580	1.487	1.209
FGQ-g-r-x1	4.917	4.229	3.730	3.371	2.726	2.596
FGQ-g-t-x1	4.917	4.227	3.715	5.898	2.934	2.810
FGQ-g-q-x1	5.094	4.395	3.983	3.574	4.920	3.301
FGQ-j-q-x3	10.684	10.046	9.586	10.021	9.393	9.092
FGQ-j-r-x3	10.704	10.053	9.478	10.091	9.444	9.110
FGQ-j-t-x3	10.783	10.014	8.843	12.730	11.736	12.291

Table 6.69. Uncorrected relative energy (ΔE, kcal/mol), relative energy corrected for ZPE ($\Delta E_{corrected}$, kcal/mol) and Gibbs free energy ($\Delta G_{corrected}$, kcal/mol) of the calculated conformers of compound FJP.

The absolute values for the lower energy conformer for $E_{corrected}$ are -1602.208430/DFT (FJP-m-s-x4) and -1594.148625/HF (FJP-m-r-x4); the absolute free energy of the lowest energy conformer is -1602.208353/DFT (FJP-m-s-x4) and -1594.209411/HF (FJP-p-q-x4).

Conformers	DFT			HF		
	ΔE (kcal/mol)	$\Delta E_{corrected}$ (kcal/mol)	$\Delta G_{corrected}$ (kcal/mol)	ΔE (kcal/mol)	$\Delta E_{corrected}$ (kcal/mol)	$\Delta G_{corrected}$ (kcal/mol)
FJP-m-r-x4	0.000	0.001	0.126	0.000	0.000	0.038
FJP-m-s-x4	0.000	0.000	0.118	2.416	2.057	0.850
FJP-m-q-x4	0.081	0.048	0.000	0.026	0.014	0.068
FJP-p-q-x4	0.342	0.264	0.035	0.427	0.309	0.000
FJP-p-s-x4	0.342	0.264	0.032	2.835	2.360	0.815
FJP-k-q-x1	1.184	1.057	0.461	1.853	1.653	0.769
FJP-p-r-x1	1.394	1.254	0.713	0.461	0.332	0.056
FJP-k-r-x1	1.394	1.255	0.722	2.095	1.867	0.941
FJP-k-s-x1	1.394	1.254	0.713	4.424	3.849	1.571
FJP-j-q-x3	18.429	17.463	16.401	17.549	16.670	16.003
FJP-j-r-x3	18.573	17.570	16.464	17.708	16.806	16.097
FJP-j-s-x3	18.573	17.569	16.460	19.802	18.571	16.793

Table 6.70. Uncorrected relative energy (ΔE, kcal/mol), relative energy corrected for ZPE ($\Delta E_{corrected}$, kcal/mol) and Gibbs free energy ($\Delta G_{corrected}$, kcal/mol) of the calculated conformers of compound FJQ.

The absolute values for the lower energy conformer for $E_{corrected}$ are (FJQ-m-r-x4) -1562.908774/DFT and -1555.131432/HF; the absolute free energy of the lowest energy conformer is -1562.970377/DFT (FJQ-p-q-x4) and -1555.190619/HF (FJQ-p-q-x4′).

Conformers	DFT			HF		
	ΔE (kcal/mol)	$\Delta E_{corrected}$ (kcal/mol)	$\Delta G_{corrected}$ (kcal/mol)	ΔE (kcal/mol)	$\Delta E_{corrected}$ (kcal/mol)	$\Delta G_{corrected}$ (kcal/mol)
FJQ-m-q-x4	0.000	0.009	0.315	0.000	0.000	0.042
FJQ-m-r-x4	0.008	0.000	0.169	0.002	0.008	0.033
FJQ-p-r-x4	0.338	0.278	0.126	0.412	0.292	0.002
FJQ-p-q-x4	0.347	0.272	0.000	0.372	0.314	0.167
FJQ-p-q-x4′	0.347	0.272	0.000	0.438	0.326	0.000
FJQ-m-q-x1	0.349	0.297	0.310	0.435	0.316	0.018
FJQ-m-r-x1	0.350	0.272	0.058	0.432	0.321	0.001
FJQ-k-q-x4	1.175	1.092	0.973	1.383	1.319	1.074
FJQ-k-d-r-x4	1.378	1.231	0.872	1.585	1.498	1.205
FJQ-j-q-x3	10.406	9.810	9.270	9.831	9.271	8.908
FJQ-j-r-x3	10.570	9.949	9.431	10.075	9.481	9.039
FJQ-j-r-x3′	10.688	10.045	9.678	10.067	9.429	9.081
FJQ-j-t-x3	10.688	10.045	9.681	12.687	11.707	12.305

FJQ-j-q-x3′	10.717	10.078	9.653	10.062	9.438	9.122

Table 6.71. Uncorrected relative energy (ΔE, kcal/mol), relative energy corrected for ZPE ($\Delta E_{corrected}$, kcal/mol) and Gibbs free energy ($\Delta G_{corrected}$, kcal/mol) of the calculated conformers of compound FLP.

The absolute values for the lower energy conformer for $E_{corrected}$ are (FLP-m-r-x4) -1528.189610/DFT and -1520.446637/HF; the absolute free energy of the lowest energy conformer is -1528.254743/DFT (FLP-p-s-x4) and -1520.508698/HF (FLP-m-r-x1).

Conformers	DFT			HF		
	ΔE (kcal/mol)	$\Delta E_{corrected}$ (kcal/mol)	$\Delta G_{corrected}$ (kcal/mol)	ΔE (kcal/mol)	$\Delta E_{corrected}$ (kcal/mol)	$\Delta G_{corrected}$ (kcal/mol)
FLP-m-r-x4	0.000	0.000	0.211	0.000	0.000	0.039
FLP-m-q-x4	0.034	0.018	0.303	0.026	0.014	0.070
FLP-m-r-x1	0.334	0.262	0.109	0.426	0.309	0.000
FLP-m-s-x4	0.334	0.262	0.117	2.446	2.086	0.868
FLP-m-s-x1	0.334	0.262	0.101	2.865	2.390	0.842
FLP-p-q-x4	0.337	0.253	0.004	0.427	0.310	0.004
FLP-p-s-x4	0.337	0.253	0.000	2.853	2.378	0.730
FLP-m-q-x1	0.378	0.298	0.160	0.461	0.332	0.050
FLP-k-q-x1	1.165	1.082	0.870	1.839	1.642	0.743
FLP-k-r-x1	1.379	1.241	0.949	2.077	1.854	0.909
FLP-k-s-x1	1.379	1.240	0.945	4.439	3.865	1.471
FLP-j-q-x3	10.374	9.839	9.306	9.641	9.041	8.416
FLP-j-r-x3	10.503	9.952	9.567	9.795	9.170	8.498
FLP-j-s-x3′	10.503	9.952	9.564	11.922	10.968	9.208
FLP-j-q-x3′	10.676	10.038	9.721	10.006	9.378	9.088
FLP-j-r-x3′	10.779	10.113	9.749	10.117	9.467	9.136
FLP-j-s-x3	10.779	10.114	9.750	12.236	11.258	9.850

Table 6.72. Uncorrected relative energy (ΔE, kcal/mol), relative energy corrected for ZPE ($\Delta E_{\text{corrected}}$, kcal/mol) and Gibbs free energies ($\Delta G_{\text{corrected}}$, kcal/mol) of the calculated conformers of compound FLQ.

The absolute values for the lower energy conformer for $E_{\text{corrected}}$ are (FLQ-p-q-x2) -1488.900683/DFT and -1481.440145/HF; the absolute free energy of the lowest energy conformer is -1488.963060/DFT (FLQ-p-r-x4′) and -1481.500008/HF (FLQ-m-r-x1).

Conformers	DFT			HF		
	ΔE (kcal/mol)	$\Delta E_{\text{corrected}}$ (kcal/mol)	$\Delta G_{\text{corrected}}$ (kcal/mol)	ΔE (kcal/mol)	$\Delta E_{\text{corrected}}$ (kcal/mol)	$\Delta G_{\text{corrected}}$ (kcal/mol)
FLQ-p-q-x2	0.000	0.000	0.168	0.007	0.000	0.021
FLQ-m-r-x4	0.001	0.006	0.212	0.000	0.003	0.037
FLQ-m-q-x4	0.009	0.004	0.100	0.005	0.000	0.051
FLQ-p-q-x4	0.339	0.284	0.126	0.429	0.314	0.002
FLQ-m-r-x1	0.339	0.286	0.073	0.431	0.316	0.000
FLQ-m-q-x1	0.347	0.287	0.097	0.430	0.306	0.016
FLQ-m-q-x1′	0.347	0.287	0.099	0.432	0.311	0.015
FLQ-p-r-x4	0.353	0.283	0.001	0.370	0.296	0.181
FLQ-p-r-x4′	0.353	0.283	0.000	0.439	0.315	0.031
FLQ-k-q-x4	1.147	1.084	1.027	1.347	1.283	1.060
FLQ-k-q-x1	1.165	1.082	0.681	1.844	1.650	0.736
FLQ-k-r-x4	1.362	1.266	1.101	1.587	1.497	1.214
FLQ-k-r-x1	1.368	1.224	0.764	2.059	1.842	0.893
FLQ-j-q-x3	10.635	9.989	9.409	9.958	9.337	9.037
FLQ-j-r-x3	10.769	10.095	9.474	10.166	9.516	9.174

Table 6.73. ZPE correction to the electronic energy (correction(ZPE), kcal/mol) and thermal correction to the Gibbs free energy (correction(TG), kcal/mol) of the calculated conformers of compound AGP.

Conformers	DFT		HF	
	Correction (ZPE) (kcal/mol)	Correction (TG) (kcal/mol)	Correction (ZPE) (kcal/mol)	Correction (TG) (kcal/mol)
AGP-m-r-u1	298.218	257.436	320.81	281.08
AGP-m-s-u1	298.218	257.435	320.45	279.50
AGP-p-t-u3	298.205	257.392	320.45	279.17
AGP-m-q-u1	298.199	257.382	320.79	281.08
AGP-p-r-u3	298.231	257.611	320.79	281.07
AGP-k-q-u1	298.153	256.893	320.73	280.68
AGP-k-r-u1	298.080	256.341	320.70	280.59
AGP-m-r-u2	298.459	258.452	321.15	282.23
AGP-g-r-u3	297.544	256.408	320.23	280.60
AGP-g-q-u3	297.564	256.528	320.24	280.62
AGP-j-q-u3	297.634	256.416	320.26	280.48
AGP-j-r-u3	297.603	256.488	320.24	280.41
AGP-j-s-u3	297.603	256.489	319.91	279.03

Table 6.74. ZPE correction to the electronic energy (correction(ZPE), kcal/mol) and thermal correction to the Gibbs free energy (correction(TG), kcal/mol) of the calculated conformers of compound AGQ.

Conformers	DFT		HF	
	Correction (ZPE) (kcal/mol)	Correction (TG) (kcal/mol)	Correction (ZPE) (kcal/mol)	Correction (TG) (kcal/mol)
AGQ-m-r-u1	280.370	240.846	301.775	263.318
AGQ-m-q-u1	280.392	241.039	301.763	263.325
AGQ-k-q-u1	280.296	240.148	301.699	262.915
AGQ-k-r-u1	280.244	239.934	301.674	262.834
AGQ-m-r-u2	280.613	241.865	302.114	264.472
AGQ-m-q-u2	280.613	241.924	302.104	264.479
AGQ-g-r-u3	279.747	240.074	301.201	262.840
AGQ-g-t-u3	279.745	240.064	300.869	261.073
AGQ-g-q-u3	279.722	239.956	301.206	262.853
AGQ-j-q-u3	279.811	240.141	301.228	262.705
AGQ-j-r-u3	279.771	239.803	301.210	262.659
AGQ-j-t-u3	279.771	239.803	300.864	263.212

Table 6.75. ZPE correction to the electronic energy (correction(ZPE), kcal/mol) and thermal correction to the Gibbs free energy (correction(TG), kcal/mol) of the calculated conformers of compound AJP.

Conformers	DFT		HF	
	Correction (ZPE) (kcal/mol)	Correction (TG) (kcal/mol)	Correction (ZPE) (kcal/mol)	Correction (TG) (kcal/mol)
AJP-m-r-u1	301.708	260.817	324.999	285.347
AJP-m-s-u1	301.706	260.805	324.640	283.758
AJP-m-q-u1	301.685	260.625	324.984	285.334
AJP-k-q-u1	301.637	260.077	324.920	284.919
AJP-k-r-u1	301.586	259.963	324.893	284.830
AJP-k-s-u1	301.583	259.929	324.546	283.138
AJP-m-r-u2	301.954	261.785	325.336	286.488
AJP-m-s-u2	301.954	261.782	324.976	284.888
AJP-m-q-u2	301.921	261.509	325.323	286.489
AJP-j-q-u3	300.842	259.120	324.201	284.105
AJP-j-r-u3	300.806	259.124	324.177	284.039
AJP-j-s-u3	300.806	259.117	323.849	282.646

Table 6.76. ZPE correction to the electronic energy (correction(ZPE), kcal/mol) and thermal correction to the Gibbs free energy (correction(TG), kcal/mol) of the calculated conformers of compound AJQ.

Conformers	DFT		HF	
	Correction (ZPE) (kcal/mol)	Correction (TG) (kcal/mol)	Correction (ZPE) (kcal/mol)	Correction (TG) (kcal/mol)
AJQ-p-q-u5	283.507	243.422	305.581	266.844
AJQ-m-q-u1	283.502	243.457	305.624	266.922
AJQ-m-q-u2	283.836	244.678	306.056	268.214
AJQ-m-r-u2	283.814	244.363	306.064	268.206
AJQ-p-q-u3	283.423	243.337	305.471	266.370
AJQ-m-r-u1	283.423	243.327	305.411	266.270
AJQ-p-q-u5	283.423	243.328	305.640	266.937
AJQ-m-s-u1	283.413	243.153	305.471	266.363
AJQ-p-r-u3	283.413	243.151	305.134	264.506
AJQ-p-s-u3	283.387	242.968	305.460	266.396
AJQ-m-q-u1	283.387	242.964	305.131	264.711
AJQ-k-q-u1	283.408	243.275	305.459	266.376
AJQ-k-q-u1	283.440	242.891	305.561	266.516
AJQ-k-r-u1	283.312	242.351	305.389	265.920
AJQ-j-q-u1	283.294	242.498	305.365	265.861
AJQ-j-r-u1	283.072	242.694	305.242	266.453
AJQ-p-q-u5	283.022	242.395	305.208	266.346

Table 6.77. ZPE correction to the electronic energy (correction(ZPE), kcal/mol) and thermal correction to the Gibbs free energy (correction(TG), kcal/mol) of the calculated conformers of compound ALP.

Conformers	DFT		HF	
	Correction (ZPE) (kcal/mol)	Correction (TG) (kcal/mol)	Correction (ZPE) (kcal/mol)	Correction (TG) (kcal/mol)
ALP-m-r-u1	310.904	268.757	334.122	293.330
ALP-m-s-u1	310.904	268.753	333.764	291.699
ALP-m-q-u1	310.866	268.617	334.109	293.328
ALP-k-q-u1	310.849	268.267	334.044	292.914
ALP-k-r-u1	310.793	268.043	334.017	292.831
ALP-k-q-u1	310.742	268.271	334.019	293.229
ALP-k-r-u1′	310.681	268.081	333.992	293.150
ALP-k-s-u1	310.682	268.087	333.643	291.366
ALP-k-r-u3	310.673	267.859	333.971	292.721
ALP-m-r-u2	311.116	269.537	334.459	294.477
ALP-m-s-u2	311.116	269.534	334.100	292.836
ALP-m-q-u2	311.108	269.549	334.447	294.480
ALP-j-q-u3	310.211	267.815	333.548	293.027
ALP-j-r-u3	310.180	267.857	333.526	292.961
ALP-j-s-u3	310.179	267.852	333.199	291.560

Table 6.78. ZPE correction to the electronic energy (correction(ZPE), kcal/mol) and thermal correction to the Gibbs free energy (correction(TG), kcal/mol) of the calculated conformers of compound ALQ.

Conformers	DFT		HF	
	Correction (ZPE) (kcal/mol)	Correction (TG) (kcal/mol)	Correction (ZPE) (kcal/mol)	Correction (TG) (kcal/mol)
ALQ-m-r-u1	292.961	252.448	315.083	276.004
ALQ-m-q-u1	292.975	252.633	315.070	276.000
ALQ-k-q-u1	292.865	251.666	315.005	275.585
ALQ-k-r-u1	292.823	251.568	314.981	275.507
ALQ-m-r-u2	293.190	253.428	315.421	277.148
ALQ-m-q-u2	293.161	253.295	315.410	277.154
ALQ-j-q-u3	292.387	251.713	314.535	275.387
ALQ-j-r-u3	292.352	251.433	314.516	275.328
ALQ-j-q-u3	292.175	251.043	314.103	273.869
ALQ-j-r-u3	292.154	250.220	314.083	273.827

Table 6.79. ZPE correction to the electronic energy (correction(ZPE), kcal/mol) and thermal correction to the Gibbs free energy (correction(TG), kcal/mol) of the calculated conformers of compound BGP.

Conformers	DFT		HF	
	Correction (ZPE) (kcal/mol)	Correction (TG) (kcal/mol)	Correction (ZPE) (kcal/mol)	Correction (TG) (kcal/mol)
BGP-p-s-v3	279.594	240.169	300.646	260.914
BGP-p-t-v3	279.594	240.171	300.649	260.647
BGP-m-r-v1	279.600	240.088	301.005	262.560
BGP-m-s-v1	279.600	240.091	300.646	260.963
BGP-m-q-v1	279.599	240.348	300.993	262.560
BGP-k-q-v3	279.541	239.696	300.963	261.977
BGP-k-r-v3	279.503	239.609	300.936	261.904
BGP-k-s-v3	279.503	239.606	300.584	260.076
BGP-m-r-v2	279.791	240.923	301.265	263.402
BGP-m-s-v2	279.791	240.921	300.905	261.800
BGP-m-q-v2	279.770	240.989	301.254	263.406
BGP-g-r-v1	278.870	238.761	300.416	261.993
BGP-g-q-v1	278.882	238.997	300.417	262.008
BGP-j-q-v5	279.010	239.221	300.362	261.928
BGP-j-r-v5	278.977	239.248	300.338	261.863
BGP-j-s-v5	278.977	239.250	300.006	260.463

Table 6.80. ZPE correction to the electronic energy (correction(ZPE), kcal/mol) and thermal correction to the Gibbs free energy (correction(TG), kcal/mol) of the calculated conformers of compound BGQ.

Conformers	DFT		HF	
	Correction (ZPE) (kcal/mol)	Correction (TG) (kcal/mol)	Correction (ZPE) (kcal/mol)	Correction (TG) (kcal/mol)
BGQ-m-r-v1	261.755	223.650	281.973	244.801
BGQ-m-q-v1	261.764	223.716	281.961	244.804
BGQ-k-q-v1	261.701	223.141	281.930	244.205
BGQ-k-r-v1	261.664	223.086	281.905	244.146
BGQ-m-r-v2	261.957	224.440	282.234	245.645
BGQ-m-q-v2	261.940	224.423	282.224	245.651
BGQ-j-q-v3	261.174	222.826	281.414	244.162
BGQ-j-r-v3	261.140	222.569	281.396	244.112
BGQ-j-t-v3	261.140	222.562	281.049	244.662

Table 6.81. ZPE correction to the electronic energy (correction(ZPE), kcal/mol) and thermal correction to the Gibbs free energy (correction(TG), kcal/mol) of the calculated conformers of compound BJP.

Conformers	DFT		HF	
	Correction (ZPE) (kcal/mol)	Correction (TG) (kcal/mol)	Correction (ZPE) (kcal/mol)	Correction (TG) (kcal/mol)
BJP-p-q-v3	283.089	243.554	305.195	266.819
BJP-p-s-v3	283.090	243.557	304.836	265.214
BJP-p-r-v3	283.082	243.500	305.183	266.813
BJP-k-q-v1	283.035	242.941	305.151	266.213
BJP-k-r-v1	283.003	243.055	305.124	266.132
BJP-k-s-v1	283.003	243.050	304.774	264.344
BJP-m-r-v2	283.305	244.444	305.456	267.655
BJP-m-s-v2	283.305	244.446	305.096	266.049
BJP-m-q-v2	283.282	244.370	305.444	267.662
BJP-j-r-v3	282.224	241.986	304.387	265.561
BJP-j-s-v3	282.184	242.014	304.363	265.492
BJP-j-q-v3	282.185	242.015	304.034	264.095

Table 6.82. ZPE correction to the electronic energy (correction(ZPE), kcal/mol) and thermal correction to the Gibbs free energy (correction(TG), kcal/mol) of the calculated conformers of compound BJQ.

Conformers	DFT		HF	
	Correction (ZPE) (kcal/mol)	Correction (TG) (kcal/mol)	Correction (ZPE) (kcal/mol)	Correction (TG) (kcal/mol)
BJQ-p-r-v3	265.030	226.405	285.968	248.517
BJQ-m-s-v1	264.876	226.070	285.502	246.863
BJQ-m-t-v1	264.876	226.072	285.507	246.454
BJQ-m-q-v2	265.209	227.130	286.229	249.370
BJQ-m-r-v2	265.203	226.966	286.239	249.361
BJQ-m-q-v1	264.887	226.206	285.822	248.404
BJQ-p-q-v3	264.798	226.019	285.836	248.415
BJQ-p-q-v3′	264.798	226.014	285.666	247.838
BJQ-p-r-v3	264.767	225.637	285.657	247.871
BJQ-p-s-v3	264.767	225.640	285.328	246.183
BJQ-j-q-v3	264.446	225.552	285.427	247.904
BJQ-j-r-v3	225.365	225.365	285.392	247.795

Table 6.83. ZPE correction to the electronic energy (correction(ZPE), kcal/mol) and thermal correction to the Gibbs free energy (correction(TG), kcal/mol) of the calculated conformers of compound BLP.

Conformers	DFT		HF	
	Correction (ZPE) (kcal/mol)	Correction (TG) (kcal/mol)	Correction (ZPE) (kcal/mol)	Correction (TG) (kcal/mol)
BLP-k-q-v1	292.079	251.014	314.174	274.296
BLP-p-s-v3	292.102	251.368	313.933	273.407
BLP-p-t-v3	292.102	251.366	313.938	273.219
BLP-m-r-v1	292.112	251.331	314.292	275.116
BLP-m-s-v1	292.112	251.333	313.932	273.495
BLP-m-r-v1′	292.080	251.373	314.278	275.112
BLP-k-r-v1	292.034	250.739	314.146	274.221
BLP-k-s-v1	292.034	250.733	313.793	272.329
BLP-p-q-v4	292.302	252.141	314.555	275.964
BLP-p-s-v4	292.302	252.145	314.193	274.250
BLP-p-t-v4	292.302	252.138	314.197	274.032
BLP-p-r-v4	292.291	252.050	314.540	275.960
BLP-j-q-v5	291.544	250.574	313.574	274.250
BLP-j-r-v5	291.516	250.510	313.549	274.182
BLP-j-s-v5	291.515	250.510	313.219	272.761

Table 6.84. ZPE correction to the electronic energy (correction(ZPE), kcal/mol) and thermal correction to the Gibbs free energy (correction(TG), kcal/mol) of the calculated conformers of compound BLQ.

Conformers	DFT		HF	
	Correction (ZPE) (kcal/mol)	Correction (TG) (kcal/mol)	Correction (ZPE) (kcal/mol)	Correction (TG) (kcal/mol)
BLQ-p-q-v3	274.339	235.198	295.279	257.478
BLQ-p-r-v3	274.329	235.152	295.270	295.270
BLQ-p-r-v3	274.324	235.074	295.269	257.476
BLQ-k-q-v1	274.250	234.585	295.237	256.894
BLQ-k-r-v1	274.242	234.693	295.212	256.816
BLQ-m-r-v1	274.162	234.744	294.808	255.542
BLQ-m-q-v1	274.119	234.300	294.806	255.653
BLQ-m-s-v1	274.117	234.276	294.462	256.487
BLQ-p-q-v4	274.524	235.970	295.540	258.319
BLQ-p-r-v4	274.495	235.788	295.530	258.325
BLQ-j-q-v3	273.733	234.120	294.644	256.612
BLQ-j-q-v5	273.734	234.119	294.559	256.611
BLQ-j-r-v3	273.738	234.306	294.625	256.554
BLQ-j-r-v5	273.738	234.302	294.539	256.555
BLQ-j-t-v5	273.738	234.304	294.201	257.191
BLQ-j-t-v3	273.738	234.301	294.287	257.211

Table 6.85. ZPE correction to the electronic energy (correction(ZPE), kcal/mol) and thermal correction to the Gibbs free energy (correction(TG), kcal/mol) of the calculated conformers of compound CGP.

Conformers	DFT		HF	
	Correction (ZPE) (kcal/mol)	Correction (TG) (kcal/mol)	Correction (ZPE) (kcal/mol)	Correction (TG) (kcal/mol)
CGP-p-q-w5	261.140	222.966	281.388	244.134
CGP-p-s-w5	261.140	222.963	281.028	242.450
CGP-p-r-w5	261.149	222.943	281.374	244.131
CGP-m-r-w1	261.128	222.769	281.327	243.862
CGP-m-s-w1	261.129	222.767	280.968	242.282
CGP-m-q-w1	261.104	222.588	281.317	243.874
CGP-m-r-w2	261.263	223.190	281.511	244.442
CGP-m-s-w2	261.263	223.184	281.149	242.816
CGP-m-q-w2	261.241	223.260	281.501	244.451
CGP-g-r-w5	260.664	222.483	280.864	243.755
CGP-g-q-w5	260.670	222.495	280.857	243.751
CGP-j-q-w5	260.654	221.930	280.915	243.609
CGP-j-r-w5	260.650	222.230	280.896	243.560
CGP-j-s-w5	260.651	222.229	280.564	242.156

Table 6.86. ZPE correction to the electronic energy (correction(ZPE), kcal/mol) and thermal correction to the Gibbs free energy (correction(TG), kcal/mol) of the calculated conformers of compound CGQ.

Conformers	DFT		HF	
	Correction (ZPE) (kcal/mol)	Correction (TG) (kcal/mol)	Correction (ZPE) (kcal/mol)	Correction (TG) (kcal/mol)
CGQ-p-q-w5	243.305	206.396	262.355	226.371
CGQ-m-q-w3	243.303	206.397	262.354	226.371
CGQ-p-r-w5	243.297	206.434	262.344	226.375
CGQ-m-r-w1	243.276	206.216	262.296	226.102
CGQ-m-q-w1	243.277	206.211	262.287	226.115
CGQ-j-q-w5	242.843	205.768	261.883	225.845
CGQ-j-r-w5	242.817	205.615	261.865	225.797
CGQ-j-t-w5	242.818	205.619	261.518	226.327

Table 6.87. ZPE correction to the electronic energy (correction(ZPE), kcal/mol) and thermal correction to the Gibbs free energy (correction(TG), kcal/mol) of the calculated conformers of compound CJP.

Conformers	DFT		HF	
	Correction (ZPE) (kcal/mol)	Correction (TG) (kcal/mol)	Correction (ZPE) (kcal/mol)	Correction (TG) (kcal/mol)
CJP-p-q-w3	264.654	226.516	285.577	248.388
CJP-p-s-w3	264.654	226.516	285.218	246.781
CJP-p- r-w3	264.622	226.109	285.564	248.384
CJP-m-r-w1	264.632	226.304	285.518	248.119
CJP-m-r-w2	264.774	226.716	285.700	248.698
CJP-m-s-w2	264.773	226.711	285.340	247.074
CJP-m-t-w2	264.773	226.714	285.343	246.595
CJP-m-q-w2	264.754	226.767	285.691	248.707
CJP-j-q-w1	263.876	224.835	284.855	247.244
CJP-j-r-w1	263.832	224.737	284.832	247.182
CJP-j-s-w1	263.832	224.743	284.502	245.775

Table 6.88. ZPE correction to the electronic energy (correction(ZPE), kcal/mol) and thermal correction to the Gibbs free energy (correction(TG), kcal/mol) of the calculated conformers of compound CJQ.

Conformers	DFT		HF	
	Correction (ZPE) (kcal/mol)	Correction (TG) (kcal/mol)	Correction (ZPE) (kcal/mol)	Correction (TG) (kcal/mol)
CJQ-m-q-w6	246.562	209.157	266.349	230.091
CJQ-m-r-w6	246.566	209.142	266.359	266.359
CJQ-p-q-w5	246.422	208.791	266.218	229.983
CJQ-m-q-w1	246.400	208.838	266.143	229.685
CJQ-p-q-w5	246.332	208.689	266.223	230.001
CJQ-p-q-w5′	246.332	208.686	266.048	229.414
CJQ-p-s-w5	246.290	208.211	265.707	227.734
CJQ-m-r-w1	246.299	208.394	265.988	229.133
CJQ-m-s-w1	246.299	208.393	265.653	227.080
CJQ-m-q-w1′	246.284	208.451	265.983	229.194
CJQ-j-q-w5	246.110	208.473	265.896	229.590
CJQ-j-r-w5	246.075	208.305	265.862	229.482

Table 6.89. ZPE correction to the electronic energy (correction(ZPE), kcal/mol) and thermal correction to the Gibbs free energy (correction(TG), kcal/mol) of the calculated conformers of compound CLP.

Conformers	DFT		HF	
	Correction (ZPE) (kcal/mol)	Correction (TG) (kcal/mol)	Correction (ZPE) (kcal/mol)	Correction (TG) (kcal/mol)
CLP-p-q-w5	273.637	234.074	294.674	256.687
CLP-p-s-w5	273.637	234.070	294.316	254.941
CLP-p-r-w5	273.649	234.082	294.661	256.686
CLP-p-r-w5′	273.649	234.081	294.654	256.678
CLP-m-r-w1	273.635	233.989	294.614	256.418
CLP-m-s-w1	273.635	233.989	294.255	254.809
CLP-m-q-w1	273.619	233.915	294.604	256.422
CLP-m-q-w2	273.778	234.515	294.796	256.990
CLP-m-s-w2	273.777	234.504	294.436	255.350
CLP-m-q-w2	273.725	234.340	294.788	257.006
CLP-j-q-w5	273.305	233.460	294.230	255.860
CLP-j-r-w5	273.292	233.561	294.207	255.791
CLP-j-s-w5	273.292	233.558	293.876	254.365
CLP-j-q-w6	272.857	232.508	293.897	255.504
CLP-j-r-w6	272.843	232.280	293.856	255.377
CLP-j-s-w6	272.840	232.254	293.552	254.053

Table 6.90. ZPE correction to the electronic energy (correction(ZPE), kcal/mol) and thermal correction to the Gibbs free energy (correction(TG), kcal/mol) of the calculated conformers of compound CLQ.

Conformers	DFT		HF	
	Correction (ZPE) (kcal/mol)	Correction (TG) (kcal/mol)	Correction (ZPE) (kcal/mol)	Correction (TG) (kcal/mol)
CLQ-p-q-w5	255.928	217.992	275.611	275.611
CLQ-p-s-w5	255.928	217.991	275.269	236.939
CLQ-m-q-w1	255.857	217.423	275.554	238.361
CLQ-m-q-w1′	255.914	217.923	275.599	238.626
CLQ-m-r-w1′	255.857	217.427	275.561	238.381
CLQ-m-r-w1	255.871	217.610	275.541	238.363
CLQ-m-s-w1	255.857	217.424	275.208	235.972
CLQ-j-q-w5	255.430	217.025	275.144	275.144
CLQ-j-r-w5	255.428	217.095	275.120	238.047
CLQ-j-s-w6	255.427	217.092	274.804	236.583

Table 6.91. ZPE correction to the electronic energy (correction(ZPE), kcal/mol) and thermal correction to the Gibbs free energy (correction(TG), kcal/mol) of the calculated conformers of compound DGP.

Conformers	DFT		HF	
	Correction (ZPE) (kcal/mol)	Correction (TG) (kcal/mol)	Correction (ZPE) (kcal/mol)	Correction (TG) (kcal/mol)
DGP-m-r	239.740	203.124	258.261	222.569
DGP-m-s	239.740	203.122	257.899	220.971
DGP-p-q	239.720	203.029	258.261	222.571
DGP-p-s	239.720	203.024	257.899	220.889
DGP-p-t	239.719	203.027	257.900	220.513
DGP-m-q	239.725	203.088	258.248	222.574
DGP-k-q	239.582	202.195	258.125	221.997
DGP-k-r	239.533	202.051	258.098	221.920
DGP-k-s	239.530	202.018	257.740	220.095
DGP-g-r	239.159	202.345	257.731	222.188
DGP-g-q	239.161	202.342	257.732	222.195
DGP-j-q	239.241	202.409	257.761	222.028
DGP-j-r	239.219	202.306	257.739	221.976
DGP-j-s	239.220	202.312	257.407	220.568

Table 6.92. ZPE correction to the electronic energy (correction(ZPE), kcal/mol) and thermal correction to the Gibbs free energy (correction(TG), kcal/mol) of the calculated conformers of compound DGQ.

Conformers	DFT		HF	
	Correction (ZPE) (kcal/mol)	Correction (TG) (kcal/mol)	Correction (ZPE) (kcal/mol)	Correction (TG) (kcal/mol)
DGQ-m-r	221.907	186.602	239.228	204.815
DGQ-p-q	221.875	186.422	239.227	204.803
DGQ-m-q	221.884	186.537	239.216	204.816
DGQ-m-q′	221.871	186.354	239.218	204.813
DGQ-k-q	221.746	185.744	239.093	204.235
DGQ-k-r	221.705	185.625	239.068	204.168
DGQ-g-r	221.339	185.871	238.697	204.422
DGQ-g-t	221.341	185.877	238.360	204.963
DGQ-g-q	221.343	185.940	238.703	204.434
DGQ-j-q	221.402	185.873	238.728	204.262
DGQ-j-r	221.388	185.836	238.709	204.220
DGQ-j-t	221.388	185.834	238.361	204.715

Table 6.93. ZPE correction to the electronic energy (correction(ZPE), kcal/mol) and thermal correction to the Gibbs free energy (correction(TG), kcal/mol) of the calculated conformers of compound DJP.

Conformers	DFT		HF	
	Correction (ZPE) (kcal/mol)	Correction (TG) (kcal/mol)	Correction (ZPE) (kcal/mol)	Correction (TG) (kcal/mol)
DJP-m-r	243.215	206.295	262.445	226.780
DJP-p-s	243.216	206.297	262.089	225.215
DJP-p-q	243.228	206.590	262.449	226.823
DJP-m-q	243.228	206.591	262.437	226.826
DJP-p-r	243.228	206.591	262.440	226.825
DJP-k-q	243.047	205.300	262.311	226.230
DJP-k-r	243.030	205.450	262.286	226.165
DJP-k-r′	243.030	205.451	262.289	226.176
DJP-k-s	243.030	205.453	261.928	224.361
DJP-j-q	242.409	204.767	261.700	225.660
DJP-j-s	242.395	204.767	261.345	224.186
DJP-j-r	242.394	204.760	261.677	225.603

Table 6.94. ZPE correction to the electronic energy (correction(ZPE), kcal/mol) and thermal correction to the Gibbs free energy (correction(TG), kcal/mol) of the calculated conformers of compound DJQ.

Conformers	DFT		HF	
	Correction (ZPE) (kcal/mol)	Correction (TG) (kcal/mol)	Correction (ZPE) (kcal/mol)	Correction (TG) (kcal/mol)
DJQ-m-q	225.153	189.222	243.233	208.528
DJQ-k-q	225.014	188.550	243.096	207.947
DJQ-k-r	224.972	188.403	243.071	207.862
DJQ-m-r	225.025	189.178	243.091	208.419
DJQ-m-s	225.025	189.176	242.755	206.852
DJQ-m-t	224.882	188.502	242.756	209.091
DJQ-m-s′	225.025	189.175	242.582	205.232
DJQ-m-q	225.001	189.024	243.077	208.415
DJQ-p-q	225.019	189.147	243.091	208.417
DJQ-m-r′	224.909	188.686	242.924	207.866
DJQ-p-q′	224.900	188.679	242.923	207.855
DJQ-p-r	224.894	188.673	242.912	207.878
DJQ-m-q	224.882	188.502	242.914	207.881
DJQ-j-q	224.873	189.086	242.890	208.460
DJQ-j-r	224.846	189.004	242.864	208.387

Table 6.95. ZPE correction to the electronic energy (correction(ZPE), kcal/mol) and thermal correction to the Gibbs free energy (correction(TG), kcal/mol) of the calculated conformers of compound DLP.

Conformers	DFT		HF	
	Correction (ZPE) (kcal/mol)	Correction (TG) (kcal/mol)	Correction (ZPE) (kcal/mol)	Correction (TG) (kcal/mol)
DLP-m-r	252.264	214.392	271.546	235.121
DLP-m-s	252.264	214.395	271.186	233.492
DLP-p-q	252.235	214.266	271.548	235.128
DLP-p-s	252.235	214.265	271.186	233.392
CLP-p-t	252.235	214.266	271.187	235.723
DLP-m-q	252.213	214.204	271.534	235.124
DLP-p-r	252.217	214.183	271.533	235.125
DLP-k-q	252.107	213.507	271.411	234.547
DLP-k-r	252.040	213.240	271.386	234.484
DLP-k-s	252.043	213.295	271.027	232.617
DLP-j-q	251.759	213.676	271.047	234.584
DLP-j-s	251.727	213.567	270.695	233.106
DLP-j-r	251.717	213.569	271.026	234.525

Table 6.96. ZPE correction to the electronic energy (correction(ZPE), kcal/mol) and thermal correction to the Gibbs free energy (correction(TG), kcal/mol) of the calculated conformers of compound DLQ.

Conformers	DFT		HF	
	Correction (ZPE) (kcal/mol)	Correction (TG) (kcal/mol)	Correction (ZPE) (kcal/mol)	Correction (TG) (kcal/mol)
DLQ-p-q	234.452	197.972	252.458	217.257
DLQ-k-q	234.329	197.259	252.323	216.685
DLQ-k-r	234.294	197.119	252.298	216.607
DLQ-m-r	234.474	198.123	252.534	217.483
DLQ-m-q	234.443	197.940	252.523	217.488
DLQ-m-r′	234.225	197.234	252.062	215.546
DLQ-m-q′	234.251	197.411	252.028	217.682
DLQ-j-q	233.977	197.325	251.958	216.713
DLQ-j-r	233.967	197.380	251.940	216.659
DLQ-j-t	233.967	197.379	251.598	217.250

Table 6.97. ZPE correction to the electronic energy (correction(ZPE), kcal/mol) and thermal correction to the Gibbs free energy (correction(TG), kcal/mol) of the calculated conformers of compound EGP.

Conformers	DFT		HF	
	Correction (ZPE) (kcal/mol)	Correction (TG) (kcal/mol)	Correction (ZPE) (kcal/mol)	Correction (TG) (kcal/mol)
EGP-m-r-x4	257.682	219.880	277.355	240.525
EGP-m-s-x4	257.681	219.878	276.995	238.928
EGP-m-q-x4	257.656	219.843	277.345	240.532
EGP-m-r-x1	257.569	219.305	277.239	240.129
EGP-m-s-x1	257.569	219.306	276.880	238.545
EGP-p-q-x3	257.545	219.201	277.238	240.119
EGP-p-s-x3	257.545	219.206	276.881	238.478
EGP-m-q-x1	257.545	219.227	277.228	240.144
EGP-k-q-x1	257.570	219.105	277.146	239.639
EGP-k-r-x2	257.531	219.045	277.237	239.790
EGP-k-q-x1′	257.532	219.054	277.119	239.555
EGP-k-s-x1	257.531	219.049	276.767	237.793
EGP-g-r-x1	257.003	218.800	276.721	239.792
EGP-g-q-x1	256.974	218.644	276.721	239.798
EGP-j-q-x3	257.054	218.790	276.736	239.622
EGP-j-r-x3	257.016	218.728	276.716	239.570
EGP-j-s-x3	257.016	218.727	276.384	238.169

Table 6.98. ZPE correction to the electronic energy (correction(ZPE), kcal/mol) and thermal correction to the Gibbs free energy (correction(TG), kcal/mol) of the calculated conformers of compound EGQ.

Conformers	DFT		HF	
	Correction (ZPE) (kcal/mol)	Correction (TG) (kcal/mol)	Correction (ZPE) (kcal/mol)	Correction (TG) (kcal/mol)
EGQ-m-r-x4	239.825	203.284	258.324	222.769
EGQ-m-q-x4	239.806	203.137	258.315	222.777
EGQ-m-r-x1	239.715	202.641	258.207	222.372
EGQ-m-q-x1	239.705	202.647	258.197	222.386
EGQ-p-q-x3	239.743	202.419	258.263	222.555
EGQ-p-r-x3	239.743	202.591	258.252	222.577
EGQ-k-q-x4	239.736	202.801	258.254	222.439
EGQ-k-r-x4	239.691	202.689	258.229	222.360
EGQ-g-r-x1	239.171	202.315	257.687	222.025
EGQ-g-t-x1	239.169	202.313	257.351	220.056
EGQ-g-q-x1	239.151	202.216	257.691	222.036
EGQ-j-q-x3	239.196	202.070	257.704	221.857
EGQ-j-r-x3	239.188	202.141	257.686	221.807
EGQ-j-t-x3	239.189	202.137	257.337	222.338

Table 6.99. ZPE correction to the electronic energy (correction(ZPE), kcal/mol) and thermal correction to the Gibbs free energy (correction(TG), kcal/mol) of the calculated conformers of compound EJP.

Conformers	DFT		HF	
	Correction (ZPE) (kcal/mol)	Correction (TG) (kcal/mol)	Correction (ZPE) (kcal/mol)	Correction (TG) (kcal/mol)
EJP-m-s-x4	261.166	223.100	281.546	244.783
EJP-m-r-x4	261.165	223.098	281.186	243.179
EJP-m-q-x4	261.149	223.253	281.534	244.788
EJP-p-s-x4	261.149	223.250	281.071	242.782
EJP-p-q-x4	261.055	222.616	281.429	244.385
EJP-p-r-x4	261.053	222.609	281.418	244.405
EJP-k-q-x1	261.044	222.356	281.334	243.885
EJP-k-r-x1	261.021	222.264	281.308	243.809
EJP-k-r-x1′	261.021	222.261	281.309	243.805
EJP-k-s-x1	261.021	222.260	280.955	242.074
EJP-j-q-x3	260.254	221.396	280.676	243.254
EJP-j-r-x3	260.183	221.068	280.653	243.189
EJP-j-s-x3	260.183	221.061	280.322	241.788

Table 6.100. ZPE correction to the electronic energy (correction(ZPE), kcal/mol) and thermal correction to the Gibbs free energy (correction(TG), kcal/mol) of the calculated conformers of compound EJQ.

Conformers	DFT		HF	
	Correction (ZPE) (kcal/mol)	Correction (TG) (kcal/mol)	Correction (ZPE) (kcal/mol)	Correction (TG) (kcal/mol)
EJQ-m-q-x4	243.076	205.992	262.319	226.494
EJQ-m-r-x4	243.086	205.987	262.328	226.482
EJQ-p-q-x4	242.850	205.299	262.070	225.979
EJQ-p-q-x4′	242.722	204.786	261.903	225.421
EJQ-m-r-x1	242.713	204.769	261.903	225.424
EJQ-m-s-x1	242.713	204.766	261.563	226.084
EJQ-p-r-x4	242.726	204.950	261.893	225.466
EJQ-p-s-x4	242.726	204.948	261.561	223.756
EJQ-m-q-x1	242.727	204.946	261.893	225.449
EJQ-k-q-x4	242.748	204.902	261.944	225.437
EJQ-k-r-x4	242.747	204.958	261.920	225.398
EJQ-j-q-x3	242.474	204.889	261.716	225.600
EJQ-j-r-x3	242.438	204.789	261.683	225.494

Table 6.101. ZPE correction to the electronic energy (correction(ZPE), kcal/mol) and thermal correction to the Gibbs free energy (correction(TG), kcal/mol) of the calculated conformers of compound ELP.

Conformers	DFT		HF	
	Correction (ZPE) (kcal/mol)	Correction (TG) (kcal/mol)	Correction (ZPE) (kcal/mol)	Correction (TG) (kcal/mol)
ELP-m-s-x4	270.198	231.128	290.643	253.079
ELP-m-q-x4	270.197	231.126	290.282	251.461
ELP-m-q-x4	270.148	230.880	290.631	253.087
ELP-m-r-x1	270.079	230.561	290.526	252.683
ELP-m-s-x1	270.081	230.564	290.168	251.073
ELP-p-s-x4	270.049	230.350	290.527	252.684
ELP-p-s-x4′	270.050	230.354	290.168	250.962
ELP-m-q-x1	270.062	230.570	290.515	252.699
ELP-k-q-x1	270.091	230.384	290.433	252.196
ELP-k-r-x1	270.030	230.177	290.406	252.117
ELP-k-s-x1	270.030	230.178	290.054	250.316
ELP-j-q-x3	269.676	230.008	290.052	251.871
ELP-j-r-x3	269.639	229.875	290.026	251.802
ELP-j-s-x3	269.640	229.879	289.696	250.380
ELP-j-q-x3′	269.554	229.926	290.023	252.178
ELP-j-r-x3′	269.540	229.963	290.002	252.116
ELP-j-s-x3′	269.540	229.956	289.673	250.707

Table 6.102. ZPE correction to the electronic energy (correction(ZPE), kcal/mol) and thermal correction to the Gibbs free energy (correction(TG), kcal/mol) of the calculated conformers of compound ELQ.

Conformers	DFT		HF	
	Correction (ZPE) (kcal/mol)	Correction (TG) (kcal/mol)	Correction (ZPE) (kcal/mol)	Correction (TG) (kcal/mol)
ELQ-m-r-x4	252.437	215.035	271.630	235.444
ELQ-m-q-x4	252.385	214.764	271.622	235.451
ELQ-m-r-x1	252.269	214.122	271.514	235.047
ELQ-m-q-x1	252.277	214.152	271.504	235.059
ELQ-k-q-x4	252.335	214.466	271.561	235.118
ELQ-k-r-x4	252.280	214.336	271.536	235.030
ELQ-j-q-x3	251.785	213.676	271.014	234.540
ELQ-j-r-x3	251.747	213.533	270.986	234.469
ELQ-j-q-x3′	251.788	213.492	270.965	234.125
ELQ-j-r-x3′	251.783	213.487	270.940	234.055
ELQ-j-s-x3	251.783	213.484	270.626	232.623

Table 6.103. ZPE correction to the electronic energy (correction(ZPE), kcal/mol) and thermal correction to the Gibbs free energy (correction(TG), kcal/mol) of the calculated conformers of compound FGP.

Conformers	DFT		HF	
	Correction (ZPE) (kcal/mol)	Correction (TG) (kcal/mol)	Correction (ZPE) (kcal/mol)	Correction (TG) (kcal/mol)
FGP-m-r-x4	275.515	236.282	296.369	258.195
FGP-m-s-x4	275.515	236.281	296.009	256.602
FGP-m-q-x4	275.482	236.141	296.358	258.201
FGP-m-r-x1	275.433	235.702	296.252	257.731
FGP-m-s-x1	275.433	235.701	295.894	256.157
FGP-p-q-x4	275.424	235.701	296.253	257.734
FGP-p-s-x4	275.424	235.700	295.895	256.078
FGP-m-q-x1	275.434	235.887	296.240	257.747
FGP-p-r-x4	275.438	235.792	296.241	257.746
FGP-k-q-x1	275.408	235.645	296.172	257.063
FGP-k-r-x1	275.377	235.648	296.145	256.989
FGP-k-r-x1	275.377	235.650	296.159	258.705
FGP-g-r-x1	274.791	234.909	295.726	257.392
FGP-g-r-x1	274.791	234.909	295.723	257.380
FGP-g-q-x1	274.792	234.934	295.726	257.400
FGP-j-q-x3	274.854	234.963	295.741	257.238
FGP-j-r-x3	274.826	234.917	295.721	257.184
FGP-j-s-x3	274.688	234.055	295.390	255.795

Table 6.104. ZPE correction to the electronic energy (correction(ZPE), kcal/mol) and thermal correction to the Gibbs free energy (correction(TG), kcal/mol) of the calculated conformers of compound FGQ.

Conformers	DFT		HF	
	Correction (ZPE) (kcal/mol)	Correction (TG) (kcal/mol)	Correction (ZPE) (kcal/mol)	Correction (TG) (kcal/mol)
FGQ-m-r-x4	257.651	219.729	277.337	240.438
FGQ-m-q-x4	257.658	219.719	277.328	240.446
FGQ-p-q-x4	257.585	219.197	277.272	240.202
FGQ-m-r-x1	257.586	219.198	277.220	239.970
FGQ-m-q-x1	257.581	219.237	277.210	239.988
FGQ-k-r-x4	257.534	219.180	277.244	240.031
FGQ-g-r-x1	256.962	218.346	276.692	239.627
FGQ-g-t-x1	256.952	218.421	276.358	237.806
FGQ-g-q-x1	256.961	218.331	276.696	239.638
FGQ-j-q-x3	257.014	218.436	276.708	239.473
FGQ-j-r-x3	256.999	218.307	276.691	239.421
FGQ-j-t-x3	256.883	217.594	276.343	239.964

Table 6.105. ZPE correction to the electronic energy (correction(ZPE), kcal/mol) and thermal correction to the Gibbs free energy (correction(TG), kcal/mol) of the calculated conformers of compound FJP.

Conformers	DFT		HF	
	Correction (ZPE) (kcal/mol)	Correction (TG) (kcal/mol)	Correction (ZPE) (kcal/mol)	Correction (TG) (kcal/mol)
FJP-m-r-x4	279.011	239.708	300.559	262.453
FJP-m-s-x4	279.011	239.701	300.200	260.849
FJP-m-q-x4	278.978	239.502	300.548	262.458
FJP-p-q-x4	278.933	239.275	300.441	261.989
FJP-p-s-x4	278.933	239.273	300.084	260.396
FJP-k-q-x1	278.884	238.859	300.360	261.331
FJP-p-r-x1	278.871	238.901	300.430	262.010
FJP-k-r-x1	278.872	238.910	300.332	261.261
FJP-k-s-x1	278.871	238.901	299.984	259.562
FJP-j-q-x3	278.045	237.555	299.681	260.871
FJP-j-r-x3	278.008	237.473	299.658	260.805
FJP-j-s-x3	278.007	237.469	299.327	259.407

Table 6.106. ZPE correction to the electronic energy (correction(ZPE), kcal/mol) and thermal correction to the Gibbs free energy (correction(TG), kcal/mol) of the calculated conformers of compound FJQ.

Conformers	DFT		HF	
	Correction (ZPE) (kcal/mol)	Correction (TG) (kcal/mol)	Correction (ZPE) (kcal/mol)	Correction (TG) (kcal/mol)
FJQ-m-q-x4	260.884	222.534	281.281	244.183
FJQ-m-r-x4	260.867	222.380	281.288	244.172
FJQ-p-r-x4	260.815	222.007	281.161	243.730
FJQ-p-q-x4	260.800	221.871	281.223	243.935
FJQ-p-q-x4′	260.800	221.871	281.169	243.703
FJQ-m-q-x1	260.823	222.180	281.162	243.723
FJQ-m-r-x1	260.797	221.927	281.170	243.710
FJQ-k-q-x4	260.793	222.016	281.218	243.832
FJQ-k-r-x4	260.727	221.712	281.194	243.760
FJQ-j-q-x3	260.279	221.082	280.722	243.218
FJQ-j-r-x3	260.254	221.080	280.687	243.105
FJQ-j-r-x3′	260.232	221.209	280.643	243.155
FJQ-j-t-x3	260.232	221.211	280.301	243.758
FJQ-j-q-x3′	260.236	221.154	280.657	243.201

Table 6.107. ZPE correction to the electronic energy (correction(ZPE), kcal/mol) and thermal correction to the Gibbs free energy (correction(TG), kcal/mol) of the calculated conformers of compound FLP.

Conformers	DFT		HF	
	Correction (ZPE) (kcal/mol)	Correction (TG) (kcal/mol)	Correction (ZPE) (kcal/mol)	Correction (TG) (kcal/mol)
FLP-m-r-x4	288.006	247.345	309.656	270.751
FLP-m-q-x4	287.991	247.404	309.645	270.756
FLP-m-r-x1	287.934	246.910	309.539	270.286
FLP-m-s-x4	287.934	246.918	309.296	269.135
FLP-m-s-x1	287.934	246.902	309.181	268.690
FLP-p-q-x4	287.922	246.801	309.540	270.289
FLP-p-s-x4	287.922	246.798	309.181	268.590
FLP-m-q-x1	287.927	246.917	309.527	270.300
FLP-k-q-x1	287.924	246.840	309.459	269.616
FLP-k-r-x1	287.868	246.705	309.433	269.544
FLP-k-s-x1	287.868	246.701	309.083	267.744
FLP-j-q-x3	287.471	246.066	309.056	269.488
FLP-j-r-x3	287.456	246.199	309.031	269.415
FLP-j-s-x3′	287.455	246.196	308.702	267.998
FLP-j-q-x3′	287.368	246.179	309.028	269.794
FLP-j-r-x3′	287.340	246.104	309.006	269.732
FLP-j-s-x3	287.340	246.105	308.678	268.326

Table 6.108. ZPE correction to the electronic energy (correction(ZPE), kcal/mol) and thermal correction to the Gibbs free energy (correction(TG), kcal/mol) of the calculated conformers of compound FLQ.

Conformers	DFT		HF	
	Correction (ZPE) (kcal/mol)	Correction (TG) (kcal/mol)	Correction (ZPE) (kcal/mol)	Correction (TG) (kcal/mol)
FLQ-p-q-x2	270.227	231.253	290.633	253.089
FLQ-m-r-x4	287.934	246.918	290.643	253.113
FLQ-m-q-x4	288.006	247.345	290.635	253.122
FLQ-p-q-x4	270.173	230.871	290.526	252.648
FLQ-m-r-x1	270.173	230.819	290.525	252.645
FLQ-m-q-x1	270.167	230.835	290.517	252.661
FLQ-m-q-x1′	270.167	230.837	290.520	252.660
FLQ-p-r-x4	270.157	230.733	290.566	252.887
FLQ-p-r-x4′	270.157	230.733	290.516	252.667
FLQ-k-q-x4	270.165	230.965	290.576	252.788
FLQ-k-q-x1	270.144	230.601	290.446	251.968
FLQ-k-r-x4	270.132	230.825	290.550	252.703
FLQ-k-r-x1	270.084	230.481	290.423	251.910
FLQ-j-q-x3	269.581	229.859	290.020	252.155
FLQ-j-r-x3	269.553	229.790	289.991	252.084

6.1.3. Parameters of the intramolecular hydrogen bonds present in the calculated conformers of the compounds considered.

This section presents the tables reporting the parameters of the intramolecular hydrogen bonds (IHBs) present in the calculated conformers of the compounds considered**.** It can be recalled that the parameters of the IHBs are the following: bond length (H···O), donor-acceptor distance (N···O) and bond angle (NĤO). For each conformer, the IHBs present are indicated individually. When two IHBs have the same donor (H11), it indicates that they are bifurcated on H11. Conformers with no IHBs do not appear in these tables (j conformers).

Table 6.109. Parameters of the hydrogen bonds in the conformers of compound AGP.

Conformers	IHB considered	H···O bond length (Å)		N···O distance (Å)		NĤO bond angle (º)	
		DFT	HF	DFT	HF	DFT	HF
AGP-m-r-u1	H11····O10	2.595	2.506	2.498	2.430	73.20	74.09
	H11····O13	2.388	2.360	2.277	2.235	71.41	70.56
	H14····O9	2.055	2.082	2.867	2.855	135.32	132.87
AGP-m-s-u1	H11····O10	2.595	2.504	2.498	2.430	73.20	74.18
	H11····O13	2.388	2.361	2.277	2.235	71.41	70.49
	H14····O9	2.055	2.087	2.867	2.860	135.32	132.87
AGP-p-t-u3	H11····O9	2.596	2.505	2.499	2.430	73.17	74.17
	H11····O13	2.388	2.362	2.277	2.236	71.42	70.49
	H14····O10	2.054	2.086	2.866	2.858	135.34	132.82
AGP-m-q-u1	H11····O10	2.591	2.499	2.497	2.428	73.34	74.34
	H11····O13	2.390	2.364	2.278	2.236	71.33	70.39
	H14····O9	2.055	2.088	2.869	2.861	135.46	132.94
AGP-p-r-u1	H11····O9	2.591	2.499	2.497	2.428	73.34	74.36
	H11····O13	2.390	2.364	2.278	2.236	71.33	70.39
	H14····O10	2.056	2.088	2.869	2.861	135.44	132.94
AGP-k-q-u1	H11····O13	2.347	2.313	2.276	2.235	73.40	72.95
	H14····O10	1.990	2.026	2.827	2.818	137.95	134.96
AGP-k-r-u1	H11····O13	2.348	2.314	2.277	2.235	73.40	72.93
	H14····O10	1.993	2.031	2.829	2.823	137.87	134.93
AGP-m-r-u2	H11····O10	2.599	2.512	2.499	2.431	73.03	73.87
	H11····O13	2.386	2.354	2.279	2.235	71.57	70.83
	H14····O9	2.040	2.070	2.864	2.853	136.86	134.11
AGP-g-r-u3	H11····O9	2.443	2.394	2.464	2.405	79.27	78.63
AGP-g-q-u3	H11····O9	2.440	2.393	2.464	2.404	79.38	78.67

Table 6.110. Parameters of the hydrogen bonds in the conformers of compound AGQ.

Conformers	IHB considered	H···O bond length (Å)		N···O distance (Å)		NĤO bond angle (°)	
		DFT	HF	DFT	HF	DFT	HF
AGQ-m-r-u1	H11····O10	2.595	2.506	2.498	2.430	73.18	74.08
	H11····O13	2.388	2.360	2.278	2.235	71.42	70.56
	H14····O9	2.054	2.082	2.866	2.854	135.35	132.87
AGQ-m-q-u1	H11····O10	2.590	2.499	2.497	2.428	73.40	74.37
	H11····O13	2.390	2.364	2.278	2.326	71.34	70.40
	H14····O9	2.059	2.089	2.871	2.862	135.38	132.94
AGQ-k-q-u1	H11····O13	2.347	2.313	2.276	2.235	73.41	72.95
	H14····O10	1.991	2.026	2.827	2.819	137.93	134.97
AGQ-k-r-u1	H11····O13	2.348	2.314	2.276	2.235	73.40	72.93
	H14····O10	1.992	2.030	2.829	2.823	137.20	134.93
AGQ-m-r-u2	H11····O10	2.598	2.512	2.499	2.431	73.07	73.86
	H11····O13	2.386	3.354	2.279	2.235	71.58	70.83
	H14····O9	2.041	2.070	2.866	2.853	136.85	134.12
AGQ-m-q-u2	H11····O10	2.594	2.504	2.498	2.429	73.21	74.17
	H11····O13	2.388	2.358	2.279	2.236	71.50	70.67
	H14····O9	2.044	2.078	2.868	2.861	136.88	134.15
AGQ-g-r-u3	H11····O9	2.443	2.390	2.464	2.405	79.28	78.63
AGQ-g-t-u3	H11····O9	2.443	2.394	2.464	2.405	79.28	78.65
AGQ-g-q-u3	H11····O9	2.440	2.392	2.464	2.404	79.38	78.68

Table 6.111. Parameters of the hydrogen bonds in the conformers of compound AJP.

Conformers	IHB considered	H···O bond length (Å)		N···O distance (Å)		NĤO bond angle (°)	
		DFT	HF	DFT	HF	DFT	HF
AJP-m-r-u1	H11····O10	2.595	2.506	2.498	2.430	73.20	74.08
	H11····O13	2.388	2.360	2.278	2.235	71.43	70.56
	H14····O9	2.056	2.083	2.867	2.855	135.25	132.82
AJP-m-s-u1	H11····O10	2.595	2.504	2.498	2.430	73.20	74.19
	H11····O13	2.388	2.361	2.278	2.235	71.43	70.49
	H14····O9	2.056	2.088	2.867	2.860	135.26	132.82
AJP-m-q-u1	H11····O10	2.592	2.499	2.498	2.429	73.34	74.35
	H11····O13	2.390	2.364	2.278	2.236	71.32	70.40
	H14····O9	2.055	2.089	2.868	2.862	135.41	132.87
AJP-k-q-u1	H11····O13	2.347	2.313	2.276	2.235	73.43	72.97
	H14····O10	1.989	2.026	2.826	2.818	137.97	134.96
AJP-k-r-u1	H11····O13	2.347	2.314	2.276	2.235	73.42	72.95
	H14····O10	1.993	2.030	2.829	2.823	137.93	134.93
AJP-k-s-u1	H11····O13	2.347	2.312	2.276	2.235	73.42	72.98
	H14····O10	1.993	2.026	2.829	2.819	137.93	134.93

AJP-m-r-u2	H11····O10	2.598	2.511	2.499	2.431	73.10	73.88
	H11····O13	2.386	2.354	2.279	2.235	71.57	70.83
	H14····O9	2.042	2.071	2.866	2.854	136.80	134.06
AJP-m-s-u2	H11····O10	2.598	2.509	2.499	2.431	73.10	73.99
	H11····O13	2.386	2.355	2.279	2.235	71.57	70.76
	H14····O9	2.042	2.077	2.866	2.859	136.80	134.06
AJP-m-q-u2	H11····O10	2.593	2.504	2.498	2.429	73.27	74.18
	H11····O13	2.388	2.358	2.279	2.236	71.48	70.65
	H14····O9	2.045	2.078	2.869	2.861	136.86	134.11

Table 6.112. Parameters of the hydrogen bonds in the conformers of compound AJQ.

Conformers	IHB considered	H···O bond length (Å)		N···O distance (Å)		NĤO bond angle (º)	
		DFT	HF	DFT	HF	DFT	HF
AJQ-p-q-u5	H11····O9	2.594	2.511	2.498	2.431	73.24	73.87
	H11····O13	2.388	2.360	2.278	2.237	71.42	70.63
	H14····O10	2.057	2.080	2.868	2.854	135.28	133.06
AJQ-m-q-u1	H11····O10	2.592	2.500	2.497	2.429	73.32	74.34
	H11····O13	2.390	2.364	2.278	2.236	71.34	70.39
	H14····O9	2.057	2.089	2.869	2.861	135.36	132.87
AJQ-m-q-u2	H11····O10	2.596	2.504	2.499	2.430	73.17	74.17
	H11····O13	2.388	2.358	2.279	2.236	71.51	70.67
	H14····O9	2.042	2.078	2.867	2.861	136.84	134.10
AJQ-m-r-u2	H11····O10	2.598	2.512	2.499	2.431	73.08	73.85
	H11····O13	2.386	2.354	2.279	2.235	71.58	70.82
	H14····O9	2.042	2.070	2.866	2.853	136.78	134.08
AJQ-p-q-u3	H11····O9	2.595	2.507	2.499	2.430	73.21	74.07
	H11····O13	2.388	2.360	2.278	2.236	71.42	70.57
	H14····O10	2.056	2.083	2.867	2.855	135.25	132.78
AJQ-m-r-u1	H11····O9	2.595	2.511	2.499	2.431	73.21	73.86
	H11····O13	2.388	2.360	2.278	2.237	71.42	70.63
	H14····O10	2.056	2.079	2.867	2.853	135.25	133.06
AJQ-p-q-u5	H11····O9	2.595	2.506	2.499	2.430	73.21	74.09
	H11····O13	2.388	2.360	2.278	2.235	71.42	70.56
	H14····O10	2.056	2.083	2.867	2.855	135.25	132.79
AJQ-m-s-u1	H11····O10	2.594	2.507	2.498	2.430	73.25	74.07
	H11····O13	2.388	2.360	2.278	2.236	71.42	70.57
	H14····O9	2.057	2.083	2.868	2.855	132.26	132.78
AJQ-p-r-u3	H11····O10	2.594	2.504	2.498	2.430	73.24	74.20
	H11····O13	2.388	2.361	2.278	2.235	71.42	70.49
	H14····O9	2.057	2.088	2.868	2.860	135.26	132.79
AJQ-p-s-u3	H11····O9	2.592	2.500	2.498	2.429	73.33	74.35
	H11····O13	2.390	2.364	2.278	2.236	71.35	70.40
	H14····O10	2.058	2.089	2.870	2.862	135.32	132.85
AJQ-m-q-u1	H11····O9	2.592	2.505	2.498	2.431	73.33	74.18
	H11····O13	2.390	2.361	2.278	2.235	71.35	70.49
	H14····O10	2.058	2.088	2.870	2.859	135.32	132.79

AJQ-k-q-u1	H11····O13	2.346	2.313	2.276	2.235	73.44	72.98
	H14····O10	1.991	2.026	2.828	2.819	137.95	134.95
AJQ-k-q-u1	H11····O13	2.346	2.312	2.276	2.235	73.44	72.99
	H14····O10	1.989	2.025	2.826	2.818	137.92	134.96
AJQ-k-r-u1	H11····O13	2.347	2.313	2.276	2.235	73.42	72.96
	H14····O10	1.992	2.031	2.828	2.823	137.93	134.92

Table 6.113. Parameters of the hydrogen bonds in the conformers of compound ALP.

Conformers	IHB considered	H···O bond length (Å)		N···O distance (Å)		NĤO bond angle (º)	
		DFT	HF	DFT	HF	DFT	HF
ALP-m-r-u1	H11····O10	2.595	2.507	2.498	2.430	73.22	74.07
	H11····O13	2.388	2.360	2.278	2.235	71.41	70.56
	H14····O9	2.055	2.082	2.867	2.854	135.34	132.85
ALP-m-s-u1	H11····O10	2.595	2.505	2.498	2.430	73.22	74.18
	H11····O13	2.388	2.361	2.278	2.235	71.42	70.49
	H14····O9	2.055	2.087	2.867	2.860	135.33	132.85
ALP-m-q-u1	H11····O10	2.591	2.499	2.497	2.428	73.37	74.35
	H11····O13	2.390	2.364	2.278	2.236	71.33	70.40
	H14····O9	2.057	2.089	2.870	2.862	135.43	132.91
ALP-k-q-u1	H11····O13	2.347	2.313	2.276	2.235	73.42	72.96
	H14····O10	1.990	2.026	2.827	2.818	137.97	134.97
ALP-k-r-u1	H11····O13	2.348	2.314	2.276	2.235	73.34	72.94
	H14····O10	1.993	2.031	2.829	2.823	137.91	134.93
ALP-k-q-u1	H11····O13	2.347	2.313	2.276	2.235	73.41	72.96
	H14····O10	1.990	2.026	2.827	2.818	137.95	134.97
ALP-k-r-u1′	H11····O13	2.348	2.314	2.277	2.235	73.40	72.93
	H14····O10	1.993	2.030	2.830	2.823	137.91	134.93
ALP-k-s-u1	H11····O13	2.348	2.313	2.277	2.235	73.40	72.97
	H14····O10	1.993	2.026	2.830	2.819	137.91	134.94
ALP-k-r-u3	H11····O13	2.344	2.308	2.275	2.234	73.53	73.14
	H14····O10	1.979	2.008	2.821	2.805	138.47	135.46
ALP-m-r-u2	H11····O10	2.592	2.512	2.499	2.430	73.07	73.87
	H11····O13	2.386	2.354	2.279	2.235	71.57	70.83
	H14····O9	2.041	2.071	2.866	2.853	136.86	134.09
ALP-m-s-u2	H11····O10	2.598	2.510	2.499	2.431	73.07	73.98
	H11····O13	2.386	2.355	2.279	2.235	71.57	70.77
	H14····O9	2.041	2.076	2.866	2.859	136.86	134.09
ALP-m-q-u2	H11····O10	2.593	2.503	2.498	2.429	73.24	74.19
	H11····O13	2.388	2.358	2.279	2.236	71.45	70.66
	H14····O9	2.042	2.078	2.868	2.861	137.02	134.14

Table 6.114. Parameters of the hydrogen bonds in the conformers of compound ALQ.

Conformers	IHB considered	H···O bond length (Å)		N···O distance (Å)		NĤO bond angle (º)	
		DFT	HF	DFT	HF	DFT	HF
ALQ-m-r-u1	H11····O10	2.596	2.506	2.499	2.430	73.17	74.08
	H11····O13	2.388	2.360	2.278	2.236	71.42	70.55
	H14····O9	2.053	2.082	2.866	2.854	135.36	132.87
ALQ-m-q-u1	H11····O10	2.590	2.499	2.497	2.428	73.39	74.37
	H11····O13	2.390	2.364	2.278	2.236	71.34	70.39
	H14····O9	2.059	2.089	2.871	2.862	135.37	132.93
ALQ-k-q-u1	H11····O13	2.347	2.313	2.276	2.235	73.40	72.95
	H14····O10	1.990	2.026	2.827	2.818	137.92	134.97
ALQ-k-r-u1	H11····O13	2.348	2.314	2.276	2.235	73.40	72.93
	H14····O10	1.993	2.030	2.829	2.823	137.90	134.93
ALQ-m-r-u2	H11····O10	2.598	2.512	2.499	2.431	73.09	73.87
	H11····O13	2.386	2.354	2.279	2.235	71.57	70.82
	H14····O9	2.041	2.070	2.866	2.853	136.86	134.11
ALQ-m-q-u2	H11····O10	2.595	2.504	2.498	2.429	73.19	74.17
	H11····O13	2.388	2.358	2.279	2.236	71.51	70.67
	H14····O9	2.043	2.078	2.868	2.861	136.87	134.15

Table 6.115. Parameters of the hydrogen bonds in the conformers of compound BGP.

Conformers	IHB considered	H···O bond length (Å)		N···O distance (Å)		NĤO bond angle (º)	
		DFT	HF	DFT	HF	DFT	HF
BGP-p-s-v3	H11····O9	2.598	2.507	2.499	2.431	73.09	74.09
	H11····O13	2.387	2.360	2.277	2.235	71.44	70.52
	H14····O10	2.047	2.082	2.863	2.856	135.72	133.04
BGP-p-t-v3	H11····O9	2.598	2.507	2.499	2.431	73.09	74.07
	H11····O13	2.387	2.361	2.277	2.236	71.44	70.52
	H14····O10	2.047	2.080	2.863	2.855	135.72	133.01
BGP-m-r-v1	H11····O10	2.598	2.509	2.499	2.431	73.08	73.97
	H11····O13	2.387	2.359	2.277	2.235	71.43	70.59
	H14····O9	2.046	2.076	2.862	2.851	135.77	133.07
BGP-m-s-v1	H11····O10	2.598	2.508	2.499	2.431	73.08	74.07
	H11····O13	2.387	2.360	2.277	2.235	71.43	70.53
	H14····O9	2.046	2.081	2.862	2.855	135.78	133.04
BGP-m-q-v1	H11····O10	2.594	2.502	2.498	2.429	73.25	74.25
	H11····O13	2.389	2.363	2.278	2.236	71.36	70.43
	H14····O9	2.050	2.082	2.866	2.857	135.76	133.12
BGP-k-q-v3	H11····O13	2.346	2.308	2.275	2.233	73.41	73.10
	H14····O10	1.980	2.011	2.822	2.813	138.52	135.91
BGP-k-r-v3	H11····O13	2.346	2.309	2.275	2.233	73.38	73.08
	H14····O10	1.980	2.016	2.822	2.818	138.53	135.87
BGP-k-s-v3	H11····O13	2.346	2.307	2.275	2.232	73.37	73.11
	H14····O10	1.980	2.010	2.822	2.812	138.53	135.92

BGP-m-r-v2	H11····O10	2.600	2.513	2.500	2.432	73.03	73.83
	H11····O13	2.384	2.351	2.278	2.234	71.64	70.94
	H14····O9	2.033	2.061	2.863	2.851	137.43	134.84
BGP-m-s-v2	H11····O10	2.600	2.511	2.500	2.432	73.03	73.93
	H11····O13	2.383	2.352	2.278	2.234	71.64	70.88
	H14····O9	2.033	2.066	2.863	2.856	137.43	134.85
BGP-m-q-v2	H11····O10	2.597	2.505	2.499	2.430	73.13	74.13
	H11····O13	2.385	2.355	2.278	2.235	71.57	70.77
	H14····O9	2.034	2.068	2.864	2.858	137.47	134.91
BGP-g-r-v1	H11····O9	2.439	2.392	2.464	2.405	79.46	78.71
BGP-g-q-v1	H11····O9	2.436	2.391	2.464	2.404	79.61	78.75

Table 6.116. Parameters of the hydrogen bonds in the conformers of compound BGQ.

Conformers	IHB considered	H···O bond length (Å)		N···O distance (Å)		NĤO bond angle (º)	
		DFT	HF	DFT	HF	DFT	HF
BGQ-m-r-v1	H11····O10	2.598	2.509	2.499	2.431	73.08	73.98
	H11····O13	2.387	2.359	2.277	2.235	71.44	70.58
	H14····O9	2.047	2.075	2.863	2.850	135.73	133.08
BGQ-m-q-v1	H11····O10	2.592	2.501	2.498	2.429	73.29	74.23
	H11····O13	2.389	2.363	2.278	2.236	71.36	70.43
	H14····O9	2.051	2.084	2.867	2.859	135.81	133.12
BGQ-k-q-v1	H11····O13	2.346	2.308	2.274	2.233	73.38	73.10
	H14····O10	1.979	2.011	2.821	2.813	138.51	135.93
BGQ-k-r-v1	H11····O13	2.344	2.309	2.275	2.233	73.39	73.08
	H14····O10	1.982	2.016	2.824	2.818	138.50	135.86
BGQ-m-r-v2	H11····O10	2.601	2.513	2.500	2.432	72.99	73.81
	H11····O13	2.383	2.350	2.277	2.234	71.63	70.95
	H14····O9	2.031	2.060	2.861	2.851	137.48	134.86
BGQ-m-q-v2	H11····O10	2.598	2.505	2.499	2.430	73.10	74.12
	H11····O13	2.385	2.354	2.278	2.235	71.58	70.79
	H14····O9	2.033	2.068	2.863	2.858	137.48	134.90

Table 6.117. Parameters of the hydrogen bonds in the conformers of compound BJP.

Conformers	IHB considered	H···O bond length (Å)		N···O distance (Å)		NĤO bond angle (º)	
		DFT	HF	DFT	HF	DFT	HF
BJP-p-q-v3	H11····O9	2.597	2.509	2.499	2.431	73.11	73.98
	H11····O13	2.387	2.359	2.277	2.235	71.45	70.59
	H14····O10	2.049	2.077	2.864	2.851	135.62	133.01
BJP-p-s-v3	H11····O9	2.598	2.507	2.499	2.431	73.11	74.08
	H11····O13	2.387	2.360	2.277	2.235	71.45	70.52
	H14····O10	2.049	2.082	2.864	2.856	135.62	132.98
BJP-p-r-v3	H11····O9	2.594	2.502	2.498	2.429	73.25	74.25

	H11····O13	2.389	2.363	2.278	2.236	71.35	70.42
	H14····O10	2.049	2.083	2.865	2.858	135.74	133.06
BJP-k-q-v1	H11····O13	2.345	2.307	2.274	2.233	73.41	73.13
	H14····O10	1.979	2.011	2.822	2.813	138.52	135.91
BJP-k-r-v1	H11····O13	2.346	2.308	2.275	2.233	73.40	73.11
	H14····O10	1.981	2.016	2.823	2.817	138.52	135.88
BJP-k-s-v1	H11····O13	2.346	2.307	2.275	2.232	73.40	73.13
	H14····O10	1.980	2.010	2.822	2.812	138.53	135.93
BJP-m-r-v2	H11····O10	2.599	2.513	2.500	2.432	73.05	73.84
	H11····O13	2.383	2.351	2.278	2.234	71.65	70.94
	H14····O9	2.034	2.062	2.864	2.852	137.35	134.78
BJP-m-s-v2	H11····O10	2.599	2.511	2.500	2.432	73.06	73.94
	H11····O13	2.383	2.352	2.278	2.234	71.65	70.88
	H14····O9	2.034	2.067	2.864	2.857	137.35	134.80
BJP-m-q-v2	H11····O10	2.596	2.505	2.499	2.430	73.15	74.14
	H11····O13	2.386	2.355	2.278	2.235	71.55	70.77
	H14····O9	2.034	2.068	2.864	2.859	137.43	134.86

Table 6.118. Parameters of the hydrogen bonds in the conformers of compound BJQ.

Conformers	IHB considered	H···O bond length (Å)		N···O distance (Å)		NĤO bond angle (°)	
		DFT	HF	DFT	HF	DFT	HF
BJQ-p-r-v3	H11····O9	2.593	2.502	2.498	2.429	73.26	74.24
	H11····O13	2.389	2.363	2.278	2.236	71.37	70.44
	H14····O10	2.051	2.083	2.867	2.857	135.75	133.07
BJQ-m-s-v1	H11····O10	2.598	2.507	2.499	2.431	73.10	74.09
	H11····O13	2.387	2.360	2.277	2.235	71.45	70.52
	H14····O9	2.048	2.083	2.863	2.856	135.64	132.96
BJQ-m-t-v1	H11····O10	2.598	2.507	2.499	2.431	73.10	74.08
	H11····O13	2.387	2.631	2.277	2.236	71.45	70.52
	H14····O9	2.048	2.082	2.863	2.855	135.63	132.92
BJQ-m-q-v2	H11····O10	2.595	2.504	2.499	2.429	73.21	74.18
	H11····O13	2.385	2.355	2.278	2.234	71.57	70.78
	H14····O9	2.036	2.070	2.866	2.861	137.44	134.86
BJQ-m-r-v2	H11····O10	2.601	2.513	2.500	2.432	73.00	73.83
	H11····O13	2.384	2.351	2.278	2.234	71.64	70.94
	H14····O9	2.033	2.061	2.862	2.851	137.36	134.80
BJQ-m-q-v1	H11····O10	2.595	2.502	2.498	2.429	73.21	74.25
	H11····O13	2.389	2.363	2.278	2.236	71.37	70.42
	H14····O9	2.049	2.083	2.865	2.857	135.73	133.04
BJQ-p-q-v3	H11····O9	2.597	2.509	2.499	2.431	73.13	73.99
	H11····O13	2.387	2.359	2.278	2.235	71.44	70.56
	H14····O10	2.049	2.077	2.864	2.851	135.62	132.98
BJQ-p-q-v3′	H11····O9	2.598	2.509	2.499	2.431	73.12	73.99
	H11····O13	2.387	2.359	2.278	2.235	71.44	70.58
	H14····O10	2.050	2.077	2.864	2.851	135.62	132.99
BJQ-p-r-v3	H11····O9	2.595	2.502	2.498	2.429	73.21	74.26

	H11····O13	2.389	2.363	2.278	2.236	71.38	70.42
	H14····O10	2.050	2.084	2.865	2.858	135.71	133.03
BJQ-p-s-v3	H11····O9	2.595	2.508	2.498	2.431	73.21	74.07
	H11····O13	2.389	2.360	2.278	2.235	71.38	70.52
	H14····O10	2.050	2.082	2.865	2.855	135.70	132.97

Table 6.119. Parameters of the hydrogen bonds in the conformers of compound BLP.

Conformers	IHB considered	H···O bond length (Å)		N···O distance (Å)		NĤO bond angle (°)	
		DFT	HF	DFT	HF	DFT	HF
BLP-k-q-v1	H11····O13	2.346	2.308	2.275	2.233	73.39	73.11
	H14····O10	1.980	2.011	2.822	2.813	138.51	135.91
BLP-p-s-v3	H11····O9	2.598	2.507	2.499	2.431	73.09	74.09
	H11····O13	2.387	2.360	2.277	2.235	71.45	70.53
	H14····O10	2.047	2.082	2.863	2.856	137.71	133.04
BLP-p-t-v3	H11····O9	2.598	2.507	2.499	2.431	73.09	74.08
	H11····O13	2.387	2.361	2.277	2.236	71.44	70.52
	H14····O10	2.047	2.081	2.863	2.855	135.72	133.01
BLP-m-r-v1	H11····O10	2.598	2.509	2.499	2.431	73.09	73.98
	H11····O13	2.387	2.359	2.277	2.235	71.44	70.59
	H14····O9	2.047	2.076	2.863	2.851	135.76	133.06
BLP-m-s-v1	H11····O10	2.598	2.507	2.499	2.431	73.09	74.07
	H11····O13	2.387	2.360	2.277	2.235	71.43	70.53
	H14····O9	2.047	2.081	2.863	2.855	135.77	133.04
BLP-m-r-v1′	H11····O10	2.594	2.502	2.498	2.429	73.23	74.25
	H11····O13	2.389	2.363	2.278	2.236	71.37	70.43
	H14····O9	2.049	2.082	2.865	2.857	135.76	133.12
BLP-k-r-v1	H11····O13	2.347	2.309	2.275	2.233	73.38	73.08
	H14····O10	1.981	2.017	2.823	2.818	138.52	135.87
BLP-k-s-v1	H11····O13	2.347	2.307	2.275	2.232	73.37	73.11
	H14····O10	1.981	2.011	2.823	2.812	138.53	135.91
BLP-p-q-v4	H11····O9	2.599	2.513	2.500	2.432	73.04	73.81
	H11····O13	2.384	2.350	2.278	2.234	71.65	70.96
	H14····O10	2.033	2.061	2.863	2.851	137.42	134.83
BLP-p-s-v4	H11····O9	2.600	2.510	2.500	2.432	73.04	73.95
	H11····O13	2.384	2.352	2.278	2.234	71.65	70.88
	H14····O10	2.033	2.067	2.863	2.857	137.42	134.84
BLP-p-t-v4	H11····O9	2.599	2.511	2.500	2.432	73.05	73.95
	H11····O13	2.384	2.353	2.278	2.234	71.65	70.86
	H14····O10	2.033	2.066	2.863	2.856	137.42	134.77
BLP-p-r-v4	H11····O9	2.597	2.505	2.499	2.430	73.13	74.14
	H11····O13	2.385	2.355	2.278	2.235	71.57	70.78
	H14····O10	2.033	2.068	2.864	2.859	137.48	134.89

Table 6.120 Parameters of the hydrogen bonds in the conformers of compound BLQ.

Conformers	IHB considered	H···O bond length (Å)		N···O distance (Å)		NĤO bond angle (°)	
		DFT	HF	DFT	HF	DFT	HF
BLQ-p-q-v3	H11····O9	2.598	2.509	2.499	2.431	73.08	73.98
	H11····O13	2.387	2.359	2.277	2.235	71.44	70.58
	H14····O10	2.047	2.076	2.863	2.850	135.72	133.06
BLQ-p-r-v3	H11····O9	2.592	2.501	2.498	2.429	73.29	74.28
	H11····O13	2.389	2.363	2.278	2.236	71.37	70.43
	H14····O10	2.051	2.084	2.867	2.859	135.80	133.11
BLQ-p-r-v3	H11····O9	2.594	2.502	2.498	2.429	73.25	74.24
	H11····O13	2.389	2.363	2.278	2.236	71.37	70.44
	H14····O10	2.050	2.082	2.866	2.857	135.78	133.12
BLQ-k-q-v1	H11····O13	2.346	2.308	2.275	2.233	73.39	73.10
	H14····O10	1.980	2.012	2.822	2.813	138.52	135.92
BLQ-k-r-v1	H11····O13	2.346	2.309	2.275	2.233	73.38	73.08
	H14····O10	1.980	2.016	2.822	2.817	138.52	135.87
BLQ-m-s-v1	H11····O10	2.593	2.508	2.498	2.431	73.26	74.06
	H11····O13	2.389	2.360	2.278	2.235	71.36	70.53
	H14····O9	2.049	2.080	2.866	2.855	135.83	133.06
BLQ-m-r-v1	H11····O10	2.597	2.509	2.499	2.431	73.11	73.97
	H11····O13	2.387	2.359	2.277	2.235	71.43	70.59
	H14····O9	2.046	2.075	2.863	2.850	135.82	133.10
BLQ-m-q-v1	H11····O10	2.593	2.502	2.498	2.429	73.26	74.26
	H11····O13	2.389	2.363	2.278	2.236	71.36	70.43
	H14····O9	2.049	2.083	2.866	2.858	135.83	133.14
BLQ-p-q-v4	H11····O9	2.600	2.513	2.500	2.432	73.02	73.82
	H11····O13	2.383	2.351	2.277	2.234	71.63	70.94
	H14····O10	2.032	2.061	2.862	2.851	137.44	134.84
BLQ-p-r-v4	H11····O9	2.595	2.504	2.499	2.429	73.20	74.16
	H11····O13	2.385	2.352	2.278	2.234	73.20	70.78
	H14····O10	2.036	2.069	2.866	2.860	137.46	134.90

Table 6.121. Parameters of the hydrogen bonds in the conformers of compound CGP.

Conformers	IHB considered	H···O bond length (Å)		N···O distance (Å)		NĤO bond angle (º)	
		DFT	HF	DFT	HF	DFT	HF
CGP-p-q-w5	H11····O9	2.587	2.498	2.497	2.428	73.51	74.40
	H11····O13	2.396	2.366	2.277	2.236	70.95	70.29
	H14····O10	2.063	2.098	2.866	2.858	134.38	131.52
CGP-p-s-w5	H11····O9	2.587	2.496	2.497	2.428	73.52	74.54
	H11····O13	2.396	2.367	2.277	2.236	70.95	70.20
	H14····O10	2.063	2.104	2.866	2.864	134.38	131.63
CGP-p-r-w5	H11····O9	2.583	2.491	2.496	2.427	73.67	74.69
	H11····O13	2.399	2.370	2.277	2.237	70.85	70.08
	H14····O10	2.065	2.104	2.869	2.865	134.52	131.71
CGP-m-r-w1	H11····O10	2.607	2.521	2.501	2.433	72.71	73.47
	H11····O13	2.389	2.356	2.282	2.237	71.59	70.85
	H14····O9	2.033	2.059	2.858	2.844	136.80	134.29
CGP-m-s-w1	H11····O10	2.607	2.519	2.501	2.433	72.70	73.59
	H11····O13	2.389	2.358	2.282	2.237	71.59	70.78
	H14····O9	2.033	2.064	2.858	2.849	136.81	134.32
CGP-m-q-w1	H11····O10	2.604	2.512	2.500	2.431	72.82	73.80
	H11····O13	2.391	2.361	2.282	2.238	71.50	70.68
	H14····O9	2.033	2.065	2.859	2.851	136.88	134.39
CGP-m-r-w2	H11····O10	2.603	2.512	2.501	2.431	72.88	73.84
	H11····O13	2.384	2.352	2.280	2.234	71.73	70.92
	H14····O9	2.025	2.058	2.852	2.845	137.10	134.38
CGP-m-s-w2	H11····O10	2.604	2.511	2.501	2.432	72.87	73.93
	H11····O13	2.384	2.353	2.280	2.234	71.73	70.85
	H14····O9	2.025	2.063	2.852	2.849	137.11	134.36
CGP-m-q-w2	H11····O10	2.600	2.505	2.500	2.430	72.99	74.14
	H11····O13	2.386	2.356	2.280	2.235	71.66	70.75
	H14····O9	2.026	2.065	2.854	2.852	137.15	134.42
CGP-g-r-w5	H11····O9	2.438	2.389	2.470	2.406	79.81	78.99
CGP-g-q-w5	H11····O9	2.435	2.386	2.470	2.406	79.95	79.10

Table 6.122. Parameters of the hydrogen bonds in the conformers of compound CGQ.

Conformers	IHB considered	H···O bond length (Å)		N···O distance (Å)		NĤO bond angle (º)	
		DFT	HF	DFT	HF	DFT	HF
CGQ-p-q-w5	H11····O9	2.587	2.498	2.497	2.428	73.53	74.42
	H11····O13	2.397	2.366	2.277	2.236	70.94	70.27
	H14····O10	2.063	2.098	2.866	2.858	134.41	131.55
CGQ-m-q-w3	H11····O10	2.587	2.498	2.497	2.428	73.53	74.40
	H11····O13	2.397	2.366	2.277	2.236	70.93	70.27
	H14····O9	2.062	2.097	2.866	2.857	134.46	131.57
CGQ-p-r-w5	H11····O9	2.582	2.491	2.495	2.427	73.72	74.70
	H11····O13	2.399	2.370	2.277	2.237	70.85	70.09
	H14····O10	2.067	2.105	2.871	2.866	134.49	131.71
CGQ-m-q-w1	H11····O10	2.602	2.512	2.500	2.431	72.89	73.82
	H11····O13	2.391	2.360	2.282	2.238	71.51	70.69
	H14····O9	2.036	2.067	2.861	2.852	136.87	134.38
CGQ-m-r-w1	H11····O10	2.607	2.521	2.501	2.433	72.72	73.46
	H11····O13	2.389	2.357	2.282	2.238	71.58	70.85
	H14····O9	2.033	2.058	2.858	2.844	136.80	134.30

Table 6.123. Parameters of the hydrogen bonds in the conformers of compound CJP.

Conformers	IHB considered	H···O bond length (Å)		N···O distance (Å)		NĤO bond angle (º)	
		DFT	HF	DFT	HF	DFT	HF
CJP-p-q-w3	H11····O9	2.587	2.489	2.497	2.428	73.53	74.40
	H11····O13	2.396	2.366	2.277	2.236	70.94	70.29
	H14····O10	2.064	2.099	2.867	2.858	134.36	131.48
CJP-p-s-w3	H11····O9	2.587	2.496	2.497	2.429	73.53	74.54
	H11····O13	2.396	2.367	2.277	2.236	73.53	70.19
	H14····O10	2.064	2.104	2.867	2.864	134.36	131.58
CJP-p- r-w3	H11····O9	2.582	2.491	2.495	2.427	73.73	74.68
	H11····O13	2.399	2.370	2.277	2.237	70.83	70.08
	H14····O10	2.066	2.104	2.870	2.865	134.48	131.64
CJP-m-r-w1	H11····O10	2.607	2.521	2.501	2.433	72.71	73.47
	H11····O13	2.389	2.356	2.282	2.237	71.59	70.85
	H14····O9	2.033	2.059	2.858	2.844	136.75	134.25
CJP-m-r-w2	H11····O10	2.603	2.512	2.501	2.432	72.90	73.84
	H11····O13	2.384	2.352	2.280	2.234	71.74	70.91
	H14····O9	2.027	2.059	2.854	2.845	137.10	134.31
CJP-m-s-w2	H11····O10	2.603	2.511	2.501	2.432	72.90	73.94
	H11····O13	2.384	2.353	2.280	2.234	71.74	70.85
	H14····O9	2.027	2.064	2.854	2.849	137.02	134.29
CJP-m-t-w2	H11····O10	2.603	2.510	2.500	2.432	72.90	73.98
	H11····O13	2.384	2.354	2.280	2.235	71.74	70.82
	H14····O9	2.027	2.065	2.854	2.850	137.01	134.22
CJP-m-q-w2	H11····O10	2.600	2.505	2.500	2.430	73.01	74.14

	H11····O13	2.386	2.356	2.280	2.235	71.65	70.75
	H14····O9	2.027	2.066	2.854	2.852	137.05	134.36

Table 6.124. Parameters of the hydrogen bonds in the conformers of compound CJQ.

Conformers	IHB considered	H···O bond length (Å)		N···O distance (Å)		NĤO bond angle (º)	
		DFT	HF	DFT	HF	DFT	HF
CJQ-m-q-w6	H11····O10	2.582	2.491	2.495	2.427	73.73	74.71
	H11····O13	2.399	2.370	2.277	2.237	70.85	70.09
	H14····O9	2.068	2.106	2.871	2.866	134.43	131.67
CJQ-m-r-w6	H11····O10	2.587	2.498	2.497	2.428	73.53	74.41
	H11····O13	2.397	2.366	2.277	2.236	70.93	70.26
	H14····O9	2.063	2.098	2.866	2.858	134.37	131.50
CJQ-p-q-w5	H11····O9	2.586	2.498	2.497	2.428	73.58	74.43
	H11····O13	2.396	2.366	2.277	2.236	70.94	70.28
	H14····O10	2.066	2.100	2.868	2.859	134.34	131.43
CJQ-m-q-w1	H11····O10	2.604	2.513	2.500	2.431	72.82	73.80
	H11····O13	2.391	2.360	2.282	2.238	71.51	70.68
	H14····O9	2.035	2.067	2.859	2.852	136.78	134.25
CJQ-p-q-w5	H11····O9	2.587	2.499	2.497	2.429	73.54	74.37
	H11····O13	2.396	2.365	2.277	2.236	70.95	70.31
	H14····O10	2.064	2.100	2.867	2.858	134.33	131.41
CJQ-p-q-w5′	H11····O9	2.587	2.498	2.497	2.429	73.54	74.41
	H11····O13	2.396	2.366	2.277	2.236	70.94	70.28
	H14····O10	2.065	2.100	2.867	2.858	134.32	131.43
CJQ-p-s-w5	H11····O9	2.583	2.496	2.496	2.429	73.67	74.52
	H11····O13	2.399	2.367	2.277	2.236	70.86	70.20
	H14····O10	2.066	2.104	2.869	2.863	134.38	131.54
CJQ-m-r-w1	H11····O10	2.607	2.521	2.501	2.433	72.72	73.47
	H11····O13	2.389	2.357	2.282	2.237	71.59	70.84
	H14····O9	2.034	2.060	2.858	2.844	136.74	134.23
CJQ-m-s-w1	H11····O10	2.607	2.518	2.501	2.433	72.71	73.61
	H11····O13	2.389	2.358	2.282	2.237	71.59	70.77
	H14····O9	2.034	2.065	2.8`58	2.850	136.74	134.27
CJQ-m-q-w1′	H11····O10	2.605	2.512	2.500	2.431	72.81	73.81
	H11····O13	2.391	2.631	2.282	2.238	71.52	70.69
	H14····O9	2.035	2.068	2.859	2.852	136.78	134.26

Table 6.125. Parameters of the hydrogen bonds in the conformers of compound CLP.

Conformers	IHB considered	H···O bond length (Å)		N···O distance (Å)		NĤO bond angle (º)	
		DFT	HF	DFT	HF	DFT	HF
CLP-p-q-w5	H11····O9	2.587	2.498	2.497	2.428	73.51	74.41
	H11····O13	2.396	2.366	2.277	2.236	70.95	70.28
	H14····O10	2.063	2.098	2.867	2.858	134.37	131.53
CLP-p-s-w5	H11····O9	2.587	2.496	2.497	2.428	73.51	74.54
	H11····O13	2.396	2.367	2.277	2.236	70.96	70.20
	H14····O10	0.063	2.104	2.866	2.864	134.37	131.62
CLP-p-r-w5	H11····O9	2.583	2.491	2.496	2.427	73.67	74.69
	H11····O13	2.399	2.370	2.277	2.237	70.85	70.08
	H14····O10	2.064	2.104	2.869	2.865	134.53	131.70
CLP-p-r-w5′	H11····O9	2.583	2.490	2.496	2.426	73.67	74.73
	H11····O13	2.399	2.371	2.277	2.237	70.85	70.04
	H14····O10	2.064	2.103	2.869	2.865	134.53	131.73
CLP-m-r-w1	H11····O10	2.607	2.521	2.501	2.433	72.72	73.47
	H11····O13	2.389	2.356	2.282	2.237	71.60	70.85
	H14····O9	2.034	2.059	2.858	2.844	136.80	134.29
CLP-m-s-w1	H11····O10	2.607	2.519	2.501	2.358	72.71	73.59
	H11····O13	2.389	2.358	2.282	2.237	71.60	70.78
	H14····O9	2.033	2.064	2.858	2.849	136.80	134.32
CLP-m-q-w1	H11····O10	2.604	2.513	2.500	2.431	72.81	73.79
	H11····O13	2.391	2.360	2.282	2.238	71.50	70.69
	H14····O9	2.032	2.065	2.858	2.851	136.89	134.37
CLP-m-q-w2	H11····O10	2.603	2.512	2.501	2.431	72.88	73.84
	H11····O13	2.384	2.352	2.280	2.234	71.73	70.92
	H14····O9	2.025	2.058	2.853	2.845	137.09	134.40
CLP-m-s-w2	H11····O10	2.603	2.511	2.501	2.432	72.88	73.93
	H11····O13	2.384	2.353	2.280	2.234	71.73	70.85
	H14····O9	2.025	2.063	2.853	2.849	137.10	134.35
CLP-m-q-w2	H11····O10	2.600	2.505	2.500	2.430	73.00	74.14
	H11····O13	2.386	2.356	2.280	2.235	71.66	70.75
	H14····O9	2.026	2.065	2.854	2.852	137.14	134.41

Table 6.126. Parameters of the hydrogen bonds in the conformers of compound CLQ.

Conformers	IHB considered	H···O bond length (Å)		N···O distance (Å)		NĤO bond angle (º)	
		DFT	HF	DFT	HF	DFT	HF
CLQ-p-q-w5	H11····O9	2.587	2.498	2.497	2.428	73.51	74.42
	H11····O13	2.396	2.366	2.277	2.236	70.94	70.28
	H14····O10	2.063	2.099	2.866	2.858	134.39	131.51
CLQ-p-s-w5	H11····O9	2.587	2.496	2.497	2.428	73.51	74.54
	H11····O13	2.396	2.367	2.277	2.236	70.95	70.20
	H14····O10	2.063	2.104	2.866	2.864	134.38	131.60
CLQ-m-q-w1	H11····O10	2.608	2.521	2.501	2.433	72.70	73.47
	H11····O13	2.389	2.356	2.282	2.237	71.58	70.85
	H14····O9	2.032	2.059	2.857	2.844	136.79	134.27
CLQ-m-q-w1′	H11····O10	2.584	2.491	2.496	2.427	73.64	74.68
	H11····O13	2.399	2.370	2.277	2.237	70.84	70.08
	H14····O9	2.063	2.104	2.867	2.865	134.51	131.68
CLQ-m-r-w1′	H11····O10	2.608	2.523	2.501	2.433	72.70	73.39
	H11····O13	2.389	2.355	2.282	2.238	71.58	70.92
	H14····O9	2.032	2.060	2.857	2.844	136.79	134.18
CLQ-m-r-w1	H11····O10	2.603	2.513	2.500	2.431	72.85	73.79
	H11····O13	2.391	2.360	2.282	2.238	71.49	70.68
	H14····O9	2.034	2.065	2.859	2.851	136.87	134.37
CLQ-m-s-w1	H11····O10	2.607	2.518	2.501	2.433	72.70	73.61
	H11····O13	2.389	2.358	2.282	2.237	71.58	70.78
	H14····O9	2.032	2.064	2.857	2.849	136.79	134.31

Table 6.127. Parameters of the hydrogen bonds in the conformers of compound DGP.

Conformers	IHB considered	H···O bond length (Å)		N···O distance (Å)		NĤO bond angle (º)	
		DFT	HF	DFT	HF	DFT	HF
DGP-m-r	H11····O10	2.599	2.511	2.499	2.431	73.03	73.89
	H11····O13	2.397	2.365	2.280	2.237	71.10	70.38
	H14····O9	2.050	2.080	2.856	2.845	134.71	132.14
DGP-m-s	H11····O10	2.599	2.509	2.499	2.431	73.03	74.00
	H11····O13	2.397	2.367	2.280	2.237	71.10	70.31
	H14····O9	2.050	2.085	2.856	2.850	134.72	132.16
DGP-p-q	H11····O9	2.559	2.511	2.499	2.431	73.03	73.88
	H11····O13	2.397	2.365	2.280	2.237	71.11	70.38
	H14····O10	2.051	2.080	2.856	2.845	134.68	132.14
DGP-p-s	H11····O9	2.599	2.509	2.499	2.431	73.03	74.01
	H11····O13	2.397	2.367	2.280	2.237	71.11	70.31
	H14····O10	2.051	2.086	2.856	2.850	134.70	132.15
DGP-p-t	H11····O9	2.599	2.508	2.499	2.431	73.03	74.02
	H11····O13	2.397	2.367	2.280	2.238	71.10	70.29
	H14····O10	2.051	2.085	2.856	2.849	134.69	132.10
DGP-m-q	H11····O10	2.595	2.503	2.498	2.429	73.19	74.19

	H11····O13	2.399	2.370	2.280	2.238	71.01	70.20
	H14····O9	2.052	2.087	2.858	2.852	134.81	132.22
DGP-k-q	H11····O13	2.358	2.320	2.280	2.237	73.08	72.75
	H14····O10	1.980	2.019	2.810	2.806	137.24	134.33
DGP-k-r	H11····O13	2.358	2.321	2.280	2.238	73.06	72.73
	H14····O10	1.981	2.023	2.810	2.809	137.24	134.31
DGP-k-s	H11····O13	2.359	2.319	2.280	2.237	73.05	72.76
	H14····O10	1.981	2.019	2.811	2.805	137.23	134.31
DGP-g-r	H11····O9	2.446	2.396	2.465	2.405	79.13	73.52
DGP-g-q	H11····O9	2.445	2.395	2.464	2.405	79.19	78.56

Table 6.128. Parameters of the hydrogen bonds in the conformers of compound DGQ.

Conformers	IHB considered	H···O bond length (Å)		N···O distance (Å)		NĤO bond angle (º)	
		DFT	HF	DFT	HF	DFT	HF
DGQ-m-r	H11····O10	2.598	2.511	2.499	2.431	73.07	73.88
	H11····O13	2.397	2.365	2.280	2.237	71.09	70.37
	H14····O9	2.050	2.079	2.856	2.845	134.76	132.08
DGQ-p-q	H11····O9	2.598	2.511	2.499	2.431	73.06	73.90
	H11····O13	2.397	2.366	2.280	2.237	71.10	70.37
	H14····O10	2.051	2.080	2.856	2.845	134.72	132.16
DGQ-m-q	H11····O10	2.594	2.502	2.498	2.429	73.20	74.21
	H11····O13	2.399	2.370	2.280	2.238	71.02	70.21
	H14····O9	2.052	2.088	2.859	2.853	134.80	132.23
DGQ-m-q′	H11····O10	2.595	2.503	2.498	2.429	73.17	74.18
	H11····O13	2.399	2.369	2.280	2.238	71.02	70.21
	H14····O9	2.051	2.087	2.857	2.852	134.82	132.22
DGQ-k-q	H11····O13	2.358	2.320	2.280	2.237	73.08	72.75
	H14····O10	1.981	2.019	2.811	2.806	137.24	134.34
DGQ-k-r	H11····O13	2.358	2.321	2.280	2.238	73.07	72.73
	H14····O10	1.981	2.024	2.810	2.810	137.23	134.29
DGQ-g-r	H11····O9	2.446	2.396	2.465	2.405	79.14	78.51
DGQ-g-t	H11····O9	2.446	2.396	2.465	2.405	79.13	78.53
DGQ-g-q	H11····O9	2.445	2.395	2.465	2.405	79.20	78.56

Table 6.129. Parameters of the hydrogen bonds in the conformers of compound DJP.

Conformers	IHB considered	H···O bond length (Å)		N···O distance (Å)		NĤO bond angle (º)	
		DFT	HF	DFT	HF	DFT	HF
DJP-m-r	H11····O10	2.598	2.513	2.499	2.431	73.08	73.81
	H11····O13	2.397	2.364	2.280	2.236	71.10	70.39
	H14····O9	2.052	2.076	2.857	2.842	134.66	132.27
DJP-p-s	H11····O9	2.598	2.509	2.499	2.431	73.08	74.16
	H11····O13	2.397	2.367	2.280	2.237	71.10	70.30
	H14····O10	2.052	2.086	2.857	2.850	134.66	132.10
DJP-p-q	H11····O9	2.595	2.511	2.498	2.431	73.18	73.91
	H11····O13	2.399	2.366	2.280	2.237	71.02	70.37
	H14····O10	2.052	2.081	2.858	2.845	134.76	132.10
DJP-m-q	H11····O10	2.595	2.503	2.498	2.429	73.17	74.19
	H11····O13	2.399	2.370	2.280	2.238	71.02	70.20
	H14····O9	2.052	2.087	2.858	2.852	134.76	132.17
DJP-p-r	H11····O9	2.595	2.504	2.498	2.429	73.17	74.17
	H11····O13	2.399	2.369	2.280	2.238	71.02	70.22
	H14····O10	2.052	2.088	2.858	2.852	134.76	132.14
DJP-k-q	H11····O13	2.357	2.319	2.280	2.237	73.10	72.77
	H14····O10	7.980	2.019	2.810	2.805	137.25	134.32
DJP-k-r	H11····O13	2.358	2.320	2.280	2.238	73.08	72.47
	H14····O10	1.981	2.024	2.810	2.809	137.25	134.29
DJP-k-r′	H11····O13	2.358	2.320	2.280	2.238	73.08	72.75
	H14····O10	1.981	2.025	2.810	2.810	137.25	134.28
DJP-k-s	H11····O13	2.358	2.319	2.280	2.237	73.07	72.77
	H14····O10	1.982	2.018	2.811	2.804	137.22	134.31

Table 6.130. Parameters of the hydrogen bonds in the conformers of compound DJQ.

Conformers	IHB considered	H···O bond length (Å)		N···O distance (Å)		NĤO bond angle (º)	
		DFT	HF	DFT	HF	DFT	HF
DJQ-m-q	H11····10	2.598	2.511	2.499	2.431	73.07	73.88
	H11····O13	2.397	2.366	2.280	2.237	71.08	70.37
	H14····O9	2.054	2.079	2.857	2.844	134.63	132.13
DJQ-k-q	H11····O13	2.358	2.320	2.280	2.237	73.08	72.75
	H14····O10	1.979	2.019	2.809	2.805	137.26	134.33
DJQ-m-r	H11····O10	2.599	2.510	2.499	2.431	73.06	73.93
	H11····O13	2.397	2.366	2.280	2.237	71.11	70.36
	H14····O9	2.052	2.082	2.857	2.846	134.60	132.07
DJQ-k-r	H11····O13	2.358	2.320	2.280	2.238	73.08	72.75
	H14····O10	1.980	2.023	2.810	2.809	137.26	134.30
DJQ-m-s	H11····O10	2.599	2.508	2.499	2.431	73.05	74.02
	H11····O13	2.397	2.367	2.280	2.237	71.11	70.30
	H14····O9	2.052	2.087	2.857	2.851	134.62	132.08
DJQ-m-t	H11····O10	2.599	2.509	2.499	2.431	73.05	74.02
	H11····O13	2.396	2.367	2.280	2.238	71.11	70.29

	H14····O9	2.052	2.086	2.857	2.850	134.60	132.01
DJQ-m-s′	H11····O10	2.599	2.508	2.499	2.431	73.06	74.03
	H11····O13	2.397	2.367	2.280	2.237	71.11	70.30
	H14····O9	2.052	2.086	2.857	2.851	134.61	132.08
DJQ-m-q	H11····O10	2.595	2.503	2.498	2.429	73.17	74.19
	H11····O13	2.398	2.370	2.280	2.238	71.03	70.20
	H14····O9	2.053	2.087	2.858	2.852	134.71	132.15
DJQ-p-q	H11····O9	2.598	2.510	2.499	2.431	73.07	73.92
	H11····O13	2.397	2.366	2.280	2.237	71.11	70.37
	H14····O10	2.053	2.082	2.857	2.846	134.61	132.07
DJQ-m-r′	H11····O10	2.598	2.511	2.499	2.431	73.07	73.89
	H11····O13	2.397	2.365	2.280	2.237	71.10	70.38
	H14····O9	2.052	2.081	2.857	2.845	134.63	132.06
DJQ-p-q′	H11····O9	2.597	2.511	2.499	2.431	73.11	73.90
	H11····O13	2.397	2.365	2.280	2.237	71.10	70.37
	H14····O10	2.054	2.081	2.858	2.846	134.62	132.06
DJQ-p-r	H11····O9	2.595	2.503	2.498	2.429	73.19	74.20
	H11····O13	2.398	2.370	2.280	2.238	71.03	70.20
	H14····O10	2.054	2.088	2.859	2.853	134.67	132.12
DJQ-m-q	H11····O10	2.596	2.503	2.498	2.429	73.16	74.18
	H11····O13	2.398	2.369	2.280	2.238	71.04	70.21
	H14····O9	2.053	2.088	2.858	2.852	134.66	132.12

Table 6.131. Parameters of the hydrogen bonds in the conformers of compound DLP.

Conformers	IHB considered	H···O bond length (Å)		N···O distance (Å)		NĤO bond angle (º)	
		DFT	HF	DFT	HF	DFT	HF
DLP-m-r	H11····O10	2.599	2.510	2.499	2.431	73.03	73.91
	H11····O13	2.397	2.366	2.280	2.237	71.10	70.37
	H14····O9	2.050	2.080	2.856	2.845	134.72	132.15
DLP-m-s	H11····O10	2.599	2.509	2.499	2.431	73.03	74.01
	H11····O13	2.397	2.367	2.280	2.237	71.10	70.31
	H14····O9	2.050	2.085	2.856	2.850	134.72	132.16
DLP-p-q	H11····O9	2.600	2.511	2.499	2.431	73.01	73.89
	H11····O13	2.397	2.365	2.280	2.237	71.11	70.38
	H14····O10	2.050	2.080	2.855	2.845	134.69	132.13
DLP-p-s	H11····O9	2.600	2.508	2.499	2.431	73.01	74.02
	H11····O13	2.397	2.367	2.280	2.237	71.11	70.31
	H14····O10	2.050	2.086	2.855	2.851	134.70	132.15
CLP-p-t	H11····O9	2.599	2.508	2.499	2.431	73.01	74.02
	H11····O13	2.396	2.367	2.280	2.238	71.11	70.29
	H14····O10	2.050	2.085	2.855	2.849	134.71	132.09
DLP-m-q	H11····O10	2.595	2.503	2.498	2.429	73.19	74.19
	H11····O13	2.399	2.370	2.280	2.238	71.02	70.20
	H14····O9	2.052	2.087	2.858	2.852	134.80	132.22
DLP-p-r	H11····O9	2.594	2.503	2.498	2.429	73.20	74.20
	H11····O13	2.399	2.370	2.280	2.238	71.01	72.20

	H14····O10	2.052	2.087	2.859	2.853	134.83	132.22
DLP-k-q	H11····O13	2.358	2.320	2.280	2.237	73.08	72.75
	H14····O10	1.980	2.019	2.810	2.805	137.24	134.33
DLP-k-r	H11····O13	2.358	2.321	2.280	2.238	73.06	72.73
	H14····O10	1.982	2.024	2.811	2.810	137.23	134.30
DLP-k-s	H11····O13	2.359	2.319	2.280	2.237	73.05	72.76
	H14····O10	1.982	2.019	2.812	2.805	137.21	134.31

Table 6.132. Parameters of the hydrogen bonds in the conformers of compound DLQ.

Conformers	IHB considered	H···O bond length (Å)		N···O distance (Å)		NĤO bond angle (°)	
		DFT	HF	DFT	HF	DFT	HF
DLQ-p-q	H11····O9	2.598	2.510	2.499	2.431	73.07	73.90
	H11····O13	2.397	2.366	2.280	2.237	71.10	70.36
	H14····O10	2.051	2.080	2.857	2.845	134.69	132.16
DLQ-k-q	H11····O13	2.358	2.320	2.280	2.237	73.07	72.74
	H14····O10	1.980	2.020	2.810	2.806	137.26	134.34
DLQ-k-r	H11····O13	2.358	2.321	2.280	2.238	73.05	72.73
	H14····O10	7.975	2.023	2.809	2.809	137.29	134.31
DLQ-m-r	H11····O10	2.598	2.511	2.499	2.431	73.08	73.90
	H11····O13	2.397	2.366	2.280	2.237	71.10	70.36
	H14····O9	2.051	2.080	2.857	2.845	134.72	132.16
DLQ-m-q	H11····O10	2.595	2.502	2.498	2.429	73.20	74.22
	H11····O13	2.398	2.370	2.280	2.238	71.03	70.19
	H14····O9	2.053	2.087	2.859	2.853	134.79	132.26
DLQ-m-r′	H11····O10	2.599	2.511	2.499	2.431	73.03	73.90
	H11····O13	2.397	2.366	2.280	2.237	71.09	70.37
	H14····O9	2.049	2.079	2.855	2.845	134.78	132.18
DLQ-m-q′	H11····O10	2.595	2.503	2.498	2.429	73.16	74.20
	H11····O13	2.398	2.370	2.280	2.238	71.03	70.20
	H14····O9	2.051	2.087	2.857	2.853	134.84	132.24

Table 6.133. Parameters of the hydrogen bonds in the conformers of compound EGP.

Conformers	IHB considered	H···O bond length (Å)		N···O distance (Å)		NĤO bond angle (º)	
		DFT	HF	DFT	HF	DFT	HF
EGP-m-r-x4	H11····O10	2.596	2.510	2.499	2.431	73.15	73.93
	H11····O13	2.391	2.360	2.279	2.236	71.30	70.55
	H14····O9	2.053	2.079	2.863	2.850	135.17	132.79
EGP-m-s-x4	H11····O10	2.597	2.508	2.499	2.431	73.14	74.02
	H11····O13	2.391	2.362	2.279	2.236	71.30	70.49
	H14····O9	2.052	2.083	2.863	2.855	135.18	132.80
EGP-m-q-x4	H11····O10	2.592	2.502	2.497	2.429	73.30	74.21
	H11····O13	2.393	2.365	2.279	2.237	71.21	70.39
	H14····O9	2.054	2.085	2.865	2.857	135.28	132.87
EGP-m-r-x1	H11····O10	2.594	2.505	2.498	2.430	73.20	74.11
	H11····O13	2.391	2.363	2.277	2.236	71.25	70.41
	H14····O9	2.054	2.085	2.865	2.853	135.22	132.44
EGP-m-s-x1	H11····O10	2.594	2.504	2.498	2.430	73.20	74.22
	H11····O13	2.391	2.364	2.277	2.236	71.25	70.35
	H14····O9	2.054	2.090	2.865	2.858	135.22	132.46
EGP-p-q-x3	H11····O9	2.595	2.505	2.498	2.430	73.18	74.12
	H11····O13	2.391	2.363	2.277	2.236	71.25	70.42
	H14····O10	2.054	2.085	2.864	2.854	135.13	132.45
EGP-p-s-x3	H11····O9	2.595	2.503	2.498	2.430	73.17	74.23
	H11····O13	2.391	2.364	2.277	2.236	71.26	70.35
	H14····O10	2.054	2.090	2.864	2.859	135.12	132.45
EGP-m-q-x1	H11····O10	2.592	2.498	2.497	2.428	73.30	74.39
	H11····O13	2.392	2.367	2.277	2.237	71.19	70.24
	H14····O9	2.054	2.091	2.866	2.860	135.32	132.52
EGP-k-q-x1	H11····O13	2.349	2.318	2.276	2.236	73.35	72.82
	H14····O10	1.975	2.028	2.814	2.816	138.27	134.48
EGP-k-r-x2	H11····O13	2.349	2.312	2.276	2.235	73.31	73.02
	H14····O10	1.974	2.009	2.814	2.803	138.26	135.23
EGP-k-q-x1′	H11····O13	2.349	2.319	2.276	2.237	73.32	72.79
	H14····O10	1.973	2.032	2.814	2.820	138.25	134.47
EGP-k-s-x1	H11····O13	2.349	2.317	2.276	2.236	73.32	72.82
	H14····O10	1.975	2.029	2.814	2.817	138.26	134.44
EGP-g-r-x1	H11····O9	2.446	2.396	2.465	2.405	79.14	78.53
EGP-g-q-x1	H11····O9	2.444	2.395	2.464	2.405	79.20	78.57

Table 6.134. Parameters of the hydrogen bonds in the conformers of compound EGQ.

Conformers	IHB considered	H···O bond length (Å)		N···O distance (Å)		NĤO bond angle (°)	
		DFT	HF	DFT	HF	DFT	HF
EGQ-m-r-x4	H11····O10	2.597	2.510	2.499	2.431	73.13	73.91
	H11····O13	2.391	2.360	2.279	2.236	71.29	70.55
	H14····O9	2.052	2.078	2.862	2.850	135.22	132.81
EGQ-m-q-x4	H11····O10	2.593	2.503	2.498	2.429	73.27	74.20
	H11····O13	2.393	2.364	2.279	2.237	71.22	70.40
	H14····O9	2.054	2.085	2.864	2.857	135.27	132.86
EGQ-m-r-x1	H11····O10	2.595	2.506	2.498	2.430	73.20	74.10
	H11····O13	2.391	2.363	2.277	2.236	71.25	70.41
	H14····O9	2.053	2.084	2.864	2.853	135.21	132.44
EGQ-m-q-x1	H11····O10	2.591	2.498	2.497	2.428	73.33	74.41
	H11····O13	2.392	2.367	2.277	2.237	71.18	70.24
	H14····O9	2.055	2.093	2.867	2.862	135.30	132.53
EGQ-p-q-x3	H11····O9	2.605	2.515	2.499	2.432	72.73	73.69
	H11····O13	2.386	2.360	2.278	2.237	71.54	70.63
	H14····O10	2.037	2.070	2.859	2.847	136.49	133.37
EGQ-p-r-x3	H11····O9	2.600	2.506	2.493	2.429	72.91	74.05
	H11····O13	2.388	2.364	2.279	2.238	71.44	70.47
	H14····O10	2.040	2.080	2.862	2.856	136.55	133.41
EGQ-k-q-x4	H11····O13	2.352	2.315	2.277	2.235	73.24	72.89
	H14····O10	1.986	2.021	2.820	2.813	137.69	134.85
EGQ-k-r-x4	H11····O13	2.352	2.316	2.278	2.236	73.23	72.88
	H14····O10	1.988	2.026	2.822	2.817	137.67	134.80
EGQ-g-r-x1	H11····O9	2.446	2.396	2.465	2.405	79.14	78.53
EGQ-g-t-x1	H11····O9	2.446	2.396	2.465	2.405	79.14	78.55
EGQ-g-q-x1	H11····O9	2.444	2.395	2.464	2.405	79.20	78.58

Table 6.135. Parameters of the hydrogen bonds in the conformers of compound EJP.

Conformers	IHB considered	H···O bond length (Å)		N···O distance (Å)		NĤO bond angle (°)	
		DFT	HF	DFT	HF	DFT	HF
EJP-m-s-x4	H11····O10	2.596	2.510	2.499	2.431	73.15	73.93
	H11····O13	2.391	2.360	2.279	2.236	71.31	70.56
	H14····O9	2.055	2.079	2.863	2.850	135.05	132.74
EJP-m-r-x4	H11····O10	2.597	2.508	2.499	2.431	73.14	74.03
	H11····O13	2.391	2.362	2.279	2.236	71.32	74.49
	H14····O9	2.054	2.084	2.863	2.855	135.05	132.75
EJP-m-q-x4	H11····O10	2.592	2.503	2.498	2.429	73.30	74.21
	H11····O13	2.393	2.365	2.279	2.237	71.21	70.38
	H14····O9	2.055	2.086	2.865	2.857	135.18	132.82
EJP-p-s-x4	H11····O9	2.593	2.503	2.498	2.430	73.29	74.22
	H11····O13	2.393	2.364	2.279	2.236	71.22	70.35
	H14····O10	2.055	2.091	2.865	2.859	135.19	132.40

EJP-p-q-x4	H11····O9	2.594	2.506	2.498	2.430	73.22	74.10
	H11····O13	2.391	2.363	2.277	2.236	71.26	70.41
	H14····O10	2.055	2.085	2.865	2.853	135.13	132.38
EJP-p-r-x4	H11····O9	2.591	2.499	2.497	2.428	73.33	74.38
	H11····O13	2.393	2.367	2.277	2.237	71.17	70.24
	H14····O10	2.055	2.092	2.866	2.860	135.28	132.47
EJP-k-q-x1	H11····O13	2.348	2.317	2.276	2.236	73.35	72.83
	H14····O10	1.974	2.028	2.814	2.816	138.26	134.45
EJP-k-r-x1	H11····O13	2.349	2.318	2.276	2.237	73.33	72.81
	H14····O10	1.975	2.033	2.814	2.821	138.25	134.44
EJP-k-r-x1′	H11····O13	2.349	2.318	2.276	2.237	73.33	72.81
	H14····O10	1.975	2.033	2.814	2.821	138.25	134.46
EJP-k-s-x1	H11····O13	2.349	2.317	2.276	2.237	73.33	72.84
	H14····O10	1.975	2.029	2.814	2.817	138.25	134.42

Table 6.136. Parameters of the hydrogen bonds in the conformers of compound EJQ.

Conformers	IHB considered	H···O bond length (Å)		N···O distance (Å)		NĤO bond angle (º)	
		DFT	HF	DFT	HF	DFT	HF
EJQ-m-q-x4	H11····O10	2.592	2.508	2.497	2.431	73.32	74.03
	H11····O13	2.393	2.362	2.279	2.236	71.22	70.49
	H14····O9	2.057	2.084	2.867	2.855	135.19	132.75
EJQ-m-r-x4	H11····O10	2.596	2.510	2.499	2.431	73.15	73.93
	H11····O13	2.392	2.360	2.279	2.236	71.29	70.56
	H14····O9	2.052	2.079	2.862	2.850	135.14	132.74
EJQ-p-q-x4	H11····O9	2.594	2.505	2.498	2.430	73.22	74.12
	H11····O13	2.391	2.363	2.277	2.236	71.26	70.41
	H14····O10	2.056	2.086	2.865	2.854	135.11	132.36
EJQ-p-q-x4′	H11····O9	2.595	2.506	2.498	2.430	73.17	74.10
	H11····O13	2.391	2.363	2.277	2.236	71.25	70.43
	H14····O10	2.055	2.086	2.864	2.854	135.04	132.35
EJQ-m-r-x1	H11····O10	2.595	2.506	2.498	2.430	73.18	74.09
	H11····O13	2.391	2.363	2.277	2.236	71.25	70.43
	H14····O9	2.055	2.086	2.865	2.853	135.06	132.35
EJQ-m-s-x1	H11····O10	2.595	2.503	2.498	2.430	73.17	74.24
	H11····O13	2.340	2.364	2.277	2.236	71.26	70.34
	H14····O9	2.055	2.091	2.864	2.859	135.06	132.38
EJQ-p-r-x4	H11····O9	2.591	2.499	2.497	2.428	73.33	74.37
	H11····O13	2.393	2.367	2.278	2.237	71.17	70.25
	H14····O10	2.056	2.090	2.867	2.861	135.19	132.43
EJQ-p-s-x4	H11····O9	2.591	2.504	2.497	2.430	73.33	74.21
	H11····O13	2.392	2.364	2.277	2.236	71.17	70.34
	H14····O10	2.056	2.090	2.867	2.858	135.20	132.37
EJQ-m-q-x1	H11····O10	2.591	2.499	2.497	2.428	73.33	74.37
	H11····O13	2.393	2.367	2.278	2.237	71.17	70.25
	H14····O9	2.056	2.092	2.866	2.860	135.19	132.43
EJQ-k-q-x4	H11····O13	2.351	2.314	2.277	2.235	73.29	72.93

	H14····O10	1.987	2.021	2.821	2.812	137.65	134.83
EJQ-k-r-x4	H11····O13	2.351	2.315	2.277	2.236	73.27	72.91
	H14····O10	1.988	2.026	2.821	2.817	137.66	134.79

Table 6.137. Parameters of the hydrogen bonds in the conformers of compound ELP.

Conformers	IHB considered	H···O bond length (Å)		N···O distance (Å)		NĤO bond angle (º)	
		DFT	HF	DFT	HF	DFT	HF
ELP-m-s-x4	H11····O10	2.597	2.510	2.499	2.431	73.14	73.93
	H11····O13	2.391	2.361	2.279	2.236	71.30	70.55
	H14····O9	2.052	2.079	2.862	2.850	135.17	132.79
ELP-m-q-x4	H11····O10	2.597	2.508	2.498	2.431	73.13	74.02
	H11····O13	2.391	2.362	2.279	2.236	71.30	70.49
	H14····O9	2.052	2.084	2.862	2.855	135.18	132.79
ELP-m-q-x4	H11····O10	2.593	2.502	2.498	2.429	73.28	74.21
	H11····O13	2.393	2.365	2.279	2.237	71.21	70.39
	H14····O9	2.054	2.085	2.865	2.857	135.28	132.87
ELP-m-r-x1	H11····O10	2.594	2.505	2.498	2.430	73.21	74.11
	H11····O13	2.391	2.363	2.277	2.236	71.25	70.41
	H14····O9	2.054	2.085	2.865	2.853	135.22	132.43
ELP-m-s-x1	H11····O10	2.494	2.504	2.498	2.430	73.20	74.22
	H11····O13	2.391	2.364	2.277	2.236	71.25	70.35
	H14····O9	2.054	2.090	2.865	2.858	135.22	132.45
ELP-p-s-x4	H11····O9	2.594	2.506	2.498	2.430	73.20	74.09
	H11····O13	2.391	2.363	2.277	2.236	71.25	70.42
	H14····O10	2.054	2.084	2.865	2.853	135.15	132.45
ELP-p-s-x4′	H11····O9	2.594	2.503	2.498	2.430	73.20	74.23
	H11····O13	2.391	2.364	2.277	2.236	71.25	70.35
	H14····O10	2.055	2.091	2.859	2.859	135.14	132.45
ELP-m-q-x1	H11····O10	2.591	2.498	2.497	2.428	73.32	74.39
	H11····O13	2.392	2.367	2.277	2.237	71.17	70.24
	H14····O9	2.054	2.091	2.866	2.860	135.35	132.54
ELP-k-q-x1	H11····O13	2.348	2.318	2.276	2.236	73.35	72.81
	H14····O10	1.974	2.028	2.813	2.816	138.27	134.47
ELP-k-r-x1	H11····O13	2.349	2.319	2.276	2.237	73.33	72.79
	H14····O10	1.977	2.033	2.816	2.821	138.24	134.45
ELP-k-s-x1	H11····O13	2.349	2.317	2.276	2.236	73.33	72.83
	H14····O10	1.977	2.029	2.816	2.817	138.24	134.43

Table 6.138. Parameters of the hydrogen bonds in the conformers of compound ELQ.

Conformers	IHB considered	H···O bond length (Å)		N···O distance (Å)		NĤO bond angle (°)	
		DFT	HF	DFT	HF	DFT	HF
ELQ-m-r-x4	H11····O10	2.597	2.510	2.499	2.431	73.13	73.90
	H11····O13	2.391	2.360	2.279	2.236	71.29	70.56
	H14····O9	2.051	2.078	2.862	2.850	135.21	132.80
ELQ-m-q-x4	H11····O10	2.593	2.503	2.498	2.429	73.26	74.21
	H11····O13	2.393	2.364	2.279	2.237	71.22	70.39
	H14····O9	2.053	2.085	2.864	2.857	135.26	132.86
ELQ-m-r-x1	H11····O10	2.594	2.505	2.498	2.430	73.23	74.11
	H11····O13	2.391	2.363	2.277	2.236	71.25	70.41
	H14····O9	2.054	2.084	2.865	2.853	135.20	132.43
ELQ-m-q-x1	H11····O10	2.591	2.498	2.497	2.428	73.32	74.40
	H11····O13	2.392	2.367	2.278	2.237	71.18	70.24
	H14····O9	2.055	2.092	2.866	2.861	135.28	132.53
ELQ-k-q-x4	H11····O13	2.352	2.315	2.278	2.236	73.25	72.89
	H14····O10	1.987	2.022	2.821	2.813	137.65	134.85
ELQ-k-r-x4	H11····O13	2.352	2.316	2.277	2.236	73.23	72.88
	H14····O10	1.988	2.026	2.821	2.816	137.67	134.81

Table 6.139. Parameters of the hydrogen bonds in the conformers of compound FGP

Conformers	IHB considered	H···O bond length (Å)		N···O distance (Å)		NĤO bond angle (°)	
		DFT	HF	DFT	HF	DFT	HF
FGP-m-r-x4	H11····O10	2.596	2.510	2.498	2.431	73.18	73.92
	H11····O13	2.391	2.360	2.279	2.236	71.33	70.58
	H14····O9	2.054	2.078	2.864	2.851	135.19	132.88
FGP-m-s-x4	H11····O10	2.596	2.508	2.498	2.431	73.18	74.02
	H11····O13	2.391	2.361	2.279	2.236	71.33	70.52
	H14····O9	2.054	2.083	2.864	2.855	135.20	132.88
FGP-m-q-x4	H11····O10	2.592	2.502	2.497	2.429	73.30	74.21
	H11····O13	2.393	2.364	2.279	2.237	71.24	70.41
	H14····O9	2.055	2.085	2.866	2.858	135.30	132.96
FGP-m-r-x1	H11····O10	2.605	2.504	2.499	2.430	72.75	74.15
	H11····O13	2.387	2.362	2.278	2.236	71.51	70.44
	H14····O9	2.037	2.085	2.859	2.855	136.46	132.61
FGP-m-s-x1	H11····O10	2.605	2.503	2.499	2.430	72.75	74.25
	H11····O13	2.387	2.363	2.278	2.236	71.51	70.38
	H14····O9	2.038	2.090	2.859	2.860	136.45	132.63
FGP-p-q-x4	H11····O9	2.605	2.505	2.499	2.430	72.76	74.13
	H11····O13	2.387	2.362	2.279	2.236	71.53	70.45
	H14····O10	2.038	2.084	2.859	2.854	136.44	132.61
FGP-p-s-x4	H11····O9	2.605	2.502	2.499	2.430	72.76	74.26
	H11····O13	2.387	2.363	2.279	2.236	71.53	70.38
	H14····O10	2.038	2.090	2.859	2.860	136.44	132.63

FGP-m-q-x1	H11····O10	2.599	2.498	2.498	2.428	72.95	74.41
	H11····O13	2.389	2.366	2.279	2.236	71.42	70.28
	H14····O9	2.040	2.091	2.862	2.862	136.54	132.68
FGP-p-r-x4	H11····O9	2.600	2.498	2.498	2.428	72.91	74.42
	H11····O13	2.389	2.366	2.279	2.236	71.43	70.27
	H14····O10	2.039	2.091	2.861	2.862	136.55	132.70
FGP-k-q-x1	H11····O13	2.349	2.315	2.277	2.236	73.37	72.88
	H14····O10	1.977	2.028	2.816	2.819	138.28	134.79
FGP-k-r-x1	H11····O13	2.349	2.316	2.277	2.236	73.34	72.86
	H14····O10	1.977	2.031	2.816	2.822	138.27	134.78
FGP-k-r-x1′	H11····O13	2.349	2.314	2.277	2.235	73.34	72.95
	H14····O10	1.977	2.029	2.816	2.823	138.27	135.15
FGP-g-r-x1	H11····O9	2.445	2.396	2.465	2.405	79.18	78.55
FGP-g-r-x1	H11····O9	2.445	2.396	2.465	2.405	79.18	78.56
FGP-g-q-x1	H11····O9	2.443	2.394	2.464	2.404	79.24	78.59

Table 6.140. Parameters of the hydrogen bonds in the conformers of compound FGQ.

Conformers	IHB considered	H···O bond length (Å)		N···O distance (Å)		NĤO bond angle (º)	
		DFT	HF	DFT	HF	DFT	HF
FGQ-m-r-x4	H11····O10	2.597	2.511	2.499	2.431	73.12	73.90
	H11····O13	2.391	2.360	2.279	2.236	71.33	70.58
	H14····O9	2.052	2.077	2.862	2.850	135.20	132.88
FGQ-m-q-x4	H11····O10	2.592	2.503	2.498	2.431	73.30	74.20
	H11····O13	2.393	2.364	2.279	2.237	71.25	70.42
	H14····O9	2.055	2.085	2.866	2.857	135.29	132.95
FGQ-p-q-x4	H11····O9	2.605	2.516	2.500	2.432	72.76	73.66
	H11····O13	2.387	2.359	2.279	2.237	71.51	70.67
	H14····O10	2.037	2.069	2.859	2.847	136.48	133.50
FGQ-m-r-x1	H11····O10	2.605	2.504	2.500	2.430	72.76	74.15
	H11····O13	2.387	2.362	2.278	2.236	71.51	70.44
	H14····O9	2.037	2.084	2.858	2.854	136.49	132.62
FGQ-m-q-x1	H11····O10	2.599	2.497	2.498	2.428	72.96	74.44
	H11····O13	2.389	2.366	2.279	2.236	71.43	70.28
	H14····O9	2.040	2.092	2.862	2.863	136.54	132.71
FGQ-k-r-x4	H11····O13	2.352	2.315	2.278	2.236	73.27	72.90
	H14····O10	1.989	2.026	2.823	2.817	137.70	134.89
FGQ-g-r-x1	H11····O9	2.445	2.396	2.465	2.405	79.19	78.55
FGQ-g-t-x1	H11····O9	2.445	2.395	2.465	2.405	79.20	78.57
FGQ-g-q-x1	H11····O9	2.444	2.394	2.464	2.404	79.23	78.60

Table 6.141. Parameters of the hydrogen bonds in the conformers of compound FJP.

Conformers	IHB considered	H···O bond length (Å)		N···O distance (Å)		NĤO bond angle (º)	
		HF	DFT	HF	DFT	HF	DFT
FJP-m-r-x4	H11····O10	2.510	2.596	2.431	2.499	73.92	73.16
	H11····O13	2.360	2.391	2.236	2.279	70.58	73.16
	H14····O9	2.079	2.054	2.851	2.863	132.82	135.14
FJP-m-s-x4	H11····O10	2.508	2.596	2.431	2.499	74.03	73.15
	H11····O13	2.361	2.391	2.236	2.279	70.52	71.34
	H14····O9	2.084	2.054	2.856	2.863	132.83	135.14
FJP-m-q-x4	H11····O10	2.503	2.592	2.429	2.498	74.21	73.30
	H11····O13	2.364	2.393	2.237	2.279	70.41	71.24
	H14····O9	2.085	2.055	2.858	2.865	132.90	135.23
FJP-p-q-x4	H11····O9	2.505	2.604	2.430	2.499	74.14	72.79
	H11····O13	2.362	2.387	2.236	2.279	70.45	71.52
	H14····O10	2.085	2.039	2.855	2.860	132.55	136.42
FJP-p-s-x4	H11····O9	2.503	2.604	2.430	2.499	74.26	72.79
	H11····O13	2.363	2.387	2.236	2.279	70.38	71.52
	H14····O10	2.091	2.039	2.860	2.860	132.57	136.41
FJP-k-q-x1	H11····O13	2.315	2.348	2.236	2.276	72.90	73.37
	H14····O10	2.028	1.975	2.819	2.815	134.75	138.29
FJP-p-r-x1	H11····O9	2.498	2.598	2.428	2.607	74.41	68.72
	H11····O13	2.366	2.387	2.236	2.276	70.28	73.35
	H14····O10	2.091	2.039	2.861	2.861	132.64	138.28
FJP-k-r-x1	H11····O13	2.316	2.349	2.236	2.276	72.87	73.36
	H14····O10	2.032	1.977	2.823	2.816	134.73	138.28
F-J-P-3a	H11····O13	2.315	2.349	2.235	2.276	72.90	73.35
	H14····O10	2.029	1.977	2.819	2.816	134.71	138.28

Table 6.142. Parameters of the hydrogen bonds in the conformers of compound FJQ.

Conformers	IHB considered	H···O bond length (Å)		N···O distance (Å)		NĤO bond angle (º)	
		DFT	HF	DFT	HF	DFT	HF
FJQ-m-q-x4	H11····O10	2.592	2.503	2.498	2.429	73.33	74.19
	H11····O13	2.393	2.364	2.279	2.237	71.26	70.42
	H14····O9	2.057	2.085	2.867	2.857	135.19	132.89
FJQ-m-r-x4	H11····O10	2.597	2.511	2.499	2.431	73.13	73.90
	H11····O13	2.391	2.360	2.279	2.236	71.33	70.57
	H14····O9	2.053	2.078	2.863	2.850	135.13	132.85
FJQ-p-r-x4	H11····O9	2.599	2.497	2.498	2.428	72.98	74.46
	H11····O13	2.389	2.366	2.279	2.236	71.44	70.27
	H14····O10	2.043	2.093	2.864	2.863	136.47	132.66
FJQ-p-q-x4	H11····O9	2.604	2.516	2.500	2.432	72.79	73.66
	H11····O13	2.387	2.359	2.279	2.237	71.51	70.67
	H14····O10	2.038	2.070	2.859	2.847	136.42	133.45
FJQ-m-q-x1	H11····O9	2.604	2.505	2.500	2.430	72.78	74.14
	H11····O13	2.387	2.362	2.278	2.236	71.49	70.44

	H14····O10	2.038	2.084	2.859	2.854	136.43	132.58
FJQ-m-r-x1	H11····O10	2.601	2.498	2.499	2.428	72.89	74.38
	H11····O13	2.389	2.366	2.279	2.236	71.44	70.30
	H14····O9	2.040	2.091	2.861	2.861	136.46	132.63
FJQ-m-r-x1	H11····O10	2.605	2.505	2.500	2.429	72.74	74.12
	H11····O13	2.387	2.362	2.278	2.236	71.49	70.44
	H14····O9	2.036	2.084	2.858	2.854	136.48	132.59
FJQ-k-q-x4	H11····O13	2.351	2.314	2.277	2.235	73.28	72.93
	H14····O10	1.986	2.021	2.820	2.813	137.73	134.93
FJQ-k-r-x4	H11····O13	2.351	2.315	2.277	2.236	73.27	72.92
	H14····O10	1.988	2.026	2.821	2.817	137.70	134.87

Table 6.143. Parameters of the hydrogen bonds in the conformers of compound FLP.

Conformers	IHB considered	H···O bond length (Å)		N···O distance (Å)		NĤO bond angle (º)	
		DFT	HF	DFT	HF	DFT	HF
FLP-m-r-x4	H11····O10	2.596	2.510	2.499	2.431	73.17	73.93
	H11····O13	2.391	2.360	2.279	2.236	71.34	70.58
	H14····O9	2.054	2.078	2.864	2.851	135.19	132.88
FLP-m-q-x4	H11····O10	2.593	2.503	2.498	2.429	73.26	74.21
	H11····O13	2.393	2.364	2.279	2.237	71.25	70.41
	H14····O9	2.053	2.085	2.865	2.857	135.31	132.95
FLP-m-r-x1	H11····O10	2.605	2.504	2.499	2.430	72.75	74.15
	H11····O13	2.387	2.362	2.278	2.236	71.52	70.45
	H14····O9	2.038	2.085	2.859	2.855	136.45	132.60
FLP-m-s-x4	H11····O10	2.605	2.508	2.499	2.431	72.74	74.02
	H11····O13	2.387	2.361	2.278	2.236	71.52	70.52
	H14····O9	2.037	2.083	2.859	2.855	136.45	132.88
FLP-m-s-x1	H11····O10	2.605	2.503	2.499	2.430	72.74	74.25
	H11····O13	2.387	2.363	2.278	2.236	71.52	70.38
	H14····O9	2.037	2.090	2.859	2.860	136.45	132.63
FLP-p-q-x4	H11····O9	2.605	2.505	2.499	2.430	72.75	74.14
	H11····O13	2.387	2.362	2.278	2.236	71.53	70.45
	H14····O10	2.038	2.084	2.859	2.854	136.44	132.60
FLP-p-s-x4	H11····O9	2.605	2.502	2.499	2.430	72.75	74.27
	H11····O13	2.387	2.364	2.278	2.236	71.53	70.37
	H14····O10	2.038	2.090	2.859	2.860	136.44	132.61
FLP-m-q-x1	H11····O10	2.601	2.498	2.498	2.428	72.91	74.41
	H11····O13	2.389	2.366	2.279	2.236	71.43	70.28
	H14····O9	2.039	2.091	2.861	2.861	136.55	132.70
FLP-k-q-x1	H11····O13	2.348	2.315	2.276	2.236	73.37	72.89
	H14····O10	1.976	2.028	2.815	2.819	138.28	134.79
FLP-k-r-x1	H11····O13	2.349	2.316	2.277	2.236	73.34	72.86
	H14····O10	1.978	2.032	2.817	2.823	138.25	134.77
FLP-k-s-x1	H11····O13	2.349	2.315	2.277	2.235	73.34	72.90
	H14····O10	1.978	2.029	2.817	2.819	138.26	134.75

Table 6.144 Parameters of the hydrogen bonds in the conformers of compound FLQ.

Conformers	IHB considered	H···O bond length (Å)		N···O distance (Å)		NĤO bond angle (º)	
		DFT	HF	DFT	HF	DFT	HF
FLQ-p-q-x2	H11····O9	2.596	2.509	2.498	2.430	73.16	73.95
	H11····O13	2.391	2.361	2.279	2.236	71.33	70.53
	H14····O10	2.054	2.076	2.864	2.850	135.18	133.02
FLQ-m-r-x4	H11····O10	2.597	2.510	2.499	2.431	73.11	73.90
	H11····O13	2.391	2.360	2.279	2.236	71.33	70.58
	H14····O9	2.052	2.077	2.862	2.850	135.19	132.89
FLQ-m-q-x4	H11····O10	2.592	2.503	2.498	2.429	73.30	74.20
	H11····O13	2.393	2.364	2.279	2.237	71.25	70.42
	H14····O9	2.055	2.085	2.866	2.858	135.28	132.94
FLQ-p-q-x4	H11····O9	2.605	2.505	2.500	2.430	72.76	74.12
	H11····O13	2.387	2.362	2.278	2.236	71.48	70.45
	H14····O10	2.036	2.084	2.858	2.854	136.51	132.62
FLQ-m-r-x1	H11····O10	2.605	2.505	2.500	2.430	72.75	74.14
	H11····O13	2.387	2.362	2.279	2.236	71.51	70.44
	H14····O9	2.036	2.084	2.858	2.854	136.49	132.62
FLQ-m-q-x1	H11····O10	2.599	2.497	2.498	2.428	72.97	74.43
	H11····O13	2.389	2.366	2.279	2.236	71.43	70.28
	H14····O9	2.039	2.092	2.863	2.863	136.53	132.70
FLQ-m-q-x1′	H11····O10	2.599	2.495	2.498	2.427	72.97	74.52
	H11····O13	2.389	2.367	2.279	2.237	71.43	70.25
	H14····O9	2.041	2.093	2.863	2.864	136.53	132.72
FLQ-p-r-x4	H11····O9	2.600	2.508	2.498	2.430	72.92	73.99
	H11····O13	2.389	2.363	2.279	2.238	71.44	70.50
	H14····O10	2.040	2.077	2.862	2.854	136.52	133.55
FLQ-p-r-x4′	H11····O9	2.600	2.498	2.498	2.428	72.92	74.41
	H11····O13	2.389	2.366	2.279	2.237	71.44	70.27
	H14····O10	2.040	2.091	2.862	2.861	136.52	132.68
FLQ-k-q-x4	H11····O13	2.351	2.314	2.277	2.235	73.27	72.91
	H14····O10	1.986	2.021	2.820	2.813	137.72	134.93
FLQ-k-q-x1	H11····O13	2.349	2.315	2.276	2.236	73.34	72.88
	H14····O10	1.975	2.028	2.815	2.819	138.30	134.80
FLQ-k-r-x4	H11····O13	2.352	2.315	2.278	2.236	73.26	72.90
	H14····O10	1.988	2.025	2.822	2.816	2.82	134.90
FLQ-k-r-x1	H11····O13	2.349	2.316	2.277	2.236	73.34	72.86
	H14····O10	1.977	2.032	2.816	2.823	138.27	134.76

6.1.4. The vibrational frequencies of the N–H bonds in the calculated conformers of each of the compounds considered.

This section presents the tables reporting the vibrational frequencies (harmonic approximations) of the N–H bonds in the conformers of each of the compounds considered. The calculated frequencies were scaled by 0.9648 for DFT calculations and 0.8992 for HF calculations. When there are two values for the same bond and in the same conformer, it shows that they correspond to two vibrations that are coupled: the symmetric and asymmetric vibrations.

Table 6.145. Vibrational frequencies of N11–H11 and N14–H14 in the calculated conformers of compound AGP.
Symbols are used to indicate the symmetric (∗) and asymmetric (э) vibrations

Conformers	Vibrational frequencies (kcal/mol)			
	N11–H11		N14–H14	
	DFT	HF	DFT	HF
AGP-m-r-u1	3465.3	3458.2	3429.9	3462.4
AGP-m-s-u1	3465.3	3457.1	3429.9	3463.7
AGP-p-t-u3	3465.2	3457.4	3429.6	3462.8
AGP-m-q-u1	3465.6	3458.5	3429.6	3462.5
AGP-p-r-u3	3465.5	3458.5	3429.8	3462.5
AGP-k-q-u1	3438.0	3435.3	3421.3	3471.6
AGP-k-r-u1	3437.4	3434.2	3422.5	3471.7
AGP.m-r-u2	3463.5	3456.5	3447.8	3480.4
AGP-g-r-u3 э	3477.5	3475.0	3479.5	3475.0
∗	3484.8	3482.9	3484.8	3482.9
AGP-g-q-u3 э	3477.9	3474.9	3477.9	3474.9
∗	3485.3	3482.8	3485.3	3482.8
AGP-j-q-u3	3429.7	3440.2	3476.3	3472.3
AGP-j-r-u3	3429.4	3440.6	3476.5	3472.7
AGP-j-s-u3	3429.4	3438.4	3476.5	3472.8

Table 6.146. Vibrational frequencies of N11–H11 and N14–H14 in the calculated conformers of compound AGQ.

Symbols are used to indicate the symmetric (∗) and asymmetric (э) vibrations

Conformers	Vibrational frequencies (cm^{-1})			
	N11–H11		N14–H14	
	DFT	HF	DFT	HF
AGQ-m-r-u1	3465.3	3458.1	3429.9	3462.3
AGQ-m-q-u1	3465.5	3458.6	3430.4	3462.7
AGQ-k-q-u1	3437.8	3435.4	3421.5	3471.5
AGQ-k-r-u1	3437.7	3434.0	3422.0	3471.6
AGQ-m-r-u2	3463.4	3456.3	3448.0	3480.4
AGQ-m-q-u2	3463.7	3456.9	3448.1	3480.7
AGQ-g-r-u3 э	3477.3	3475.0	3477.3	3475.0
∗	3484.6	3482.9	3484.6	3482.9
AGQ-g-t-u3 э	3477.3	3474.6	3477.3	3474.6
∗	3484.7	3482.5	3484.7	3482.5
AGQ-g-q-u3 э	3477.9	3474.9	3477.9	3474.9
∗	3485.3	3482.8	3485.3	3482.8
AGQ-j-q-u3	3429.5	3440.3	3476.5	3472.3
AGQ-j-r-u3	3429.3	3440.9	3476.5	3472.5
AGQ-j-t-u3	3429.3	3438.2	3476.5	3472.8

Table 6.147. Vibrational frequencies of N11–H11 and N14–H14 in the calculated conformers of compound AJP.

Conformers	Vibrational frequencies (cm^{-1})			
	N11–H11		N14–H14	
	DFT	HF	DFT	HF
AJP-m-r-u1	3464.8	3458.0	3430.1	3462.3
AJP-m-s-u1	3464.9	3457.0	3430.1	3463.6
AJP-m-q-u1	3465.6	3458.2	3429.9	3462.6
AJP-k-q-u1	3437.9	3435.0	3421.4	3471.9
AJP-k-r-u1	3437.1	3434.6	3422.0	3471.9
AJP-k-s-u1	3437.1	3432.8	3422.0	3473.6
AJP-m-r-u2	3463.5	3456.3	3448.1	3480.4
AJP-m-s-u2	3463.5	3455.3	3448.1	3481.9
AJP-m-q-u2	3464.0	3456.6	3448.6	3480.8
AJP-j-q-u3	3429.0	3439.7	3476.5	3472.4
AJP-j-r-u3	3428.9	3440.1	3476.7	3472.7
AJP-j-s-u3	3429.0	3437.9	3476.8	3472.9

Table 6.148. Vibrational frequencies of N11–H11 and N14–H14 in the calculated conformers of compound AJQ.

Conformers	Vibrational frequencies (cm^{-1})			
	N11–H11		N14–H14	
	DFT	HF	DFT	HF
AJQ-p-q-u5	3465.1	3457.3	3430.3	3474.7
AJQ-m-q-u1	3465.4	3458.1	3430.2	3462.5
AJQ-m-q-u2	3463.6	3456.8	3447.9	3480.5
AJQ-m-r-u2	3463.1	3456.1	3448.3	3480.5
AJQ-p-q-u3	3464.7	3458.0	3430.2	3462.4
AJQ-m-r-u1	3464.8	3457.7	3430.3	3462.3
AJQ-p-q-u5	3464.7	3457.2	3430.2	3474.7
AJQ-m-s-u1	3464.7	3457.0	3430.3	3463.6
AJQ-p-r-u3	3465.3	3458.1	3430.5	3462.5
AJQ-p-s-u3	3465.3	3456.9	3430.5	3463.6
AJQ-m-q-u1	3465.2	3458.1	3430.2	3462.4
AJQ-k-q-u1	3437.3	3434.9	3421.8	3472.1
AJQ-k-q-u1	3437.6	3434.9	3422.1	3472.1
AJQ-k-r-u1	3437.3	3434.4	3422.5	3472.2
AJQ-j-q-u1	3428.6	3439.7	3476.6	3472.5
AJQ-j-r-u1	3429.0	3440.3	3476.6	3472.6

Table 6.149. Vibrational frequencies of N11–H11 and N14–H14 in the calculated conformers of compound ALP.

Conformers	Vibrational frequencies (cm^{-1})			
	N11–H11		N14–H14	
	DFT	HF	DFT	HF
ALP-m-r-u1	3465.2	3458.0	3429.9	3462.3
ALP-m-s-u1	3465.2	3457.1	3429.9	3463.6
ALP-m-q-u1	3465.6	3458.4	3429.9	3462.5
ALP-k-q-u1	3436.8	3435.2	3421.2	3471.7
ALP-k-r-u1	3437.3	3434.8	3422.1	3471.8
ALP-k-q-u1	3438.0	3435.3	3421.4	3471.6
ALP-k-r-u1′	3437.3	3434.7	3422.0	3471.7
ALP-k-s-u1	3437.2	3433.0	3422.0	3473.3
ALP-k-r-u3	3437.9	3434.1	3419.8	3476.2
ALP-m-r-u2	3463.8	3456.4	3447.9	3480.4
ALP-m-s-u2	3463.8	3455.5	3447.8	3481.8
ALP-m-q-u2	3464.6	3456.8	3447.7	3480.8
ALP-j-q-u3	3429.6	3440.3	3476.2	3472.2
ALP-j-r-u3	3429.4	3440.5	3476.5	3472.7
ALP-j-s-u3	3429.4	3438.6	3476.6	3472.8

Table 6.150. Vibrational frequencies of N11–H11 and N14–H14 in the calculated conformers of compound ALQ.

Conformers	Vibrational frequencies (cm^{-1})			
	N11–H11		N14–H14	
	DFT	HF	DFT	HF
ALQ-m-r-u1	3465.2	3458.1	3429.7	3462.2
ALQ-m-q-u1	3465.4	3458.6	3430.4	3462.6
ALQ-k-q-u1	3438.1	3435.3	3421.6	3471.6
ALQ-k-r-u1	3437.6	3434.8	3422.2	3471.7
ALQ-m-r-u2	3463.5	3456.3	3447.9	3480.4
ALQ-m-q-u2	3463.7	3456.9	3448.1	3480.7
ALQ-j-q-u3	3429.5	3440.2	3476.4	3472.3
ALQ-j-r-u3	3429.5	3440.8	3476.5	3472.6
ALQ-j-q-u3	3429.7	3440.5	3476.5	3472.3
ALQ-j-r-u3	3429.8	3441.0	3476.5	3472.6

Table 6.151. Vibrational frequencies of N11–H11 and N14–H14 in the calculated conformers of compound BGP.

Conformers	Vibrational frequencies (cm^{-1})			
	N11–H11		N14-H14	
	DFT	HF	DFT	HF
BGP-p-s-v3	3464.1	3456.6	3429.6	3463.9
BGP-p-t-v3	3464.1	3456.7	3429.5	3463.0
BGP-m-r-v1	3464.4	3457.5	3429.4	3462.7
BGP-m-s-v1	3464.4	3456.4	3429.4	3463.9
BGP-m-q-v1	3464.4	3457.8	3429.8	3462.7
BGP-k-q-v3	3438.3	3435.0	3419.3	3467.8
BGP-k-r-v3	3438.3	3434.4	3420.1	3467.9
BGP-k-s-v3	3438.4	3432.9	3420.1	3469.6
BGP-m-r-v2	3462.7	3455.9	3438.8	3475.0
BGP-m-s-v2	3462.7	3454.9	3438.8	3476.5
BGP-m-q-v2	3471.4	3456.4	3438.9	3475.3
BGP-g-r-v1 э	3479.1	3475.9	3479.1	3475.9
*	3488.6	3484.3	3488.6	3484.3
BGP-g-q-v1 э	3479.4	3475.9	3479.4	3475.9
*	3489.6	3484.0	3489.6	3484.0
BGP-j-q-v5	3429.7	3440.6	3480.5	3479.5
BGP-j-r-v5	3429.6	3441.0	3480.9	3480.1
BGP-j-s-v5	3429.6	3438.8	3480.9	3480.6

Table 6.152. Vibrational frequencies of N11–H11 and N14–H14 in the calculated conformers of compound BGQ.

Conformers	Vibrational frequencies (cm^{-1})			
	N11–H11		N14–H14	
	DFT	HF	DFT	HF
BGQ-m-r-v1	3464.3	3457.5	3429.7	3462.5
BGQ-m-q-v1	3464.6	3457.5	3430.1	3462.9
BGQ-k-q-v1	3438.7	3435.0	3419.6	3467.7
BGQ-k-r-v1	3438.0	3434.5	3420.1	3468.0
BGQ-m-r-v2	3463.1	3455.7	3438.5	3474.9
BGQ-m-q-v2	3462.9	3456.3	3438.6	3475.3
BGQ-j-q-v3	3429.7	3440.1	3480.5	3474.2
BGQ-j-r-v3	3429.7	3440.6	3480.8	3474.5
BGQ-j-t-v3	3429.7	3437.9	3480.8	3474.7

Table 6.153. Vibrational frequencies of N11–H11 and N14–H14 in the calculated conformers of compound BJP.

Conformers	Vibrational frequencies (cm^{-1})			
	N11–H11		N14–H14	
	DFT	HF	DFT	HF
BJP-p-q-v3	3463.9	3457.7	3430.0	3462.7
BJP-p-s-v3	3463.9	3456.3	3430.0	3463.9
BJP-p-r-v3	3464.4	3457.5	3430.0	3462.7
BJP-k-q-v1	3438.4	3434.7	3419.8	3468.1
BJP-k-r-v1	3438.1	3434.2	3420.4	3468.3
BJP-k-s-v1	3438.2	3432.7	3420.4	3469.9
BJP-m-r-v2	3462.6	3455.8	3439.2	3475.0
BJP-m-s-v2	3462.6	3454.8	3439.2	3476.5
BJP-m-q-v2	3463.0	3456.1	3439.1	3475.4
BJP-j-r-v3	3429.2	3439.9	3481.1	3474.7
BJP-j-s-v3	3429.3	3437.7	3481.0	3474.6
BJP-j-q-v3	3429.1	3439.5	3480.7	3474.4

Table 6.154. Vibrational frequencies of N11–H11 and N14–H14 in the calculated conformers of compound BJQ.

Conformers	Vibrational frequencies (cm^{-1})			
	N11–H11		N14–H14	
	DFT	HF	DFT	HF
BJQ-p-r-v3	3464.5	3457.7	3430.2	3462.7
BJQ-m-s-v1	3464.1	3456.2	3430.1	3464.0
BJQ-m-t-v1	3464.0	3456.5	3430.1	3463.0
BJQ-m-q-v2	3463.0	3456.3	3439.5	3475.5
BJQ-m-r-v2	3462.6	3455.7	3438.9	3474.8
BJQ-m-q-v1	3464.3	3457.4	3430.2	3462.7
BJQ-p-q-v3	3463.8	3457.2	3430.2	3462.6
BJQ-p-q-v3′	3463.8	3457.2	3430.2	3462.6
BJQ-p-r-v3	3464.4	3457.5	3430.3	3462.8
BJQ-p-s-v3	3464.3	3456.2	3430.3	3463.9
BJQ-j-q-v3	3429.0	3439.5	3481.0	3474.5
BJQ-j-r-v3	3429.3	3440.1	3481.0	3474.6

Table 6.155. Vibrational frequencies of N11–H11 and N14–H14 in the calculated conformers of compound BLP.

Conformers	Vibrational frequencies (cm^{-1})			
	N11–H11		N14–H14	
	DFT	HF	DFT	HF
BLP-k-q-v1	3438.4	3435.0	3419.4	3467.8
BLP-p-s-v3	3464.0	3456.5	3429.6	3464.0
BLP-p-t-v3	3464.1	3456.7	3429.6	3463.0
BLP-m-r-v1	3464.4	3457.5	3429.5	3462.6
BLP-m-s-v1	3429.5	3456.4	3464.4	3464.0
BLP-m-r-v1′	3464.3	3457.8	3429.7	3462.7
BLP-k-r-v1	3438.0	3434.3	3419.8	3467.9
BLP-k-s-v1	3438.0	3432.9	3419.9	3469.6
BLP-p-q-v4	3462.7	3455.8	3438.8	3474.9
BLP-p-s-v4	3462.7	3455.1	3438.8	3476.4
BLP-p-t-v4	3462.7	3455.2	3438.8	3475.4
BLP-p-r-v4	3462.8	3456.2	3438.9	3475.4
BLP-j-q-v5	3429.8	3440.6	3480.4	3479.4
BLP-j-r-v5	3429.6	3441.0	3480.8	3479.9
BLP-j-s-v5	3429.6	3438.9	3480.9	3480.2

Table 6.156. Vibrational frequencies of N11–H11 and N14–H14 in the calculated conformers of compound BLQ.

Conformers	Vibrational frequencies (cm^{-1})			
	N11–H11		N14–H14	
	DFT	HF	DFT	HF
BLQ-p-q-v3	3464.2	3457.4	3429.7	3462.5
BLQ-p-r-v3	3464.6	3457.8	3430.2	3462.9
BLQ-p-r-v3	3464.5	3457.8	3429.9	3462.7
BLQ-k-q-v1	3438.3	3434.7	3419.4	3467.8
BLQ-k-r-v1	3438.4	3434.6	3420.0	3467.9
BLQ-m-r-v1	3464.4	3457.5	3429.4	3462.5
BLQ-m-q-v1	3464.6	3458.0	3429.6	3462.8
BLQ-p-q-v4	3463.0	3455.9	3438.6	3474.8
BLQ-p-r-v4	3463.0	3456.4	3439.2	3475.4
BLQ-m-s-v1	3464.6	3456.6	3429.6	3463.7
BLQ-j-q-v3	3429.8	3440.1	3480.5	3474.2
BLQ-j-q-v5	3429.8	3440.7	3480.5	3479.4
BLQ-j-r-v3	3430.0	3440.7	3480.9	3474.6
BLQ-j-t-v5	3429.9	3438.7	3480.9	3480.0
BLQ-j-r-v5	3429.9	3441.4	3480.9	3479.8
BLQ-j-t-v3	3429.8	3437.8	3481.0	3474.7

Table 6.157. Vibrational frequencies of N11–H11 and N14–H14 in the calculated conformers of compound CGP.

Conformers	Vibrational frequencies (cm^{-1})			
	N11–H11		N14–H14	
	DFT	HF	DFT	HF
CGP-p-q-w5	3467.8	3458.1	3432.5	3463.4
CGP-p-s-w5	3467.8	3457.5	3432.5	3464.4
CGP-p-r-w5	3468.1	3458.7	3432.4	3463.4
CGP-m-r-w1	3460.8	3455.3	3438.0	3480.9
CGP-m-s-w1	3460.9	3454.4	3437.9	3482.4
CGP-m-q-w1	3461.2	3455.8	3438.2	3481.5
CGP-m-r-w2	3463.0	3456.5	3434.6	3469.7
CGP-m-s-w2	3463.0	3455.4	3434.6	3471.1
CGP-m-q-w2	3463.1	3456.8	3434.8	3470.0
CGP-g-r-w5	3456.6	3464.4	3479.9	3484.7
CGP-g-q-w5	3455.8	3464.2	3480.8	3485.2
CGP-j-q-w5	3431.2	3440.2	3469.2	3467.9
CGP-j-r-w5	3431.1	3440.4	3469.6	3468.3
CGP-j-s-w5	3431.0	3438.5	3469.5	3468.4

Table 6.158. Vibrational frequencies of N11–H11 and N14–H14 in the calculated conformers of compound CGQ.

Conformers	Vibrational frequencies (cm^{-1})			
	N11–H11		N14–H14	
	DFT	HF	DFT	HF
CGQ-p-q-w5	3467.8	3458.2	3432.3	3463.4
CGQ-m-q-w3	3467.9	3458.1	3432.2	3463.4
CGQ-p-r-w5	3468.3	3458.8	3432.5	3463.4
CGQ-m-r-w1	3460.7	3455.3	3437.9	3480.8
CGQ-m-q-w1	3461.2	3455.8	3438.5	3481.6
CGQ-j-q-w5	3431.2	3440.2	3469.2	3467.9
CGQ-j-r-w5	3431.1	3440.5	3469.6	3468.3
CGQ-j-t-w5	3431.0	3438.1	3469.5	3468.4

Table 6.159. Vibrational frequencies of N11–H11 and N14–H14 in the calculated conformers of compound CJP.

Conformers	Vibrational frequencies (cm^{-1})			
	N11–H11		N14–H14	
	DFT	HF	DFT	HF
CJP-p-q-w3	3467.7	3457.9	3432.6	3463.3
CJP-p-s-w3	3467.6	3457.3	3432.6	3464.4
CJP-p- r-w3	3468.3	3458.5	3432.4	3463.3
CJP-m-r-w1	3460.6	3455.1	3438.2	3480.9
CJP-m-r-w2	3462.9	3456.3	3435.1	3469.7
CJP-m-s-w2	3462.9	3455.2	3435.1	3471.2
CJP-m-t-w2	3462.9	3455.7	3435.1	3470.1
CJP-m-q-w2	3463.1	3456.6	3435.2	3470.0
CJP-j-q-w1	3430.1	3439.6	3469.2	3468.1
CJP-j-r-w1	3430.3	3439.8	3469.5	3468.4
CJP-j-s-w1	3430.5	3437.9	3469.5	3468.5

Table 6.160. Vibrational frequencies of N11–H11 and N14–H14 in the calculated conformers of compound CJQ.

Conformers	Vibrational frequencies (cm^{-1})			
	N11–H11		N14–H14	
	DFT	HF	DFT	HF
CJQ-m-q-w6	3468.1	3458.7	3432.8	3463.5
CJQ-m-r-w6	3467.6	3458.0	3432.3	3463.3
CJQ-p-q-w5	3467.6	3463.4	3432.8	3463.4
CJQ-m-q-w1	3460.7	3455.5	3438.6	3481.8
CJQ-p-q-w5	3467.6	3457.7	3432.7	3463.6
CJQ-p-q-w5′	3467.5	3457.8	3432.8	3463.4
CJQ-p-s-w5	3467.8	3457.1	3432.6	3464.3
CJQ-m-r-w1	3460.4	3455.0	3438.4	3480.9
CJQ-m-s-w1	3460.4	3454.3	3438.4	3482.5
CJQ-m-q-w1′	3460.7	3455.3	3438.5	3481.7
CJQ-j-q-w5	3430.2	3439.5	3469.5	3468.2
CJQ-j-r-w5	3430.4	3440.2	3469.5	3468.3

Table 6.161. Vibrational frequencies of N11–H11 and N14–H14 in the calculated conformers of compound CLP.

Conformers	Vibrational frequencies (cm^{-1})			
	N11–H11		N14–H14	
	DFT	HF	DFT	HF
CLP-p-q-w5	3467.8	3458.2	3432.6	3463.4
CLP-p-s-w5	3467.8	3457.5	3432.5	3464.4
CLP-p-r-w5	3468.1	3458.7	3432.3	3463.4
CLP-p-r-w5′	3468.1	3458.9	3432.3	3463.2
CLP-m-r-w1	3460.7	3455.3	3438.1	3480.9
CLP-m-s-w1	3460.8	3454.4	3438.0	3482.5
CLP-m-q-w1	3461.1	3455.7	3438.0	3481.5
CLP-m-q-w2	3463.1	3456.5	3434.6	3469.6
CLP-m-s-w2	3463.1	3455.4	3434.7	3471.2
CLP-m-q-w2	3463.1	3456.8	3434.8	3470.0
CLP-j-q-w5	3430.9	3440.0	3469.3	3468.0
CLP-j-r-w5	3430.7	3440.2	3469.4	3468.3
CLP-j-s-w5	3431.0	3438.3	3469.5	3468.4
CLP-j-q-w6	3433.9	3445.1	3500.2	3506.2
CLP-j-r-w6	3438.1	3447.7	3494.3	3505.6
CLP-j-s-w6	3437.8	3443.7	3494.7	3505.5

Table 6.162. Vibrational frequencies of N11–H11 and N14–H14 in the calculated conformers of compound CLQ.

Conformers	Vibrational frequencies (cm^{-1})			
	N11–H11		N14–H14	
	DFT	HF	DFT	HF
CLQ-p-q-w5	3467.8	3458.1	3432.4	3463.4
CLQ-p-s-w5	3467.8	3457.4	3432.4	3464.4
CLQ-m-q-w1	3468.1	3458.6	3432.0	3463.4
CLQ-m-r-w1	3460.7	3454.5	3437.9	3480.7
CLQ-m-r-w1′	3460.7	3455.2	3437.9	3480.9
CLQ-m-q-w1′	3461.1	3455.6	3438.3	3481.5
CLQ-m-s-w1	3460.8	3454.5	3437.9	3482.4
CLQ-j-q-w5	3430.6	3440.0	3469.3	3468.0
CLQ-j-r-w5	3430.5	3440.2	3469.6	3468.4
CLQ-j-s-w6	3430.7	3438.2	3469.7	3468.5

Table 6.163. Vibrational frequencies of N11–H11 and N14–H14 in the calculated conformers of compound DGP.

Conformers	Vibrational frequencies (cm^{-1})			
	N11–H11		N14–H14	
	DFT	HF	DFT	HF
DGP-m-r	3466.9	3458.3	3451.9	3477.9
DGP-m-s	3466.9	3457.3	3451.8	3479.2
DGP-p-q	3466.9	3458.3	3451.9	3477.9
DGP-p-s	3467.0	3457.4	3451.7	3479.3
DGP-p-a-t	3467.0	3457.7	3451.8	3478.9
DGP-m-q	3467.3	3458.7	3451.5	3478.1
DGP-k-q	3439.5	3435.6	3448.7	3491.1
DGP-k-r	3439.4	3435.0	3449.4	3491.1
DGP-k-s	3439.4	2534.3	3449.4	3493.1
DGP-g-r	3480.9	3477.6	3502.6	3493.4
DGP-g-q	3481.6	3477.9	3502.6	3492.9
DGP-j-q	3430.8	3439.6	3497.4	3486.1
DGP-j-r	3430.6	3439.9	3497.9	3486.6
DGP-j-s	3430.6	3437.9	3497.7	3486.6

Table 6.164. Vibrational frequencies of N11–H11 and N14–H14 in the calculated conformers of compound DGQ.

Conformers	Vibrational frequencies (cm^{-1})			
	N11–H11		N14–H14	
	DFT	HF	DFT	HF
DGQ-m-r	3466.9	3458.2	3451.7	3478.1
DGQ-p-q	3466.8	3458.4	3451.8	3477.9
DGQ-m-q	3467.4	3458.8	3451.8	3478.2
DGQ-m-q′	3467.4	3458.8	3451.3	3478.1
DGQ-k-q	3439.4	3435.6	3448.7	3491.0
DGQ-k-r	3439.5	3435.0	3449.4	3491.2
DGQ-g-r	3481.0	3477.7	3502.7	3493.3
DGQ-g-t	3480.9	3476.9	3502.7	3493.4
DGQ-g-q	3481.8	3477.9	3502.7	3492.9
DGQ-j-q	3430.8	3439.6	3497.5	3486.1
DGQ-j-r	3430.8	3440.1	3497.5	3486.4
DGQ-j-t	3430.7	3437.5	3497.6	3486.6

Table 6.165. Vibrational frequencies of N11–H11 and N14–H14 in the calculated conformers of compound DJP.

Conformers	Vibrational frequencies (cm^{-1})			
	N11–H11		N14–H14	
	DFT	HF	DFT	HF
DJP-m-r	3466.9	3459.1	3452.0	3478.2
DJP-p-s	3466.8	3457.2	3432.7	3479.2
DJP-p-q	3467.2	3458.2	3451.7	3477.9
DJP-m-q	3467.1	3458.5	3451.7	3478.1
DJP-p-r	3467.1	3458.3	3451.7	3478.1
DJP-k-q	3439.4	3435.3	3449.1	3491.6
DJP-k-r	3439.3	3434.8	3449.6	3491.5
DJP-k-r′	3439.3	3434.7	3449.6	3491.4
DJP-k-s	3439.2	3433.3	3449.7	3493.6
DJP-j-q	3430.2	3439.0	3497.8	3486.3
DJP-j-s	3430.2	3437.2	3497.8	3486.8
DJP-j-r	3430.2	3439.2	3497.9	3486.5

Table 6.166. Vibrational frequencies of N11–H11 and N14–H14 in the calculated conformers of compound DJQ.

Conformers	Vibrational frequencies (cm^{-1})			
	N11–H11		N14–H14	
	DFT	HF	DFT	HF
DJQ-m-q	3466.7	3457.9	3451.7	3478.0
DJQ-k-q	3439.3	3435.1	3449.1	3491.4
DJQ-k-r	3439.7	3435.1	3449.6	3491.4
DJQ-m-r	3466.7	3458.2	3452.2	3478.0
DJQ-m-s	3466.7	3457.1	3452.1	3479.2
DJQ-m-t	3466.6	3457.5	3452.1	3478.2
DJQ-m-s′	3466.8	3457.2	3452.1	3479.1
DJQ-m-q	3467.0	3458.4	3452.1	3478.1
DJQ-p-q	3466.8	3458.1	3452.2	3477.9
DJQ-m-r′	3466.7	3457.9	3452.2	3477.9
DJQ-p-q′	3466.7	3458.0	3452.3	3477.8
DJQ-p-r	3466.9	3458.4	3452.2	3478.1
DJQ-m-q	3466.8	3458.3	3452.1	3477.9
DJQ-j-q	3430.2	3439.1	3497.6	3486.4
DJQ-j-r	3430.1	3439.5	3498.1	3486.6

Table 6.167. Vibrational frequencies of N11–H11 and N14–H14 in the calculated conformers of compound DLP.

Conformers	Vibrational frequencies (cm^{-1})			
	N11–H11		N14–H14	
	DFT	HF	DFT	HF
DLP-m-r	3466.9	3458.4	3451.8	3478.0
DLP-m-s	3466.9	3457.3	3451.8	3479.2
DLP-p-q	3466.8	3458.3	3451.8	3477.9
DLP-p-s	3466.9	3457.4	3451.7	3479.3
DLP-p-t	3466.9	3457.7	3451.6	3478.4
DLP-m-q	3467.2	3458.7	3451.7	3478.1
DLP-p-r	3467.3	3458.7	3451.6	3478.2
DLP-k-q	3439.7	3435.6	3448.7	3491.2
DLP-k-r	3439.2	3435.0	3449.3	3491.2
DLP-k-s	3439.1	3433.5	3449.3	3493.2
DLP-j-q	3430.9	3439.6	3497.5	3486.1
DLP-j-s	3430.6	3437.9	3497.7	3486.7
DLP-j-r	3430.6	3439.8	3497.8	3486.5

Table 6.168. Vibrational frequencies of N11–H11 and N14–H14 in the calculated conformers of compound DLQ.

Conformers	Vibrational frequencies (cm^{-1})			
	N11–H11		N14–H14	
	DFT	HF	DFT	HF
DLQ-p-q	3466.9	3458.4	3451.9	3477.9
DLQ-k-q	3439.6	3435.6	3448.5	3491.0
DLQ-k-r	3440.0	3435.2	3449.3	3491.1
DLQ-m--r	3466.9	3458.3	3451.8	3477.9
DLQ-m-q	3467.4	3458.9	3451.9	3478.0
DLQ-m-r′	3466.9	3458.4	3451.4	3477.9
DLQ-m-q′	3467.3	3459.0	3451.5	3478.2
DLQ-j-q	3430.8	3439.6	3497.4	3486.1
DLQ-j-r	3430.9	3440.0	3497.6	3486.4
DLQ-j-t	3430.8	3437.6	3497.6	3486.7

Table 6.169. Vibrational frequencies of N11–H11 and N14–H14 in the calculated conformers of compound EGP.

Symbols are used to indicate the symmetric (∗) and asymmetric (э) vibrations

Conformers	Vibrational frequencies (cm^{-1})			
	N11–H11		N14–H14	
	DFT	HF	DFT	HF
EGP-m-r-x4	3465.4	3457.8	3443.3	3471.6
EGP-m-s-x4	3465.4	3456.8	3443.3	3472.8
EGP-m-q-x4	3465.9	3458.2	3443.1	3471.7
EGP-m-r-x1	3467.1	3458.6	3435.2	3464.3
EGP-m-s-x1	3467.1	3457.6	3435.2	3465.5
EGP-p-q-x3	3466.9	3458.6	3435.3	3464.5
EGP-p-s-x3	3466.9	3457.7	3435.3	3465.6
EGP-m-q-x1	3467.3	3459.0	3434.9	3464.4
EGP-k-q-x1	3439.3	3435.4	3434.5	3475.5
EGP-k-r-x2	3439.6	3434.5	3435.4	3485.6
EGP-k-q-x1′	3439.3	3434.9	3435.4	3475.5
EGP-k-s-x1	3439.4	3433.2	3435.4	3477.3
EGP-g-r-x1 э	3478.9	3474.8	3478.9	3474.8
∗	3486.8	3482.1	3486.8	3482.1
EGP-g-q-x1 э	3479.5	3474.8	3479.5	3474.8
∗	3487.2	3482.1	3487.2	3482.1
EGP-j-q-x3	3430.1	3439.8	3481.0	3472.4
EGP-j-r-x3	3429.9	3440.1	3481.4	3472.9
EGP-j-s-x3	3429.8	3438.2	3481.4	3473.0

Table 6.170. Vibrational frequencies of N11–H11 and N14–H14 in the calculated conformers of compound EGQ.

Symbols are used to indicate the symmetric (∗) and asymmetric (э) vibrations

Conformers	Vibrational frequencies (cm^{-1})			
	N11–H11		N14–H14	
	DFT	HF	DFT	HF
EGQ-m-r-x4	3465.6	3457.7	3443.1	3471.5
EGQ-m-q-x4	3465.8	3458.2	3443.0	3471.6
EGQ-m-r-x1	3467.0	3458.6	3435.0	3464.2
EGQ-m-q-x1	3467.4	3459.1	3435.4	3464.6
EGQ-p-q-x3	3464.7	3457.3	3446.6	3484.4
EGQ-p-r-x3	3465.2	3457.8	3447.8	3485.1
EGQ-k-q-x4	3438.6	3435.3	3436.8	3481.8
EGQ-k-r-x4	3438.5	3434.8	3437.9	3481.9
EGQ-g-r-x1 э	3479.0	3474.8	3479.0	3474.8
∗	3486.9	3482.1	3486.9	3482.1
EGQ-g-t-x1 э	3479.0	3474.5	3479.0	3474.5
∗	3486.9	3481.8	3486.9	3481.8
EGQ-g-q-x1 э	3479.5	3474.7	3479.5	3474.7
∗	3487.2	3482.0	3487.2	3482.0
EGQ-j-q-x3	3430.0	3439.9	3481.1	3472.4
EGQ-j-r-x3	3430.1	3440.3	3481.3	3472.7
EGQ-j-t-x3	3429.9	3437.8	3481.3	3473.0

Table 6.171. Vibrational frequencies of N11–H11 and N14–H14 in the calculated conformers of compound EJP.

Conformers	Vibrational frequencies (cm^{-1})			
	N11–H11		N14–H14	
	DFT	HF	DFT	HF
EJP-m-r-x4	3465.3	3456.6	3443.7	3472.8
EJP-m-s-x4	3465.3	3457.6	3443.7	3471.4
EJP-m-q-x4	3465.7	3458.0	3443.6	3471.7
EJP-p-s-x4	3465.7	3457.5	3443.6	3465.5
EJP-p-q-x4	3466.9	3458.4	3435.5	3464.3
EJP-p-r-x4	3467.3	3458.7	3435.2	3464.3
EJP-k-q-x1	3468.4	3435.1	3434.9	3476.0
EJP-k-r-x1	3439.4	3434.7	3435.7	3475.8
EJP-k-r-x1′	3439.4	3434.7	3435.7	3475.7
EJP-k-s-x1	3439.4	3432.8	3435.7	3477.7
EJP-j-q-x3	3429.5	3439.3	3481.4	3472.6
EJP-j-r-x3	3429.5	3439.4	3481.5	3472.8
EJP-j-s-x3	3429.4	3437.5	3481.4	3473.1

Table 6.172. Vibrational frequencies of N11–H11 and N14–H14 in the calculated conformers of compound EJQ.

Conformers	Vibrational frequencies (cm^{-1})			
	N11–H11		N14–H14	
	DFT	HF	DFT	HF
EJQ-m-q-x4	3465.9	3458.2	3443.6	3471.8
EJQ-m-r-x4	3465.2	3457.7	3443.1	3471.3
EJQ-p-q-x4	3466.8	3458.4	3435.6	3464.3
EJQ-p-q-x4′	3466.8	3458.2	3435.6	3464.2
EJQ-m-r-x1	3466.8	3458.1	3435.6	3464.2
EJQ-m-s-x1	3466.7	3457.5	3435.6	3465.5
EJQ-p-r-x4	3466.9	3458.5	3435.5	3464.5
EJQ-p-s-x4	3466.9	3457.3	3435.5	3465.5
EJQ-m-q-x1	3466.9	3458.6	3435.4	3464.3
EJQ-k-q-x4	3438.2	3434.9	3437.8	3482.4
EJQ-k-r-x4	3438.5	3434.3	3438.0	3482.4
EJQ-j-q-x3	3429.4	3439.3	3481.4	3472.8
EJQ-j-r-x3	3429.7	3439.9	3481.4	3472.8

Table 6.173. Vibrational frequencies of N11–H11 and N14–H14 in the calculated conformers of compound ELP.

Conformers	Vibrational frequencies (cm^{-1})			
	N11–H11		N14–H14	
	DFT	HF	DFT	HF
ELP-m-q-x4	3465.4	3456.7	3443.3	3472.8
ELP-m-s-x4	3465.4	3457.8	3443.2	3471.5
ELP-m-q-x4	3465.9	3458.2	3443.1	3471.6
ELP-m-r-x1	3466.9	3458.6	3435.3	3464.3
ELP-m-s-x1	3466.9	3457.6	3435.2	3465.6
ELP-p-s-x4	3467.0	3458.6	3435.4	3464.3
ELP-p-s-x4′	3466.9	3457.8	3435.3	3465.6
ELP-m-q-x1	3467.3	3459.0	3434.9	3464.4
ELP-k-q-x1	3439.7	3435.4	3430.7	3475.6
ELP-k-r-x1	3438.8	3434.9	3435.3	3475.5
ELP-k-s-x1	3438.8	3433.1	3435.3	3477.3
ELP-j-q-x3	3429.9	3439.6	3481.2	3472.5
ELP-j-r-x3	3429.9	3440.0	3481.4	3472.9
ELP-j-s-x3	3429.9	3437.9	3481.4	3473.1
ELP-j-q-x3′	3430.1	3439.8	3481.0	3472.4
ELP-j-r-x3′	3429.9	3440.0	3481.5	3472.9
ELP-j-s-x3′	3429.8	3438.1	3481.5	3473.0

Table 6.174. Vibrational frequencies of N11–H11 and N14–H14 in the calculated conformers of compound ELQ.

Conformers	Vibrational frequencies (cm^{-1})			
	N11–H11		N14–H14	
	DFT	HF	DFT	HF
ELQ-m-r-x4	3465.6	3457.6	3443.0	3471.5
ELQ-m-q-x4	3465.8	3458.2	3443.0	3471.6
ELQ-m-r-x1	3467.0	3458.6	3435.2	3464.2
ELQ-m-q-x1	3467.4	3459.1	3435.3	3464.5
ELQ-k-q-x4	3438.4	3435.1	3437.4	3481.9
ELQ-k-r-x4	3438.5	3434.9	3437.8	3481.9
ELQ-j-q-x3	3430.0	3439.7	3481.0	3472.6
ELQ-j-r-x3	3430.0	3440.2	3481.3	3472.8
ELQ-j-q-x3′	3429.9	3439.6	3481.1	3472.5
ELQ-j-r-x3′	3429.7	3439.8	3481.5	3472.9
ELQ-j-s-x3	3429.6	3437.9	3481.6	3473.1

Table 6.175. Vibrational frequencies of N11–H11 and N14–H14 in the calculated conformers of compound FGP.

Symbols are used to indicate the symmetric (∗) and asymmetric (э) vibrations

Conformers	Vibrational frequencies (cm^{-1})			
	N11–H11		N14–H14	
	DFT	HF	DFT	HF
FGP-m-r-x4	3465.1	3457.8	3444.2	3472.4
FGP-m-s-x4	3465.2	3456.7	3444.2	3473.7
FGP-m-q-x4	3465.6	3458.2	3444.0	3472.5
FGP-m-r-x1	3465.0	3458.7	3448.5	3464.2
FGP-m-s-x1	3465.0	3457.7	3448.5	3465.5
FGP-p-q-x4	3464.8	3458.7	3448.1	3464.2
FGP-p-s-x4	3464.8	3457.9	3448.1	3465.5
FGP-m-q-x1	3465.3	3459.1	3448.9	3464.3
FGP-p-r-x4	3465.2	3459.0	3448.6	3464.4
FGP-k-q-x1	3438.8	3435.5	3435.2	3473.2
FGP-k-r-x1	3438.7	3435.0	3436.0	3473.2
FGP-k-r-x1	3438.7	3434.8	3436.0	3471.6
FGP-g-r-x1 э	3478.8	3475.3	3478.8	3475.3
∗	3488.1	3482.7	3487.3	3482.7
FGP-g-r-x1 э	3478.8	3475.5	3478.6	3475.5
∗	3488.1	3482.9	3488.1	3482.9
FGP-g-q-x1 э	3479.4	3475.3	3479.4	3475.3
∗	3488.5	3482.6	3488.5	3482.6
FGP-j-q-x3	3429.5	3439.8	3482.9	3473.5
FGP-j-r-x3	3429.5	3440.2	3483.3	3474.0

FGP-j-s-x3	3430.2	3437.9	3514.0	3474.1

Table 6.176. Vibrational frequencies of N11–H11 and N14–H14 in the calculated conformers of compound FGQ.

Conformers	Vibrational frequencies (cm^{-1})			
	N11–H11		N14–H14	
	DFT	HF	DFT	HF
FGQ-m-r-x4	3465.2	3457.6	3443.9	3472.4
FGQ-m-q-x4	3465.5	3458.2	3444.0	3472.5
FGQ-p-q-x4	3464.8	3457.2	3448.2	3484.7
FGQ-m-r-x1	3464.8	3458.7	3448.1	3464.1
FGQ-m-q-x1	3465.2	3459.2	3448.9	3464.5
FGQ-k-r-x4	3438.0	3457.2	3438.7	3484.7
FGQ-g-r-x1	3478.9	3475.3	3488.2	3482.7
FGQ-g-t-x1	3478.9	3474.9	3488.3	3482.5
FGQ-g-q-x1	3479.6	3475.3	3488.0	3482.6
FGQ-j-q-x3	3429.5	3439.8	3483.1	3473.5
FGQ-j-r-x3	3429.6	3440.3	3483.2	3473.8
FGQ-j-t-x3	3430.2	3437.7	3513.7	3474.1

Table 6.177. Vibrational frequencies of N11–H11 and N14–H14 in the calculated conformers of compound FJP.

Conformers	Vibrational frequencies (cm^{-1})			
	N11–H11		N14–H14	
	DFT	HF	DFT	HF
FJP-m-r-x4	3465.0	3457.6	3444.2	3472.3
FJP-m-s-x4	3465.0	3456.6	3444.1	3473.6
FJP-m-q-x4	3465.5	3457.9	3444.2	3472.5
FJP-p-q-x4	3464.8	3458.5	3448.9	3464.2
FJP-p-s-x4	3464.7	3457.5	3448.9	3465.5
FJP-k-q-x1	3439.1	3435.2	3435.6	3473.7
FJP-p-r-x1	3438.6	3458.8	3436.1	3464.3
FJP-k-r-x1	3438.6	3434.8	3436.1	3473.8
FJP-k-s-x1	3438.7	3432.9	3436.2	3475.3
FJP-j-q-x3	3428.9	3439.2	3483.0	3473.7
FJP-j-r-x3	3429.0	3439.5	3483.2	3474.0
FJP-j-s-x3	3428.9	3437.4	3483.3	3474.2

Table 6.178. Vibrational frequencies of N11–H11 and N14–H14 in the calculated conformers of compound FJQ.

Conformers	Vibrational frequencies (cm^{-1})			
	N11–H11		N14–H14	
	DFT	HF	DFT	HF
FJQ-m-q-x4	3465.2	3458.1	3444.3	3472.3
FJQ-m-r-x4	3464.9	3457.4	3444.2	3472.4
FJQ-p-r-x4	3465.0	3459.1	3449.4	3464.6
FJQ-p-q-x4	3464.7	3457.0	3448.6	3484.7
FJQ-p-q-x4′	3464.7	3458.5	3448.6	3464.2
FJQ-m-q-x1	3465.0	3458.9	3448.9	3464.4
FJQ-m-r-x1	3464.7	3458.3	3448.4	3464.2
FJQ-k-q-x4	3438.5	3435.2	3437.9	3482.4
FJQ-k-r-x4	3438.3	3434.5	3439.2	3482.5
FJQ-j-q-x3	3428.9	3439.2	3483.0	3473.8
FJQ-j-r-x3	3429.2	3439.8	3483.4	3473.9
FJQ-j-r-x3′	3429.3	3440.0	3483.2	3473.8
FJQ-j-t-x3	3429.2	3437.2	3483.2	3474.4
FJQ-j-q-x3′	3429.0	3439.4	3483.3	3473.6

Table 6.179. Vibrational frequencies of N11–H11 and N14–H14 in the calculated conformers of compound FLP.

Conformers	Vibrational frequencies (cm^{-1})			
	N11–H11		N14–H14	
	DFT	HF	DFT	HF
FLP-m-r-x4	3465.1	3457.8	3444.1	3472.3
FLP-m-q-x4	3465.5	3458.2	3443.9	3472.5
FLP-m-r-x1	3465.0	3458.7	3448.4	3464.3
FLP-m-s-x4	3465.0	3456.7	3448.5	3473.7
FLP-m-s-x1	3465.0	3457.7	3448.4	3465.6
FLP-p-q-x4	3464.8	3458.7	3448.2	3464.2
FLP-p-s-x4	3464.9	3457.9	3448.2	3465.5
FLP-m-q-x1	3465.2	3459.0	3448.5	3464.4
FLP-k-q-x1	3439.2	3435.4	3435.3	3473.2
FLP-k-r-x1	3438.5	3435.0	3436.1	3473.2
FLP-k-s-x1	3438.5	3433.1	3436.0	3474.8
FLP-j-q-x3	3429.4	3439.6	3483.1	3473.6
FLP-j-r-x3	3429.4	3440.0	3483.1	3474.0
FLP-j-s-x3′	3429.4	3437.9	3483.2	3474.1
FLP-j-q-x3′	3429.6	3439.8	3482.8	3473.5
FLP-j-r-x3′	3429.5	3440.0	3483.5	3474.0

FLP-j-s-x3	3429.4	3438.1	3483.5	3474.1

Table 6.180. Vibrational frequencies of N11–H11 and N14–H14 in the calculated conformers of compound FLQ.

Conformers	Vibrational frequencies (cm^{-1})			
	N11–H11		N14–H14	
	DFT	HF	DFT	HF
FLQ-p-q-x2	3465.2	3458.3	3444.0	3473.5
FLQ-m-r-x4	3465.2	3457.6	3443.9	3472.4
FLQ-m-q-x4	3465.5	3458.2	3444.0	3472.5
FLQ-p-q-x4	3465.0	3458.5	3448.4	3464.2
FLQ-m-r-x1	3464.8	3458.7	3448.2	3464.2
FLQ-m-q-x1	3465.1	3459.1	3449.0	3464.6
FLQ-m-q-x1′	3465.1	3459.3	3449.0	3464.2
FLQ-p-r-x4	3465.0	3457.6	3448.6	3485.1
FLQ-p-r-x4′	3465.0	3459.1	3448.6	3464.3
FLQ-k-q-x4	3438.5	3435.1	3437.9	3482.2
FLQ-k-q-x1	3439.2	3435.5	3435.2	3473.1
FLQ-k-r-x4	3438.1	3434.9	3438.5	3482.2
FLQ-k-r-x1	3436.1	3435.0	3439.0	3473.2
FLQ-j-q-x3	3429.4	3439.7	3483.0	3473.7
FLQ-j-r-x3	3429.4	3440.2	3483.2	3473.8

6.1.5. Changes in the vibrational frequencies, caused by the formation of IHBs.

This section presents the tables reporting the changes in the vibrational frequencies of N11–H11 and H14–H14 bonds when they form IHBs. The table also indicate the IHB formed by the given N–H bonds. The changes are calculated as the difference between the average vibrational frequency of the given N–H bond over the conformer where it does not form any IHB and its vibrational frequency in a conformer where it forms an IHB. In this way, a negative change indicates an increase of the vibrational frequency, that is a blue shift, and a positive change indicates a decrease of the vibrational frequencies, that is a red shift.

Table 6.181. Changes in the IR vibrational frequencies of the N11–H11 and N14–H14 bonds in the conformers of compound AGP containing IHBs.

Conformers	Vibrational frequency change (cm^{-1})					
	N11–H11			N14–H14		
	IHB	DFT	HF	IHB	DFT	HF
AGP-m-r-u1	H11····O10 H11····O13	-35.8	-18.7	H14····O9	46.5	10.2
AGP-m-s-u1	H11····O10 H11····O13	-35.8	-17.6	H14····O9	46.5	8.9
AGP-p-t-u3	H11····O9 H11····O13	-35.7	-17.9	H14····O10	46.8	9.8
AGP-m-q-u1	H11····O10 H11····O13	-36.1	-19.0	H14····O9	46.8	10.1
AGP-p-r-u3	H11····O9 H11····O13	-36.0	-19.0	H14····O10	46.6	10.1
AGP-k-q-u1	H11····O13	-8.5	4.2	H14····O10	55.1	1.0
AGP-k-r-u1	H11····O13	-7.9	5.3	H14····O10	53.9	0.9
AGP-m-r-u2	H11····O10 H11····O13	-34.0	-17.0	H14····O9	28.6	-7.8
AGP-g-r-u3	H11····O9	-48.0	-35.5			
		-55.3	-43.4			
AGP-g-q-u3	H11····O9	-48.4	-35.4			
		-55.8	-43.3			

Table 6.182. Changes in the IR vibrational frequencies of the N11–H11 and N14–H14 bonds in the conformers of compound AGQ containing IHBs.

Conformers	Vibrational frequency change (cm^{-1})					
	N11–H11			N14–H14		
	IHB	DFT	HF	IHB	DFT	HF
AGQ-m-r-u1	H11····O10 H11····O13	-35.9	-18.3	H14····O9	46.6	10.2
AGQ-m-q-u1	H11····O10 H11····O13	-36.1	-18.8	H14····O9	46.1	9.8
AGQ-k-q-u1	H11····O13	-8.4	4.4	H14····O10	55.0	1.0
AGQ-k-r-u1	H11····O13	-8.3	5.8	H14····O10	54.5	0.9
AGQ-m-r-u2	H11····O10 H11····O13	-34.0	-16.5	H14····O9	28.5	-7.9
AGQ-m-q-u2	H11····O10 H11····O13	-34.3	-17.1	H14····O9	28.4	-8.2
AGQ-g-r-u3	H11····O9	-47.9	-35.2			
		-55.2	-43.1			
AGQ-g-t-u3	H11····O9	-47.9	-34.8			
		-55.3	-42.7			
AGQ-g-q-u3	H11····O9	-48.5	-35.1			
		-55.9	-43.0			

Table 6.183. Changes in the IR vibrational frequencies of the N11–H11 and N14–H14 bonds in the conformers of compound AJP containing IHBs.

Conformers	Vibrational frequency change (cm^{-1})					
	N11–H11			N14–H14		
	IHB	DFT	HF	IHB	DFT	HF
AJP-m-r-u1	H11····O10 H11····O13	-35.8	-18.8	H14····O9	46.4	10.4
AJP-m-s-u1	H11····O10 H11····O13	-35.9	-17.8	H14····O9	46.4	9.1
AJP-m-q-u1	H11····O10 H11····O13	-36.6	-19.0	H14····O9	46.6	10.1
AJP-k-q-u1	H11····O13	-8.9	4.2	H14····O10	55.1	0.8
AJP-k-r-u1	H11····O13	-8.1	4.6	H14····O10	54.5	0.8
AJP-k-s-u1	H11····O13	-8.1	6.4	H14····O10	54.5	-0.9
AJP-m-r-u2	H11····O10 H11····O13	-34.5	-17.1	H14····O9	28.4	-7.7
AJP-m-s-u2	H11····O10 H11····O13	-34.5	-16.1	H14····O9	28.4	-9.2
AJP-m-q-u2	H11····O10 H11····O13	-35.0	-17.4	H14····O9	27.9	-8.1

Table 6.184. Changes in the IR vibrational frequencies of the N11–H11 and N14–H14 bonds in the conformers of compound AJQ containing IHBs.

Conformers	Vibrational frequency change (cm^{-1})					
	N11–H11			N14–H14		
	IHB	DFT	HF	IHB	DFT	HF
AJQ-p-q-u5	H11····O9 H11····O13	-35.8	-17.3	H14····O10	46.3	-2.1
AJQ-m-q-u1	H11····O10 H11····O13	-36.1	-18.1	H14····O9	46.4	10.1
AJQ-m-q-u2	H11····O10 H11····O13	-34.3	-16.8	H14····O9	28.7	-7.9
AJQ-m-r-u2	H11····O10 H11····O13	-33.8	-16.1	H14····O9	28.3	-7.9
AJQ-p-q-u3	H11····O9 H11····O13	-35.4	-18.0	H14····O10	46.4	10.2
AJQ-m-r-u1	H11····O10 H11····O13	-35.5	-17.7	H14····O9	46.3	10.3
AJQ-p-q-u5	H11····O9 H11····O13	-35.4	-17.2	H14····O10	46.4	-2.1
AJQ-m-s-u1	H11····O10 H11····O13	-35.4	-17.0	H14····O9	46.3	9.0
AJQ-p-r-u3	H11····O9 H11····O13	-36.0	-18.1	H14····O10	46.1	10.1
AJQ-p-s-u3	H11····O9 H11····O13	-36.0	-16.9	H14····O10	46.1	9.0
AJQ-m-q-u1	H11····O10 H11····O13	-35.9	-18.1	H14····O9	46.4	10.2
AJQ-k-q-u1	H11····O13	-8.0	5.1	H14····O10	54.8	0.5
AJQ-k-q-u1	H11····O13	-8.3	5.1	H14····O10	54.5	0.5

Table 6.185. Changes in the IR vibrational frequencies of the N11–H11 and N14–H14 bonds in the conformers of compound ALP containing IHBs.

Conformers	Vibrational frequency change (cm^{-1})					
	N11–H11			N14–H14		
	IHB	DFT	HF	IHB	DFT	HF
ALP-m-r-u1	H11····O10 H11····O13	-35.7	-18.2	H14····O9	46.5	10.3
ALP-m-s-u1	H11····O10 H11····O13	-35.7	-17.3	H14····O9	46.5	9.0
ALP-m-q-u1	H11····O10 H11····O13	-36.1	-18.6	H14····O9	46.5	10.1
ALP-k-q-u1	H11····O13	-7.3	4.6	H14····O10	55.2	0.9
ALP-k-r-u1	H11····O13	-7.8	5.0	H14····O10	54.3	0.8

ALP-k-q-u1	H11····O13	-8.5	4.5	H14····O10	55.0	1.0
ALP-k-r-u1′	H11····O13	-7.8	5.1	H14····O10	54.4	0.9
ALP-k-s-u1	H11····O13	-7.7	6.8	H14····O10	54.4	-0.7
ALP-k-r-u3	H11····O13	-8.4	5.7	H14····O10	56.6	-3.6
ALP-m-r-u2	H11····O10 H11····O13	-34.3	-16.6	H14····O9	28.5	-7.8
ALP-m-s-u2	H11····O10 H11····O13	-34.3	-15.7	H14····O9	28.6	-9.2
ALP-m-q-u2	H11····O10 H11····O13	-35.1	-17.0	H14····O9	28.7	-8.2

Table 6.186. Changes in the IR vibrational frequencies of the N11–H11 and N14–H14 bonds in the conformers of compound ALQ containing IHBs.

Conformers	Vibrational frequency change (cm^{-1})					
	N11–H11			N14–H14		
	IHB	DFT	HF	IHB	DFT	HF
ALQ-m-r-u1	H11····O10 H11····O13	-35.6	-17.5	H14····O9	46.8	10.3
ALQ-m-q-u1	H11····O10 H11····O13	-35.8	-18.0	H14····O9	46.1	9.9
ALQ-k-q-u1	H11····O13	-8.5	5.3	H14····O10	54.9	0.9
ALQ-k-r-u1	H11····O13	-8.0	5.8	H14····O10	54.3	0.8
ALQ-m-r-u2	H11····O10 H11····O13	-33.9	-15.7	H14····O9	28.6	-7.9
ALQ-m-q-u2	H11····O10 H11····O13	-34.1	-16.3	H14····O9	28.4	-8.2

Table 6.187. Changes in the IR vibrational frequencies of the N11–H11 and N14–H14 bonds in the conformers of compound BGP containing IHBs.

Conformers	Vibrational frequency change (cm^{-1})					
	N11–H11			N14–H14		
	IHB	DFT	HF	IHB	DFT	HF
BGP-p-s-v3	H11····O9 H11····O13	-34.5	-16.5	H14····O10	51.2	16.2
BGP-p-t-v3	H11····O9 H11····O13	-34.5	-16.6	H14····O10	51.3	17.1
BGP-m-r-v1	H11····O10 H11····O13	-34.8	-17.4	H14····O9	51.4	17.4
BGP-m-s-v1	H11····O10 H11····O13	-34.8	-16.3	H14····O9	51.4	16.2
BGP-m-q-v1	H11····O10 H11····O13	-34.8	-17.7	H14····O9	51.0	17.4

BGP-k-q-v3	H11····O13	-8.7	5.1	H14····O10	61.5	12.3
BGP-k-r-v3	H11····O13	-8.7	5.7	H14····O10	60.7	12.2
BGP-k-s-v3	H11····O13	-8.8	7.2	H14····O10	60.7	10.5
BGP-m-r-v2	H11····O10 H11····O13	-33.1	-15.8	H14····O9	42.0	5.1
BGP-m-s-v2	H11····O10 H11····O13	-33.1	-14.8	H14····O9	42.0	3.6
BGP-m-q-v2	H11····O10 H11····O13	-41.8	-16.3	H14····O9	41.9	4.8
BGP-g-r-v1	H11····O9	-49.5	-35.8			
		-59.0	-44.2			
BGP-g-q-v1	H11····O9	-49.8	-35.8			
		-60.0	-43.9			

Table 6.188. Changes in the IR vibrational frequencies of the N11–H11 and N14–H14 bonds in the conformers of compound BGQ containing IHBs.

Conformers	Vibrational frequency change (cm^{-1})					
	N11–H11			N14–H14		
	IHB	DFT	HF	IHB	DFT	HF
BGQ-m-r-v1	H11····O10 H11····O13	-34.6	-18.0	H14····O9	51.0	12.0
BGQ-m-q-v1	H11····O10 H11····O13	-34.9	-18.0	H14····O9	50.6	11.6
BGQ-k-q-v1	H11····O13	-9.0	4.5	H14····O10	61.1	6.8
BGQ-k-r-v1	H11····O13	-8.3	5.0	H14····O10	60.6	6.5
BGQ-m-r-v2	H11····O10 H11····O13	-33.4	-16.2	H14····O9	42.2	-0.4
BGQ-m-q-v2	H11····O10 H11····O13	-33.2	-16.8	H14····O9	42.1	-0.8

Table 6.189. Changes in the IR vibrational frequencies of the N11–H11 and N14–H14 bonds in the conformers of compound BJP containing IHBs.

Conformers	Vibrational frequency change (cm^{-1})					
	N11–H11			N14–H14		
	IHB	DFT	HF	IHB	DFT	HF
BJP-p-q-v3	H11····O9 H11····O13	-34.7	-18.0	H14····O10	50.9	11.9
BJP-p-s-v3	H11····O9 H11····O13	-34.7	-16.6	H14····O10	50.9	10.7
BJP-p-r-v3	H11····O9 H11····O13	-35.2	-17.8	H14····O10	50.9	11.9
BJP-k-q-v1	H11····O13	-9.2	5.0	H14····O10	61.1	6.5
BJP-k-r-v1	H11····O13	-8.9	5.5	H14····O10	60.5	6.3
BJP-k-s-v1	H11····O13	-9.0	7.0	H14····O10	60.5	4.7
BJP-m-r-v2	H11····O10 H11····O13	-33.4	-16.1	H14····O9	41.7	-0.4
BJP-m-s-v2	H11····O10 H11····O13	-33.4	-15.1	H14····O9	41.7	-1.9
BJP-m-q-v2	H11····O10 H11····O13	-33.8	-16.4	H14····O9	41.8	-0.8

Table 6.190. Changes in the IR vibrational frequencies of the N11–H11 and N14–H14 bonds in the conformers of compound BJQ containing IHBs.

Conformers	Vibrational frequency change (cm^{-1})					
	N11–H11			N14–H14		
	IHB	DFT	HF	IHB	DFT	HF
BJQ-p-r-v3	H11····O9 H11····O13	-35.2	-18.0	H14····O10	50.8	11.8
BJQ-m-s-v1	H11····O10 H11····O13	-34.8	-16.5	H14····O9	50.9	10.5
BJQ-m-t-v1	H11····O10 H11····O13	-34.7	-16.8	H14····O9	50.9	11.5
BJQ-m-q-v2	H11····O10 H11····O13	-33.7	-16.6	H14····O9	41.5	-1.0
BJQ-m-r-v2	H11····O10 H11····O13	-33.3	-16.0	H14····O9	42.1	-0.3
BJQ-m-q-v1	H11····O10 H11····O13	-35.0	-17.7	H14····O9	50.8	11.8
BJQ-p-q-v3	H11····O9 H11····O13	-34.5	-17.5	H14····O10	50.8	11.9
BJQ-p-q-v3′	H11····O9	-34.5	-17.5	H14····O10	50.8	11.9

	H11····O13					
BJQ-p-r-v3	H11····O9 H11····O13	-35.1	-17.8	H14····O10	50.7	11.7
BJQ-p-s-v3	H11····O9 H11····O13	-35.0	-16.5	H14····O10	50.7	10.6

Table 6.191. Changes in the IR vibrational frequencies of the N11–H11 and N14–H14 bonds in the conformers of compound BLP containing IHBs.

Conformers	Vibrational frequency change (cm^{-1})					
	N11–H11			N14–H14		
	IHB	DFT	HF	IHB	DFT	HF
BLP-k-q-v1	H11····O13	-8.7	5.2	H14····O10	61.3	12.0
BLP-p-s-v3	H11····O9 H11····O13	-34.3	-16.3	H14····O10	51.1	15.8
BLP-p-t-v3	H11····O9 H11····O13	-34.4	-16.5	H14····O10	51.1	16.8
BLP-m-r-v1	H11····O10 H11····O13	-34.7	-17.3	H14····O9	51.2	17.2
BLP-m-s-v1	H11····O10 H11····O13	-34.7	-16.2	H14····O9	51.0	15.8
BLP-m-r-v1′	H11····O10 H11····O13	-34.6	-17.6	H14····O9	51.0	17.1
BLP-k-r-v1	H11····O13	-8.3	5.9	H14····O10	60.9	11.9
BLP-k-s-v1	H11····O13	-8.3	7.3	H14····O10	60.8	10.2
BLP-p-q-v4	H11····O9 H11····O13	-33.0	-15.6	H14····O10	41.9	4.9
BLP-p-s-v4	H11····O9 H11····O13	-33.0	-14.9	H14····O10	41.9	3.4
BLP-p-t-v4	H11····O9 H11····O13	-33.0	-15.0	H14····O10	41.9	4.4
BLP-p-r-v4	H11····O9 H11····O13	-33.1	-16.0	H14····O10	41.8	4.4

Table 6.192. Changes in the IR vibrational frequencies of the N11–H11 and N14–H14 bonds in the conformers of compound BLQ containing IHBs.

Conformers	Vibrational frequency change (cm^{-1})					
	N11–H11			N14–H14		
	IHB	DFT	HF	IHB	DFT	HF
BLQ-p-q-v3	H11····O9 H11····O13	-34.3	-17.5	H14····O10	51.1	14.6
BLQ-p-r-v3	H11····O9 H11····O13	-34.7	-17.9	H14····O10	50.6	14.2
BLQ-p-r-v3	H11····O9 H11····O13	-34.6	-17.9	H14····O10	50.9	14.4
BLQ-k-q-v1	H11····O13	-8.4	5.2	H14····O10	61.4	9.3
BLQ-k-r-v1	H11····O13	-8.5	5.3	H14····O10	60.8	9.2
BLQ-m-r-v1	H11····O10 H11····O13	-34.5	-17.6	H14····O9	51.4	14.6
BLQ-m-q-v1	H11····O10 H11····O13	-34.7	-18.1	H14····O9	51.2	14.3
BLQ-p-q-v4	H11····O9 H11····O13	-33.1	-16.0	H14····O10	42.2	2.3
BLQ-p-r-v4	H11····O9 H11····O13	-33.1	-16.5	H14····O10	41.6	1.7
BLQ-m-s-v1	H11····O9 H11····O13	-34.7	-16.7	H14····O10	51.2	13.4

Table 6.193. Changes in the IR vibrational frequencies of the N11–H11 and N14–H14 bonds in the conformers of compound CGP containing IHBs.

Conformers	Vibrational frequency change (cm^{-1})					
	N11–H11			N14–H14		
	IHB	DFT	HF	IHB	DFT	HF
CGP-p-q-w5	H11····O9 H11····O13	-36.7	-18.4	H14····O10	36.9	4.8
CGP-p-s-w5	H11····O9 H11····O13	-36.7	-17.8	H14····O10	36.9	3.8
CGP-p-r-w5	H11····O9 H11····O13	-37.0	-19.0	H14····O10	37.0	4.8
CGP-m-r-w1	H11····O10 H11····O13	-29.7	-15.6	H14····O9	31.4	-12.7
CGP-m-s-w1	H11····O10 H11····O13	-29.8	-14.7	H14····O9	31.5	-14.2
CGP-m-q-w1	H11····O10 H11····O13	-30.1	-16.1	H14····O9	31.2	-13.3

CGP-m-r-w2	H11····O10 H11····O13	-31.9	-16.8	H14····O9	34.8	-1.5
CGP-m-s-w2	H11····O10 H11····O13	-31.9	-15.7	H14····O9	34.8	-2.9
CGP-m-q-w2	H11····O10 H11····O13	-32.0	-17.1	H14····O9	34.6	-1.8
CGP-g-r-w5	H11····O9	-25.5	-24.7			
CGP-g-q-w5	H11····O9	-24.7	-24.5			

Table 6.194. Changes in the IR vibrational frequencies of the N11–H11 and N14–H14 bonds in the conformers of compound CGQ containing IHBs.

Conformers	Vibrational frequency change (cm^{-1})					
	N11–H11			N14–H14		
	IHB	DFT	HF	IHB	DFT	HF
CGQ-p-q-w5	H11····O9 H11····O13	-36.7	-18.6	H14····O10	37.1	4.8
CGQ-m-q-w3	H11····O10 H11····O13	-36.8	-18.5	H14····O9	37.2	4.8
CGQ-p-r-w5	H11····O9 H11····O13	-37.2	-19.2	H14····O10	36.9	4.8
CGQ-m-r-w1	H11····O10 H11····O13	-29.6	-15.7	H14····O9	31.5	-12.6
CGQ-m-q-w1	H11····O10 H11····O13	-30.1	-16.2	H14····O9	30.9	-13.4

Table 6.195. Changes in the IR vibrational frequencies of the N11–H11 and N14–H14 bonds in the conformers of compound CJP containing IHBs.

Conformers	Vibrational frequency change (cm^{-1})					
	N11–H11			N14–H14		
	IHB	DFT	HF	IHB	DFT	HF
CJP-p-q-w3	H11····O9 H11····O13	-37.4	-18.8	H14····O10	36.8	5.0
CJP-p-s-w3	H11····O9 H11····O13	-37.3	-18.2	H14····O10	36.8	3.9
CJP-p- r-w3	H11····O9 H11····O13	-38.0	-19.4	H14····O10	37.0	5.0
CJP-m-r-w1	H11····O10 H11····O13	-30.3	-16.0	H14····O9	31.2	-12.6
CJP-m-r-w2	H11····O10 H11····O13	-32.6	-17.2	H14····O9	34.3	-1.4
CJP-m-s-w2	H11····O10 H11····O13	-32.6	-16.1	H14····O9	34.3	-2.9

CJP-m-t-w2	H11····O10 H11····O13	-32.6	-16.6	H14····O9	34.3	-1.8
CJP-m-q-w2	H11····O10 H11····O13	-32.8	-17.5	H14····O9	34.2	-1.7

Table 6.196. Changes in the IR vibrational frequencies of the N11–H11 and N14–H14 bonds in the conformers of compound CJQ containing IHBs.

Conformers	Vibrational frequency change (cm^{-1})					
	N11–H11			N14–H14		
	IHB	DFT	HF	IHB	DFT	HF
CJQ-m-q-w6	H11····O10 H11····O13	-37.8	-18.8	H14····O9	36.7	4.8
CJQ-m-r-w6	H11····O10 H11····O13	-37.3	-18.1	H14····O9	37.2	5.0
CJQ-p-q-w5	H11····O10 H11····O13	-37.3	-23.5	H14····O10	36.7	4.9
CJQ-m-q-w1	H11····O10 H11····O13	-30.4	-15.6	H14····O9	30.9	-13.5
CJQ-p-q-w5	H11····O10 H11····O13	-37.3	-17.8	H14····O10	36.8	4.7
CJQ-p-q-w5′	H11····O10 H11····O13	-37.2	-17.9	H14····O10	36.7	4.9
CJQ-p-s-w5	H11····O10 H11····O13	-37.5	-17.2	H14····O10	36.9	4.0
CJQ-m-r-w1	H11····O10 H11····O13	-30.1	-15.1	H14····O9	31.1	-12.6
CJQ-m-s-w1	H11····O10 H11····O13	-30.1	-14.4	H14····O9	31.1	-14.2
CJQ-m-q-w1′	H11····O10 H11····O13	-30.4	-15.4	H14····O9	31.0	-13.4

Table 6.197. Changes in the IR vibrational frequencies of the N11–H11 and N14–H14 bonds in the conformers of compound CLP containing IHBs.

Conformers	Vibrational frequency change (cm^{-1})					
	N11–H11			N14–H14		
	IHB	DFT	HF	IHB	DFT	HF
CLP-p-q-w5	H11····O9 H11····O13	-34.1	-15.7	H14····O10	50.8	23.6
CLP-p-s-w5	H11····O9 H11····O13	-34.1	-15.0	H14····O10	50.9	22.6
CLP-p-r-w5	H11····O9 H11····O13	-34.4	-16.2	H14····O10	51.1	23.6

CLP-p-r-w5′	H11····O9 H11····O13	-34.4	-16.4	H14····O10	51.1	23.8
CLP-m-r-w1	H11····O10 H11····O13	-27.0	-12.8	H14····O9	45.3	6.1
CLP-m-s-w1	H11····O10 H11····O13	-27.1	-11.9	H14····O9	45.4	4.5
CLP-m-q-w1	H11····O10 H11····O13	-27.4	-13.2	H14····O9	45.4	5.5
CLP-m-q-w2	H11····O10 H11····O13	-29.4	-14.0	H14····O9	48.8	17.4
CLP-m-s-w2	H11····O10 H11····O13	-29.4	-12.9	H14····O9	48.7	15.8
CLP-m-q-w2	H11····O10 H11····O13	-29.4	-14.3	H14····O9	48.6	17.0

Table 6.198. Changes in the IR vibrational frequencies of the N11–H11 and N14–H14 bonds in the conformers of compound CLQ containing IHBs.

Conformers	Vibrational frequency change (cm^{-1})					
	N11–H11			N14–H14		
	IHB	DFT	HF	IHB	DFT	HF
CLQ-p-q-w5	H11····O9 H11····O13	-37.2	-18.6	H14····O10	37.1	4.9
CLQ-p-s-w5	H11····O9 H11····O13	-37.2	-17.9	H14····O10	37.1	3.9
CLQ-m-q-w1	H11····O10 H11····O13	-37.5	-19.1	H14····O9	37.5	4.9
CLQ-m-r-w1	H11····O10 H11····O13	-30.1	-15.0	H14····O9	31.6	-12.4
CLQ-m-r-w1′	H11····O10 H11····O13	-30.1	-15.7	H14····O9	31.6	-12.6
CLQ-m-q-w1′	H11····O10 H11····O13	-30.5	-16.1	H14····O9	31.2	-13.2
CLQ-m-s-w1	H11····O10 H11····O13	-30.2	-15.0	H14····O9	31.6	-14.1

Table 6.199. Changes in the IR vibrational frequencies of the N11–H11 and N14–H14 bonds in the conformers of compound DGP containing IHBs.

Conformers	Vibrational frequency change (cm^{-1})					
	N11–H11			N14–H14		
	IHB	DFT	HF	IHB	DFT	HF
DGP-m-r	H11····O10 H11····O13	-36.2	-19.2	H14····O9	45.8	8.5
DGP-m-s	H11····O10 H11····O13	-36.2	-18.2	H14····O9	45.9	7.2
DGP-p-q	H11····O9 H11····O13	-36.2	-19.2	H14····O10	45.8	8.5
DGP-p-s	H11····O9 H11····O13	-36.3	-18.3	H14····O10	46.0	7.1
DGP-p-t	H11····O9 H11····O13	-36.3	-18.6	H14····O10	45.9	7.5
DGP-m-q	H11····O10 H11····O13	-36.6	-19.6	H14····O9	46.2	8.3
DGP-k-q	H11····O13	-8.8	3.5	H14····O10	49.0	-4.7
DGP-k-r	H11····O13	-8.7	4.1	H14····O10	48.3	-4.7
DGP-k-s	H11····O13	-8.7	4.8	H14····O10	48.3	-6.7
DGP-g-r	H11····O9	-50.2	-38.5			
DGP-g-q	H11····O9	-50.9	-38.8			

Table 6.200. Changes in the IR vibrational frequencies of the N11–H11 and N14–H14 bonds in the conformers of compound DGQ containing IHBs.

Conformers	Vibrational frequency change (cm^{-1})					
	N11–H11			N14–H14		
	IHB	DFT	HF	IHB	DFT	HF
DGQ-m-r	H11····O10 H11····O13	-36.1	-19.1	H14····O9	45.8	8.3
DGQ-p-q	H11····O9 H11····O13	-36.0	-19.3	H14····O10	45.7	8.5
DGQ-m-q	H11····O10 H11····O13	-36.6	-19.7	H14····O9	45.7	8.2
DGQ-m-q′	H11····O10 H11····O13	-36.6	-19.7	H14····O9	46.2	8.3
DGQ-k-q	H11····O13	-8.6	3.5	H14····O10	48.8	-4.6
DGQ-k-r	H11····O13	-8.7	4.1	H14····O10	48.1	-4.8
DGQ-g-r	H11····O9	-50.2	-38.6			
DGQ-g-t	H11····O9	-50.1	-37.8			
DGQ-g-q	H11····O9	-51.0	-38.8			

Table 6.201. Changes in the IR vibrational frequencies of the N11–H11 and N14–H14 bonds in the conformers of compound CJP containing IHBs.

Conformers	Vibrational frequency change (cm^{-1})					
	N11–H11			N14–H14		
	IHB	DFT	HF	IHB	DFT	HF
DJP-m-r	H11····O10 H11····O13	-36.7	-19.6	H14····O9	45.8	8.3
DJP-p-s	H11····O9 H11····O13	-36.6	-17.7	H14····O10	65.1	7.3
DJP-p-q	H11····O9 H11····O13	-37.0	-18.7	H14····O10	46.1	8.6
DJP-m-q	H11····O10 H11····O13	-36.9	-19.0	H14····O9	46.1	8.4
DJP-p-r	H11····O9 H11····O13	-36.9	-18.8	H14····O10	46.1	8.4
DJP-k-q	H11····O13	-9.2	4.2	H14····O10	48.7	-5.1
DJP-k-r	H11····O13	-9.1	4.7	H14····O10	48.2	-5.0
DJP-k-r′	H11····O13	-9.1	4.8	H14····O10	48.2	-4.9
DJP-k-s	H11····O13	-9.0	6.2	H14····O10	48.1	-7.1

Table 6.202. Changes in the IR vibrational frequencies of the N11–H11 and N14–H14 bonds in the conformers of compound CJQ containing IHBs.

Conformers	Vibrational frequency change (cm^{-1})					
	N11–H11			N14–H14		
	IHB	DFT	HF	IHB	DFT	HF
DJQ-m-q	H11····O10 H11····O13	-36.5	-18.6	H14····O9	46.2	8.5
DJQ-k-q	H11····O13	-9.1	4.2	H14····O10	48.8	-4.9
DJQ-k-r	H11····O13	-9.5	4.2	H14····O10	48.3	-4.9
DJQ-m-r	H11····O10 H11····O13	-36.5	-18.9	H14····O9	45.7	8.5
DJQ-m-s	H11····O10 H11····O13	-36.5	-17.8	H14····O9	45.8	7.3
DJQ-m-t	H11····O10 H11····O13	-36.4	-18.2	H14····O9	45.8	8.3
DJQ-m-s′	H11····O10 H11····O13	-36.6	-17.9	H14····O9	45.8	7.4
DJQ-m-q	H11····O10 H11····O13	-36.8	-19.1	H14····O9	45.8	8.4
DJQ-p-q	H11····O9 H11····O13	-36.6	-18.8	H14····O10	45.7	8.6
DJQ-m-r′	H11····O10 H11····O13	-36.5	-18.6	H14····O9	45.7	8.6
DJQ-p-q′	H11····O9	-36.5	-18.7	H14····O10	45.6	8.7

	H11····O13					
DJQ-p-r	H11····O9 H11····O13	-36.7	-19.1	H14····O10	45.7	8.4
DJQ-m-q	H11····O10 H11····O13	-36.6	-19.0	H14····O9	45.8	8.6

Table 6.203. Changes in the IR vibrational frequencies of the N11–H11 and N14–H14 bonds in the conformers of compound DLP containing IHBs.

Conformers	Vibrational frequency change (cm^{-1})					
	N11–H11			N14–H14		
	IHB	DFT	HF	IHB	DFT	HF
DLP-m-r	H11····O10 H11····O13	-36.2	-19.3	H14····O9	45.9	8.4
DLP-m-s	H11····O10 H11····O13	-36.2	-18.2	H14····O9	45.9	7.2
DLP-p-q	H11····O9 H11····O13	-36.1	-19.2	H14····O10	45.9	8.5
DLP-p-s	H11····O9 H11····O13	-36.2	-18.3	H14····O10	46.0	7.1
DLP-p-t	H11····O9 H11····O13	-36.2	-18.6	H14····O10	46.1	8.0
DLP-m-q	H11····O10 H11····O13	-36.5	-19.6	H14····O9	46.0	8.3
DLP-p-r	H11····O9 H11····O13	-36.6	-19.6	H14····O10	46.1	8.2
DLP-k-q	H11····O13	-9.0	3.5	H14····O10	49.0	-4.8
DLP-k-r	H11····O13	-8.5	4.1	H14····O10	48.4	-4.8
DLP-k-s	H11····O13	-8.4	5.6	H14····O10	48.4	-6.8

Table 6.204. Changes in the IR vibrational frequencies of the N11–H11 and N14–H14 bonds in the conformers of compound DLQ containing IHBs.

Conformers	Vibrational frequency change (cm^{-1})					
	N11–H11			N14–H14		
	IHB	DFT	HF	IHB	DFT	HF
DLQ-p-q	H11····O9 H11····O13	-36.1	10.7	H14····O10	45.6	8.5
DLQ-k-q	H11····O13	-8.8	33.5	H14····O10	49.0	-4.6
DLQ-k-r	H11····O13	-9.2	33.9	H14····O10	48.2	-4.7
DLQ-m--r	H11····O10 H11····O13	-36.1	10.8	H14····O9	45.7	8.5
DLQ-m-q	H11····O10 H11····O13	-36.6	10.2	H14····O9	45.6	8.4
DLQ-m-r′	H11····O10 H11····O13	-36.1	10.7	H14····O9	46.1	8.5
DLQ-m-q′	H11····O10 H11····O13	-36.5	10.1	H14····O9	46.0	8.2

Table 6.205. Changes in the IR vibrational frequencies of the N11–H11 and N14–H14 bonds in the conformers of compound EGP containing IHBs.

Conformers	Vibrational frequency change (cm^{-1})					
	N11–H11			N14–H14		
	IHB	DFT	HF	IHB	DFT	HF
EGP-m-r-x4	H11····O10 H11····O13	-35.5	-18.4	H14····O9	38.0	1.2
EGP-m-s-x4	H11····O10 H11····O13	-35.5	-17.4	H14····O9	38.0	0.0
EGP-m-q-x4	H11····O10 H11····O13	-36.0	-18.8	H14····O9	38.2	1.1
EGP-m-r-x1	H11····O10 H11····O13	-37.2	-19.2	H14····O9	46.1	8.5
EGP-m-s-x1	H11····O10 H11····O13	-37.2	-18.2	H14····O9	46.1	7.3
EGP-p-q-x3	H11····O9 H11····O13	-37.0	-19.2	H14····O10	46.0	8.3
EGP-p-s-x3	H11····O9 H11····O13	-37.0	-18.3	H14····O10	46.0	7.2
EGP-m-q-x1	H11····O10 H11····O13	-37.4	-19.6	H14····O9	46.4	8.4
EGP-k-q-x1	H11····O13	-9.4	4.0	H14····O10	46.8	-2.7
EGP-k-r-x2	H11····O13	-9.7	4.9	H14····O10	45.9	-12.8
EGP-k-q-x1′	H11····O13	-9.4	4.5	H14····O10	45.9	-2.7
EGP-k-s-x1	H11····O13	-9.5	6.2	H14····O10	45.9	-4.5
EGP-g-r-x1	H11····O9	-49.0	-35.4			

		-56.9	-42.7			
EGP-g-q-x1	H11····O9	-49.6	-35.4			
		-57.3	-42.7			

Table 6.206. Changes in the IR vibrational frequencies of the N11–H11 and N14–H14 bonds in the conformers of compound EGQ containing IHBs.

Conformers	Vibrational frequency change (cm^{-1})					
	N11–H11			N14–H14		
	IHB	DFT	HF	IHB	DFT	HF
EGQ-m-r-x4	H11····O10 H11····O13	-35.6	-18.4	H14····O9	38.1	1.2
EGQ-m-q-x4	H11····O10 H11····O13	-35.8	-18.9	H14····O9	38.2	1.1
EGQ-m-r-x1	H11····O10 H11····O13	-37.0	-19.3	H14····O9	46.2	8.5
EGQ-m-q-x1	H11····O10 H11····O13	-37.4	-19.8	H14····O9	45.8	8.1
EGQ-p-q-x3	H11····O9 H11····O13	-34.7	-18.0	H14····O10	34.6	-11.7
EGQ-p-r-x3	H11····O9 H11····O13	-35.2	-18.5	H14····O10	33.4	-12.4
EGQ-k-q-x4	H11····O13	-8.6	4.0	H14····O10	44.4	-9.1
EGQ-k-r-x4	H11····O13	-8.5	4.5	H14····O10	43.3	-9.2
EGQ-g-r-x1	H11····O9	-49.0	-35.5			
		-56.9	-42.8			
EGQ-g-t-x1	H11····O9	-49.0	-35.2			
		-56.9	-42.5			
EGQ-g-q-x1	H11····O9	-49.5	-35.4			
		-57.2	-42.7			

Table 6.207. Changes in the IR vibrational frequencies of the N11–H11 and N14–H14 bonds in the conformers of compound EJP containing IHBs.

Conformers	Vibrational frequency change (cm^{-1})					
	N11–H11			N14–H14		
	IHB	DFT	HF	IHB	DFT	HF
EJP-m-r-x4	H11····O10 H11····O13	-35.8	-17.2	H14····O9	37.7	0.0
EJP-m-s-x4	H11····O10 H11····O13	-35.8	-18.2	H14····O9	37.7	1.4
EJP-m-q-x4	H11····O10 H11····O13	-36.2	-18.6	H14····O9	37.8	1.1
EJP-p-s-x4	H11····O9 H11····O13	-36.2	-18.1	H14····O10	37.8	7.3
EJP-p-q-x4	H11····O9 H11····O13	-37.4	-19.0	H14····O10	45.9	8.5
EJP-p-r-x4	H11····O9 H11····O13	-37.8	-19.3	H14····O10	46.2	8.5
EJP-k-q-x1	H11····O13	-8.9	4.3	H14····O10	46.5	-3.2
EJP-k-r-x1	H11····O13	-9.9	4.7	H14····O10	45.7	-3.0
EJP-k-r-x1′	H11····O13	-9.9	4.7	H14····O10	45.7	-2.9
EJP-k-s-x1	H11····O13	-9.9	6.6	H14····O10	45.7	-4.9

Table 6.208. Changes in the IR vibrational frequencies of the N11–H11 and N14–H14 bonds in the conformers of compound EJQ containing IHBs.

Conformers	Vibrational frequency change (cm^{-1})					
	N11–H11			N14–H14		
	IHB	DFT	HF	IHB	DFT	HF
EJQ-m-q-x4	H11····O10 H11····O13	-36.4	-18.6	H14····O9	37.8	1.0
EJQ-m-r-x4	H11····O10 H11····O13	-35.7	-18.1	H14····O9	38.3	1.5
EJQ-p-q-x4	H11····O9 H11····O13	-37.3	-18.8	H14····O10	45.8	8.5
EJQ-p-q-x4′	H11····O9 H11····O13	-37.3	-18.6	H14····O10	45.8	8.6
EJQ-m-r-x1	H11····O10 H11····O13	-37.3	-18.5	H14····O9	45.8	8.6
EJQ-m-s-x1	H11····O10 H11····O13	-37.2	-17.9	H14····O9	45.8	7.3
EJQ-p-r-x4	H11····O9 H11····O13	-37.4	-18.9	H14····O10	45.9	8.3
EJQ-p-s-x4	H11····O9 H11····O13	-37.4	-17.7	H14····O10	45.9	7.3
EJQ-m-q-x1	H11····O10	-37.4	-19.0	H14····O9	46.0	8.5

	H11····O13					
EJQ-k-q-x4	H11····O13	-8.7	4.7	H14····O10	43.6	-9.6
EJQ-k-r-x4	H11····O13	-9.0	5.3	H14····O10	43.4	-9.6

Table 6.209. Changes in the IR vibrational frequencies of the N11–H11 and N14–H14 bonds in the conformers of compound ELP containing IHBs.

Conformers	Vibrational frequency change (cm^{-1})					
	N11–H11			N14–H14		
	IHB	DFT	HF	IHB	DFT	HF
ELP-m-q-x4	H11····O10 H11····O13	-35.5	-17.5	H14····O9	38.0	0.0
ELP-m-s-x4	H11····O10 H11····O13	-35.5	-18.6	H14····O9	38.1	1.3
ELP-m-q-x4	H11····O10 H11····O13	-36.0	-19.0	H14····O9	38.2	1.2
ELP-m-r-x1	H11····O10 H11····O13	-37.0	-19.4	H14····O9	46.0	8.5
ELP-m-s-x1	H11····O10 H11····O13	-37.0	-18.4	H14····O9	46.1	7.2
ELP-p-s-x4	H11····O9 H11····O13	-37.1	-19.4	H14····O10	45.9	8.5
ELP-p-s-x4′	H11····O9 H11····O13	-37.0	-18.6	H14····O10	46.0	7.2
ELP-m-q-x1	H11····O10 H11····O13	-37.4	-19.8	H14····O9	46.4	8.4
ELP-k-q-x1	H11····O13	-9.8	3.8	H14····O10	50.6	-2.8
ELP-k-r-x1	H11····O13	-8.9	4.3	H14····O10	46.0	-2.7
ELP-k-s-x1	H11····O13	-8.9	6.1	H14····O10	46.0	-4.5

Table 6.210. Changes in the IR vibrational frequencies of the N11–H11 and N14–H14 bonds in the conformers of compound ELQ containing IHBs.

Conformers	Vibrational frequency change (cm^{-1})					
	N11–H11			N14–H14		
	IHB	DFT	HF	IHB	DFT	HF
ELQ-m-r-x4	H11····O10 H11····O13	-35.8	-17.8	H14····O9	38.3	1.3
ELQ-m-q-x4	H11····O10 H11····O13	-36.0	-18.4	H14····O9	38.3	1.2
ELQ-m-r-x1	H11····O10 H11····O13	-37.2	-18.8	H14····O9	46.1	8.6
ELQ-m-q-x1	H11····O10 H11····O13	-37.6	-19.3	H14····O9	46.0	8.3

ELQ-k-q-x4	H11····O13	-8.6	4.7	H14····O10	43.9	-9.1
ELQ-k-r-x4	H11····O13	-8.7	4.9	H14····O10	43.5	-9.1

Table 6.211. Changes in the IR vibrational frequencies of the N11–H11 and N14–H14 bonds in the conformers of compound FGP containing IHBs.

Conformers	Vibrational frequency change (cm^{-1})					
	N11–H11			N14–H14		
	IHB	DFT	HF	IHB	DFT	HF
FGP-m-r-x4	H11····O10 H11····O13	-35.4	-18.5	H14····O9	49.2	1.5
FGP-m-s-x4	H11····O10 H11····O13	-35.5	-17.4	H14····O9	49.2	0.2
FGP-m-q-x4	H11····O10 H11····O13	-35.9	-18.9	H14····O9	49.4	1.4
FGP-m-r-x1	H11····O10 H11····O13	-35.3	-19.4	H14····O9	44.9	9.7
FGP-m-s-x1	H11····O10 H11····O13	-35.3	-18.4	H14····O9	44.9	8.4
FGP-p-q-x4	H11····O9 H11····O13	-35.1	-19.4	H14····O10	45.3	9.7
FGP-p-s-x4	H11····O9 H11····O13	-35.1	-18.6	H14····O10	45.3	8.4
FGP-m-q-x1	H11····O10 H11····O13	-35.6	-19.8	H14····O9	44.5	9.6
FGP-p-r-x4	H11····O9 H11····O13	-35.5	-19.7	H14····O10	44.8	9.5
FGP-k-q-x1	H11····O13	-9.1	3.8	H14····O10	58.2	0.7
FGP-k-r-x1	H11····O13	-9.0	4.3	H14····O10	57.4	0.7
FGP-k-r-x1	H11····O13	-9.0	4.5	H14····O10	57.4	2.3
FGP-g-r-x1	H11····O9	-49.1	-36.0			
		-58.4	-43.4			
FGP-g-r-x1	H11····O9	-49.1	-36.2			
		-58.4	-43.6			
FGP-g-q-x1	H11····O9	-49.7	-36.0			
		-58.8	-43.3			

Table 6.212. Changes in the IR vibrational frequencies of the N11–H11 and N14–H14 bonds in the conformers of compound FGQ containing IHBs.

Conformers	Vibrational frequency change (cm^{-1})					
	N11–H11			N14–H14		
	IHB	DFT	HF	IHB	DFT	HF
FGQ-m-r-x4	H11····O10 H11····O13	-35.4	-18.3	H14····O9	49.2	1.4
FGQ-m-q-x4	H11····O10 H11····O13	-35.7	-18.9	H14····O9	49.1	1.3
FGQ-p-q-x4	H11····O10 H11····O13	-35.0	-17.9	H14····O9	44.9	-10.9
FGQ-m-r-x1	H11····O10 H11····O13	-35.0	-19.4	H14····O9	45.0	9.7
FGQ-m-q-x1	H11····O10 H11····O13	-35.4	-19.9	H14····O9	44.2	9.3
FGQ-k-r-x4	H11····O13	-8.2	7.9	H14····O10	54.4	-10.9
FGQ-g-r-x1	H11····O9	-49.1	-36.0			
FGQ-g-t-x1	H11····O9	-49.1	-35.6			
FGQ-g-q-x1	H11····O9	-49.8	-36.0			

Table 6.213. Changes in the IR vibrational frequencies of the N11–H11 and N14–H14 bonds in the conformers of compound FJP containing IHBs.

Conformers	Vibrational frequency change (cm^{-1})					
	N11–H11			N14–H14		
	IHB	DFT	HF	IHB	DFT	HF
FJP-m-r-x4	H11····O10 H11····O13	-36.1	-18.4	H14····O9	39.0	2.7
FJP-m-s-x4	H11····O10 H11····O13	-36.1	-17.4	H14····O9	39.1	1.4
FJP-m-q-x4	H11····O10 H11····O13	-36.6	-18.7	H14····O9	39.0	2.5
FJP-p-q-x4	H11····O9 H11····O13	-35.9	-19.3	H14····O10	34.3	10.8
FJP-p-s-x4	H11····O9 H11····O13	-35.8	-18.3	H14····O10	34.3	9.5
FJP-k-q-x1	H11····O13	-10.2	4.0	H14····O10	47.6	1.3
FJP-p-r-x1	H11····O9 H11····O13	-36.6	-19.6	H14····O10	34.4	10.7
FJP-k-r-x1	H11····O13	-9.7	4.4	H14····O10	47.1	1.2
FJP-k-s-x1	H11····O13	-9.8	6.3	H14····O10	47.0	-0.3

Table 6.214. Changes in the IR vibrational frequencies of the N11–H11 and N14–H14 bonds in the conformers of compound FJQ containing IHBs.

Conformers	Vibrational frequency change (cm^{-1})					
	N11–H11			N14–H14		
	IHB	DFT	HF	IHB	DFT	HF
FJQ-m-q-x4	H11····O10 H11····O13	-36.1	-19.0	H14····O9	38.9	1.6
FJQ-m-r-x4	H11····O10 H11····O13	-35.8	-18.3	H14····O9	39.0	1.5
FJQ-p-r-x4	H11····O9 H11····O13	-35.9	-20.0	H14····O10	33.8	9.3
FJQ-p-q-x4	H11····O9 H11····O13	-35.6	-17.9	H14····O10	34.6	-10.8
FJQ-p-q-x4′	H11····O9 H11····O13	-35.6	-19.4	H14····O10	34.6	9.7
FJQ-m-q-x1	H11····O10 H11····O13	-35.9	-19.8	H14····O9	34.3	9.5
FJQ-m-r-x1	H11····O10 H11····O13	-35.6	-19.2	H14····O9	34.8	9.7
FJQ-k-q-x4	H11····O13	-9.4	3.9	H14····O10	45.3	-8.5
FJQ-k-r-x4	H11····O13	-9.2	4.6	H14····O10	44.0	-8.6

Table 6.215. Changes in the IR vibrational frequencies of the N11–H11 and N14–H14 bonds in the conformers of compound FLP containing IHBs.

Conformers	Vibrational frequency change (cm^{-1})					
	N11–H11			N14–H14		
	IHB	DFT	HF	IHB	DFT	HF
FLP-m-r-x4	H11····O10 H11····O13	-35.6	-18.6	H14····O9	39.1	1.6
FLP-m-q-x4	H11····O10 H11····O13	-36.0	-19.0	H14····O9	39.3	1.4
FLP-m-r-x1	H11····O10 H11····O13	-35.5	-19.5	H14····O9	34.8	9.6
FLP-m-s-x4	H11····O10 H11····O13	-35.5	-17.5	H14····O9	34.7	0.2
FLP-m-s-x1	H11····O10 H11····O13	-35.5	-18.5	H14····O9	34.8	8.3
FLP-p-q-x4	H11····O9 H11····O13	-35.3	-19.5	H14····O10	35.0	9.7
FLP-p-s-x4	H11····O9 H11····O13	-35.4	-18.7	H14····O10	35.0	8.4
FLP-m-q-x1	H11····O10 H11····O13	-35.7	-19.8	H14····O9	34.7	9.5

FLP-k-q-x1	H11····O13	-9.7	3.8	H14····O10	47.9	0.7
FLP-k-r-x1	H11····O13	-9.0	4.2	H14····O10	47.1	0.7
FLP-k-s-x1	H11····O13	-9.0	6.1	H14····O10	47.2	-0.9

Table 6.216. Changes in the IR vibrational frequencies of the N11–H11 and N14–H14 bonds in the conformers of compound FLQ containing IHBs.

Conformers	Vibrational frequency change (cm^{-1})					
	N11–H11			N14–H14		
	IHB	DFT	HF	IHB	DFT	HF
FLQ-p-q-x2	H11····O9 H11····O13	-35.8	-18.3	H14····O10	39.1	0.3
FLQ-m-r-x4	H11····O10 H11····O13	-35.8	-17.6	H14····O9	39.2	1.4
FLQ-m-q-x4	H11····O10 H11····O13	-36.1	-18.2	H14····O9	39.1	1.3
FLQ-p-q-x4	H11····O9 H11····O13	-35.6	-18.5	H14····O10	34.7	9.6
FLQ-m-r-x1	H11····O10 H11····O13	-35.4	-18.7	H14····O9	34.9	9.6
FLQ-m-q-x1	H11····O10 H11····O13	-35.7	-19.1	H14····O9	34.1	9.2
FLQ-m-q-x1′	H11····O10 H11····O13	-35.7	-19.3	H14····O9	34.1	9.6
FLQ-p-r-x4	H11····O9 H11····O13	-35.6	-17.6	H14····O10	34.5	-11.3
FLQ-p-r-x4′	H11····O9 H11····O13	-35.6	-19.1	H14····O10	34.5	9.5
FLQ-k-q-x4	H11····O13	-9.1	4.9	H14····O10	45.2	-8.4
FLQ-k-q-x1	H11····O13	-9.8	4.5	H14····O10	47.9	0.7
FLQ-k-r-x4	H11····O13	-8.7	5.1	H14····O10	44.6	-8.4
FLQ-k-r-x1	H11····O13	-6.7	5.0	H14····O10	44.1	0.6

Tables 6.217. Ranges of the Vibrational frequency changes according to compound and conformer type.

Compound	Conformer type	Ranges of vibrational frequency changes (cm^{-1})					
		N11–H11			N14–H14		
		IHB	DFT	HF	IHB	DFT	HF
AGP	m	H11····O10 H11····O13	-34.0 – (-36.1)	-17.0 – (-19.0)	H14····O9	28.6 – 46.8	-7.8 –10.2
	p	H11····O9 H11····O13	-35.7 – (-36.0)	-17.9 – (-19.0)	H14····O10	46.6 – 46.8	9.8 – 10.1
	k	H11····O13	-7.9 – (-8.5)	4.2 – 5.3	H14····O10	53.9 – 55.1	0.9 – 1.0
	g	H11····O9	-48.0 – (-48.4)	-35.4 – (-35.5)			
			-55.3 – (-55.8)	-43.3 – (-43.4)			
AGQ	m	H11····O10 H11····O13	-34.0 – (-36.1)	-16.5 – (-18.8)	H14····O9	28.4 – 46.6	-8.2 – 10.2
	k	H11····O13	-8.3 – (-8.4)	4.4 – 5.8	H14····O10	54.5 – 55.0	0.9 – 1.0
	g	H11····O9	-47.9 – (-48.5)	-34.8 – (-35.2)			
			-55.2 – (-55.9)	-42.7 – (-43.1)			
AJP	m	H11····O10 H11····O13	-34.5 – (-36.6)	-16.1 – (-19.0)	H14····O9	27.9 – 46.6	-9.2 – 10.4
	k	H11····O13	-8.1 – (-8.9)	4.6 – 6.4	H14····O10	54.5 – 55.1	0.8
AJQ	m	H11····O10 H11····O13	-34.3 – (-.53.9)	-16.1 – (-18.1)	H14····O9	28.3 – 46.4	-7.9 – 10.3
	p	H11····O9 H11····O13	-35.4 – (-36.0)	-16.9 – (-18.1)	H14····O10	46.1 – 46.4	-2.1 – 10.2
	k	H11····O13	-8.0 – (-8.3)	5.1	H14····O10	54.5 – 54.8	0.5
ALP	m	H11····O10 H11····O13	-34.3 – (-36.1)	-15.7– 18.6	H14····O9	28.5 – 46.5	-9.2 – 10.3
	k	H11····O13	-7.3 – (-8.5)	4.5 – 6.8	H14····O10	54.4 – 56.6	-3.6 – 1.0
ALQ	m	H11····O10 H11····O13	-33.9 – (-35.8)	-15.7– (-18.0)	H14····O9	28.4 – 46.8	-8.2 – 10.3
	k	H11····O13	-8.0 – (-8.5)	5.3 – 5.8	H14····O10		0.8 – 0.9
BGP	m	H11····O10 H11····O13	-33.1 – (-41.8)	-14.8 – (-17.7)	H14····O9	41.9 – 51.4	3.6 – 17.4
	p	H11····O9 H11····O13	-34.5	-16.4 – (-16.5)	H14····O10	51.2 – 51.3	16.2 – 17.1
	k	H11····O13	-8.7 – (-8.8)	5.1 – 7.2	H14····O10	60.7 – 61.5	10.5 – 12.3
	g	H11····O9	-49.8 – (-49.9)	-35.8			

			-59.0 – (-60)	-43.9 – (-44.2)			
BGQ	m	H11····O10 H11····O13	-33.4 – (-34.9)	-16.2 – (-18.0)	H14····O9	42.1 – 51.0	-0.8 – 12.0
	k	H11····O13	-8.3 – (-9.0)	4.5 – 5.0	H14····O10	60.6 – 61.1	6.5 – 6.8
BJP	m	H11····O10 H11····O13	-33.4 – (-33.8)	-15.1 – (-16.1)	H14····O9	41.7 – 41.8	-1.9 – (-0.4)
	p	H11····O9 H11····O13	-34.7 – (-35.2)	-16.6 – (-18.0)	H14····O10	50.9	10.7 – 11.9
	k	H11····O13	-.8.9 – (-9.2)	5.0 – 7.0	H14····O10	60.5 – 61.1	4.7 – 6.5
BJQ	m	H11····O10 H11····O13	-33.3 – (-35.0)	16.0 – (-16.8)	H14····O9	41.5 – 50.9	-1.0 – 11.8
	p	H11····O9 H11····O13	-34.5 – (-35.2)	-16.5 – (-18.0)	H14····O10	50.7 – 50.8	10.6 – 11.9
BLP	m	H11····O10 H11····O13	-34.6 – (-34.7)	-16.2 – (-17.6)	H14····O9	51.0 – 51.2	15.8 – 17.2
	p	H11····O9 H11····O13	-33.4 – (-34.4)	-14.9 – (-16.5)	H14····O10	41.5 – 51.1	3.4 – 16.8
	k	H11····O13	-8.3 – (-8.7)	5.2 – 7.3	H14····O10	60.8 – 61.3	10.2 – 12.0
BLQ	m	H11····O10 H11····O13	-34.5 – (-34.7)	-16.7 – (-18.1)	H14····O9	51.2 – 51.4	13.4 – 14.6
	p	H11····O9 H11····O13	-33.1 – (-34.7)	-16.0 – (-17.9)	H14····O10	41.6 – 51.1	1.7 – 14.6
	k	H11····O13	-8.4 – (-8.5)	5.2 – 5.3	H14····O10	60.8 – 61.4	9.2 – 9.3
CGP	m	H11····O10 H11····O13	-29.7 – (-32.0)	-14.7 – (-17.1)	H14····O9	31.2 – 34.8	-14.2 – (-1.5)
	p	H11····O9 H11····O13	-36.7 – (-37.0)	-17.8 – (-19.0)	H14····O10	36.9 – 37.0	3.8 – 4.8
	g	H11····O9	-24.7 – (-25.5)	-24.5 – (-24.7)			
CGQ	m	H11····O10 H11····O13	-36.7	-18.6	H14····O9	37.1	4.8
	p	H11····O9 H11····O13	-29.6 – (-37.2)	-15.7 – (19.2)	H14····O10	30.9 – 37.2	-13.4 – 4.8
CJP	m	H11····O10 H11····O13	-30.3 – (-32.8)	-16.0 – (-17.5)	H14····O9	31.2 – 34.3	-12.6 – (-1.4)
	p	H11····O9 H11····O13	-37.3 – (-38.0)	-18.2 – (-19.4)	H14····O10	36.8 – 37.0	3.9 – 5.0
CJQ	m	H11····O10 H11····O13	-30.1 – (-37.8)	-14.4 – (-18.8)	H14····O9	31.0 – 37.2	-14.2 – 5.0
	p	H11····O9 H11····O13	-37.2 – (-37.5)	-17.2 – (-23.5)	H14····O10	36.7 – 36.9	4.0 – 4.9
CLP	m	H11····O10 H11····O13	-27.0 – (-29.4)	-11.9 – (-14.3)	H14····O9	45.3 – 48.8	4.5 – 17.4
	p	H11····O9 H11····O13	-34.1 – (-34.4)	-15.0 – (-16.4)	H14····O10	50.8 – 51.1	22.6 – 23.8

CLQ	m	H11····O10 H11····O13	-30.1 – (-37.5)	-15.0 – (-19.1)	H14····O9	31.2 – 37.5	-14.1 – 4.9
	p	H11····O9 H11····O13	-37.2	-17.9 – (-18.6)	H14····O10	37.1	3.9 – 4.9
DGP	m	H11····O10 H11····O13	36.2 – (-36.6)	-18.2 – (-19.6)	H14····O9	45.8 – 46.2	7.2 – 8.5
	p	H11····O9 H11····O13	-36.2 – (-36.3)	-18.3 – (-19.2)	H14····O10	45.8 – 46.0	7.1 – 8.5
	k	H11····O13	-8.7 – (-8.8)	3.5 – 4.8	H14····O10	48.3 – 49.0	-6.7 – (-4.7)
	g	H11····O9	-50.2 – (-50.9)	-38.5 – (-38.8)			
DGQ	m	H11····O10 H11····O13	-36.1 – (-36.6)	-19.1 – (-19.7)	H14····O9	45.7 – 46.2	8.2 – 8.3
	p	H11····O9 H11····O13	-36.0	-19.3	H14····O10	45.7	8.5
	k	H11····O13	-8.6 – (-8.7)	3.5 – 4.1	H14····O10	48.1 – 48.8	-4.8 – (-4.6)
	g	H11····O9	-50.1 – (-51.0)	-37.8 – (-38.8)			
DJP	m	H11····O10 H11····O13	-36.7 – (-36.9)	-19.0 – (-19.6)	H14····O9	45.8 – 46.1	8.3 – 8.4
	p	H11····O9 H11····O13	-36.6 – (-37.0)	-17.7 – (-18.8)	H14····O10	46.1 – 65.1	7.3 – 8.6
	k	H11····O13	-9.0 – (-9.2)	4.2 – 6.2	H14····O10	48.1 – 48.7	-7.1 – (-4.9)
DJQ	m	H11····O10 H11····O13	-36.4 – (-36.8)	-17.8 – (-19.1)	H14····O9	45.7 – 46.2	7.3 – 8.6
	p	H11····O9 H11····O13	-36.5 – (-36.7)	-18.7 – (-19.1)	H14····O10	45.6 – 45.8	8.4 – 8.7
	k	H11····O13	-9.1 – (-9.5)	4.2	H14····O10	48.3 – 48.4	-4.9
DLP	m	H11····O10 H11····O13	-36.2 – (36.5)	-18.2 – (-19.6)	H14····O9	45.9 – 46.0	7.2 – 8.4
	p	H11····O9 H11····O13	-36.1 – (-36.6)	-18.3 – (-19.6)	H14····O10	45.9 – 46.1	7.1 – 8.5
	k	H11····O13	-8.4 – (-9.0)	3.5 – 5.6	H14····O10	48.4 – 49.0	-6.8 – (-4.8)
DLQ	m	H11····O10 H11····O13	-36.1 – (-36.6)	10.1 – 10.8	H14····O9	45.6 – 46.1	8.2 – 8.5
	p	H11····O9 H11····O13	-36.1	10.7	H14····O10	45.6	8.5
	k	H11····O13	-8.8 – (-9.2)	33.5 – 33.9	H14····O10	48.2 – 49.0	–4.7 – (-4.6)
EGP	m	H11····O10 H11····O13	-35.5 – (37.4)	-17.4 – (-19.6)	H14····O9	38.0 – 46.4	0.0 – 8.5
	p	H11····O9 H11····O13	-37.0	-18.3 – (-19.2)	H14····O10	46.0	7.2 – 8.3
	k	H11····O13	-9.4 – (-9.7)	4.0 – 6.2	H14····O10	45.9 – 46.8	-12.8 – (-2.7)

	g	H11····O9	-49.0 – (49.6)	-35.4			
			-56.9 – (-57.3)	-42.7			
EGQ	m	H11····O10 H11····O13	-35.6 – (-37.4)	-18.4 – (-19.8)	H14····O9	38.1 – 46.2	1.1 – 8.5
	p	H11····O9 H11····O13	-34.7 – (-35.2)	-18.0 – (-18.5)	H14····O10	33.4 – 34.6	-12.4 – (-11.7)
	k	H11····O13	-8.5 – (-8.6)	4.0 – 4.5	H14····O10	43.3 – 44.4	-9.2 – (-9.1)
	g	H11····O9	-49.0 – (-49.5)	-35.2 – (-35.5)			
			-56.9 – (-57.2)	-42.5 – (-42.8)			
EJP	m	H11····O10 H11····O13	-35.8 – (-36.2)	-17.2 – (-18.6)	H14····O9	37.7 – 37.8	0.0 – 1.4
	p	H11····O9 H11····O13	-36.2 – (-37.8)	-18.1 – (-19.0)	H14····O10	37.8 – 46.2	7.3 – 8.5
	k	H11····O13	-8.9 – (-9.9)	4.3 – 6.6	H14····O10	45.7 – 46.5	-4.9 – (-2.9)
EJQ	m	H11····O10 H11····O13	35.7 – (-37.4)	-17.9 – (-19.0)	H14····O9	37.8 – 46.0	1.0 – 8.5
	p	H11····O9 H11····O13	-37.3 – (.37.4)	-17.7 – (-18.9)	H14····O10	45.8 – 45.9	7.3 – 8.6
	k	H11····O13	-8.7 – (-9.0)	4.7 – 5.3	H14····O10	43.4 – 43.6	-9.6
ELP	m	H11····O10 H11····O13	-35.5 – (-37.4)	-17.5 – (-19.8)	H14····O9	38.0 – 46.4	0.0 – 8.5
	p	H11····O9 H11····O13	-37.0 – (-37.1)	-18.6 – (-19.4)	H14····O10	45.9 – 46.0	7.2 – 8.5
	k	H11····O13	-8.9 – (-9.8)	3.8 – 6.1	H14····O10	46.0 – 50.6	-4.5 – (-2.7)
ELQ	m	H11····O10 H11····O13	-35.8 – (-37.6)	-17.8 – (-19.3)	H14····O9	38.3 – 46.1	1.2 – 8.6
	k	H11····O13	-8.6 – (-8.7)	4.7 – 4.9	H14····O10	43.5 – 43.9	-9.1
FGP	m	H11····O10 H11····O13	-35.3 – (35.9)	-17.4 – (-19.8)	H14····O9	44.5 – 49.4	0.2 – 9.7
	p	H11····O9 H11····O13	-35.1 – (-35.5)	-18.6 – (-19.7)	H14····O10	44.8 – 45.3	8.4 – 9.7
	k	H11····O13	-9.0 – (-9.1)	3.8 – 4.5	H14····O10	57.4 – 58.2	0.7 – 2.3
	g	H11····O9	-49.1 – (-49.7)	-36.0 – (-36.2)			
			-58.4 – (-58.8)	-43.3 – (-43.6)			
FGQ	m	H11····O10 H11····O13	-35.0 – (-35.7)	-18.3 – (-19.9)	H14····O9	44.2 – 49.2	1.3 – 9.7
	p	H11····O9 H11····O13	-35.0	-17.9	H14····O10	44.9	-10.9

	k	H11····O13	-8.2	7.9	H14····O10	54.4	-10.9
	g	H11····O9	-49.1 – (-49.8)	-35.6 – (-36.0)			
FJP	m	H11····O10 H11····O13	-36.1 – (-36.6)	-17.4 – (-18.7)	H14····O9	39.0 – 39.1	1.4 – 2.7
	p	H11····O9 H11····O13	-35.8 – (-35.9)	-18.3 – (-19.6)	H14····O10	34.3 – 34.4	9.5 –10.8
	k	H11····O13	-9.7 – (-10.2)	4.0 – 6.3	H14····O10	47.0 – 47.6	-0.3 – 1.3
FJQ	m	H11····O10 H11····O13	-35.6 – (-36.2)	-18.3 – (-19.8)	H14····O9	34.3 – (39.0)	1.5 – 9.7
	p	H11····O9 H11····O13	-35.6 – (-35.9)	-17.9 – (-20.0)	H14····O10	33.8 – 34.6	-10.8 – 9.7
	k	H11····O13	-9.2 – (-9.4)	3.9 – 4.6	H14····O10	45.3 – 44.0	-8.6 – (-8.5)
FLP	m	H11····O10 H11····O13	-35.5 – (-36.0)	-17.5 – (-19.8)	H14····O9	34.7 – 39.1	8.4 – 9.7
	p	H11····O9 H11····O13	-35.3 – (-35.4)	-18.7 – (-19.5)	H14····O10	35.0	8.4 – 9.4
	k	H11····O13	-9.0 – (-9.7)	3.8 – 6.1	H14····O10	47.1 – 47.9	-0.9 – 0.7
FLQ	m	H11····O10 H11····O13	-35.4 – (-36.1)	-17.6 – (-19.3)	H14····O9	34.1 – 39.2	1.3 – 9.6
	p	H11····O9 H11····O13	-35.6 – (-35.8)	-17.6 – (-19.1)	H14····O10	34.5 – 39.1	-11.3 – 9.6
	k	H11····O13	-6.7 – (-9.8)	4.5 – 5.1	H14····O10	44.1 – 47.9	-8.4 – 0.6

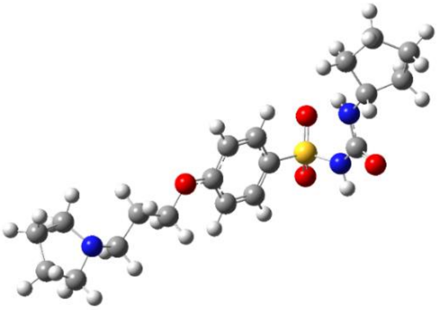
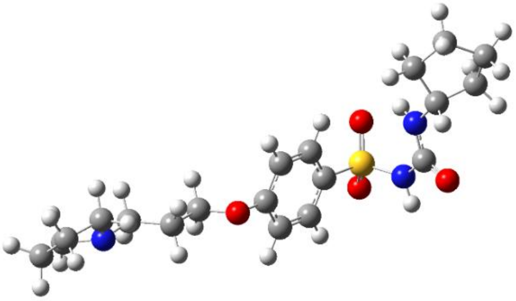
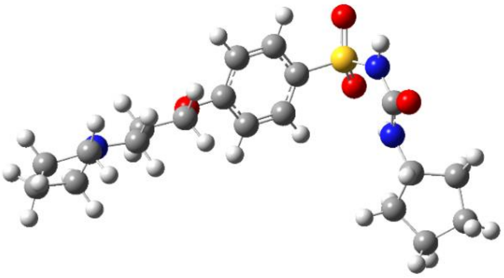
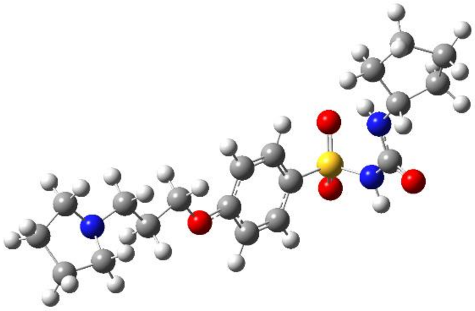
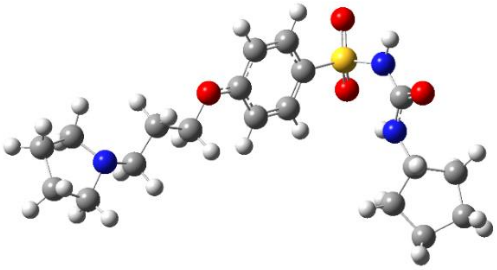
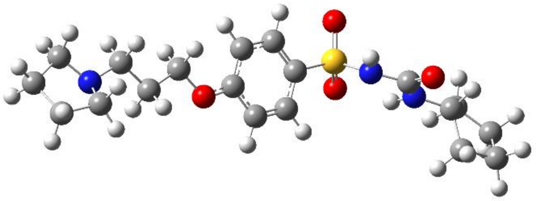
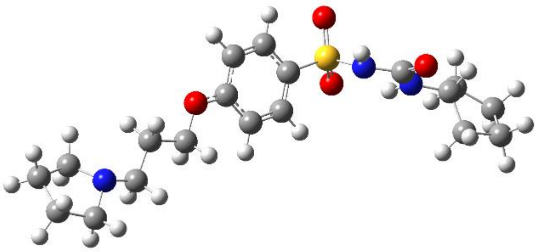
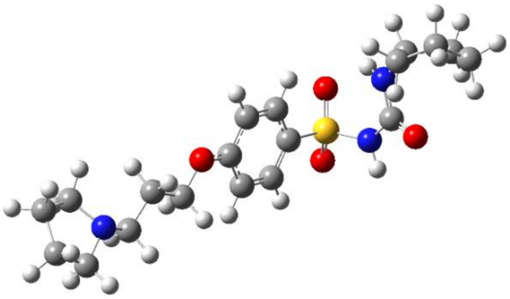
6.2. Figures presenting molecular structures

This section presents the figures of the molecular structures of the optimized geometries of all the calculated conformers and the shapes of the HOMO and LUMO frontier molecular orbitals. The results are obtained from full optimization calculations. The conformers are listed in order of increasing DFT relative energy. All the figures are presented with a similar orientation (the thiourea group on the right side of the benzene ring, and the chain to which R′ is attached on the left side of the benzene ring) to facilitate geometry comparisons.

6.2.1. Optimized geometries of the calculated conformers of all the compounds considered.

This section presents the figures of the optimized geometries of the calculated conformers of each of the compounds considered. The geometries reported are from the HF results. This is because some of the inputs optimized to the same conformer with DFT calculations, and it is interesting to view the additional conformers obtained from HF calculations (Appendix A show the inputs which optimized to the same output). In most cases conformers, the geometry types are similar in the DFT and HF results, and the interesting parameters to differentiate are the parameters of the IHBs which are reported in tables separately (section 6.1.3).

Figure 6.1: Optimized geometries of the calculated conformers of compound AGP.

	
AGP-m-r-u1	AGP-m-s-u1
	
AGP-p-t-u3	AGP-m-q-u1
	
AGP-p-r-u3	AGP-k-q-u1
	
AGP-k-r-u1	AGP-m-r-u2

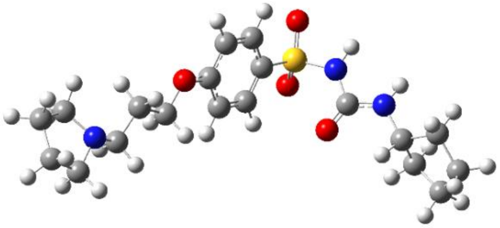
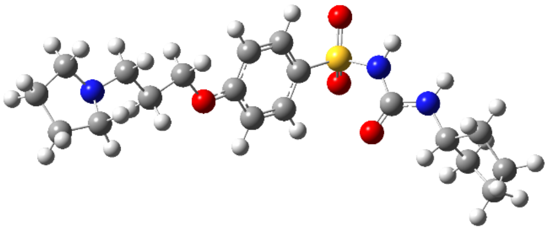
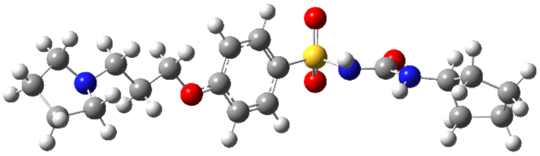
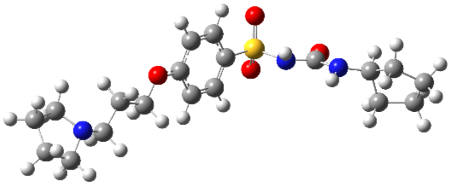
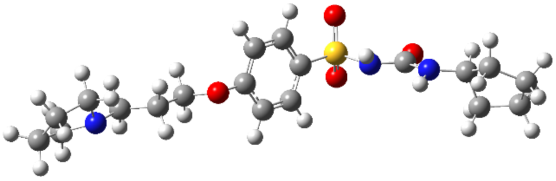
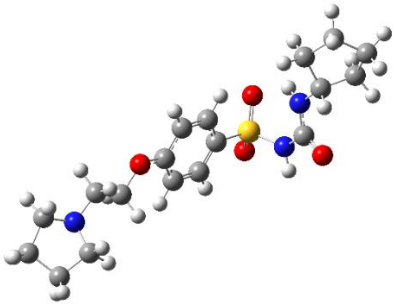
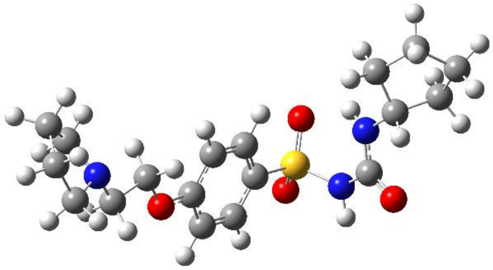
	
AGP-g-r-u3	AGP-g-q-u3
	
AGP-j-q-u3	AGP-j-r-u3
	
AGP-j-s-u3	

Figure 6.2: Optimized geometries of the calculated conformers of compound AGQ.

	
AGQ-m-r-u1	AGQ-m-q-u1

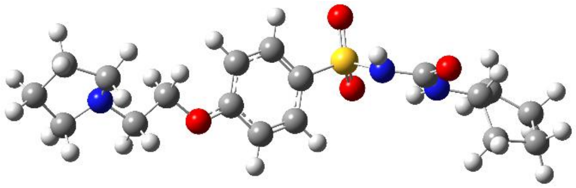
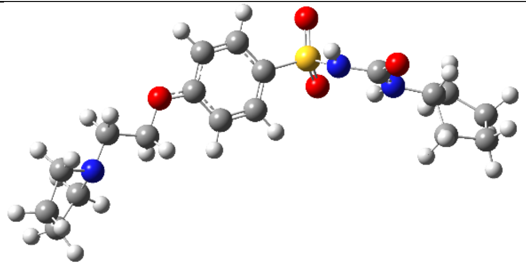
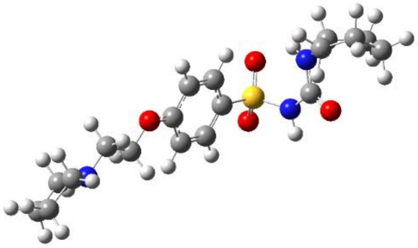
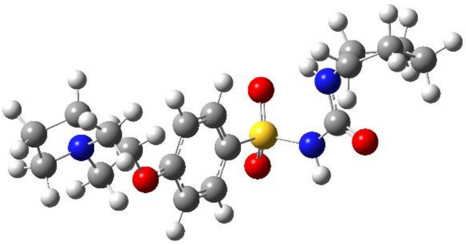
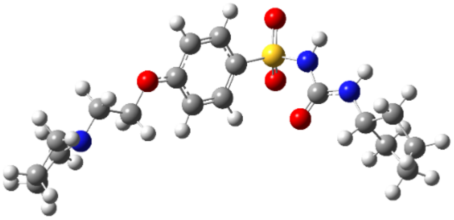
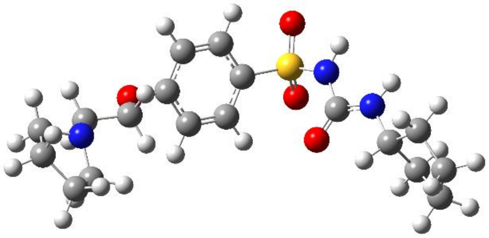
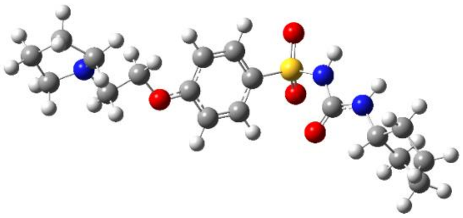
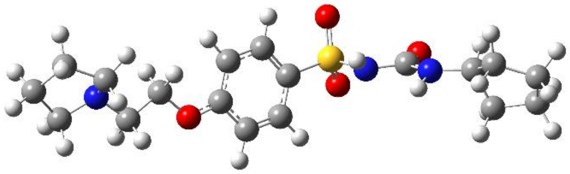
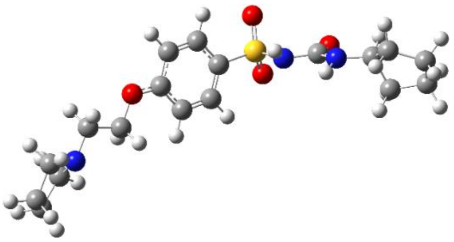
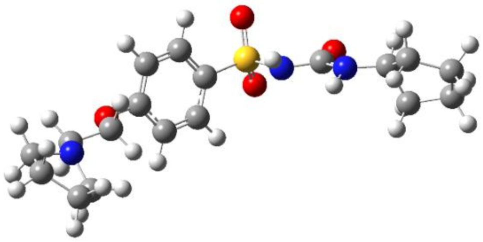
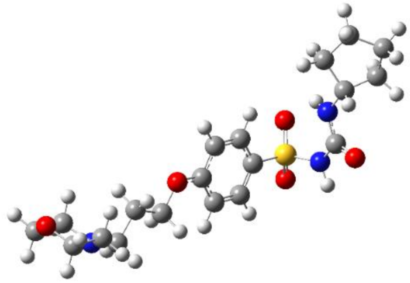
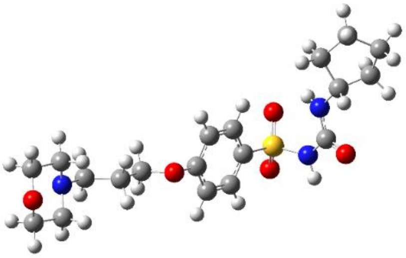
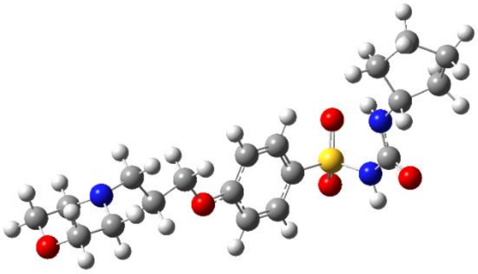
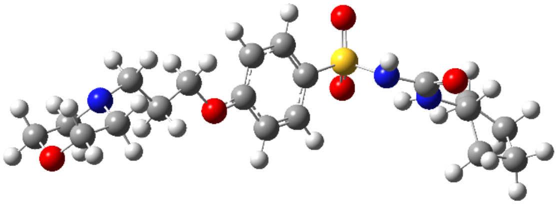
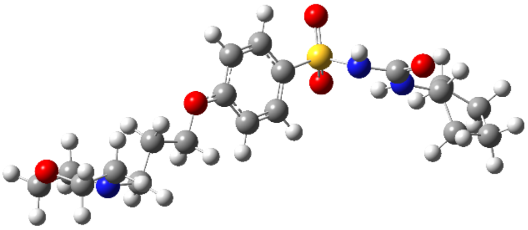
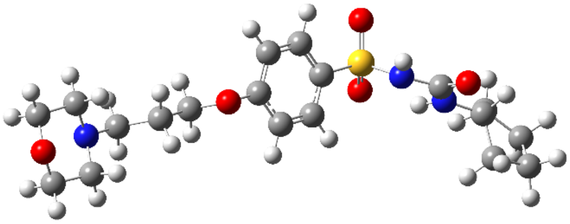
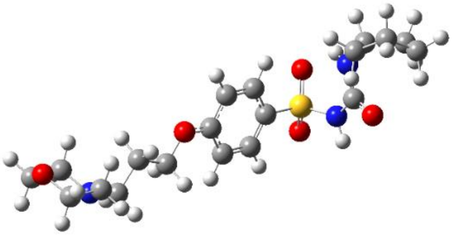
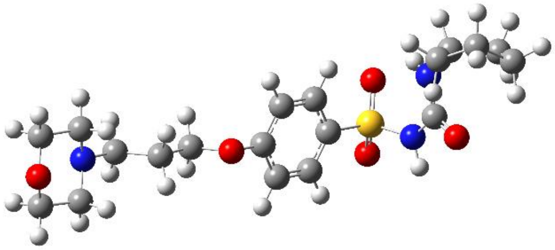
	
AGQ-k-q-u1	AGQ-k-r-u1
	
AGQ-m-r-u2	AGQ-m-q-u2
	
AGQ-g-r-u3	AGQ-g-t-u3
	
AGQ-g-q-u3	AGQ-j-q-u3
	
AGQ-j-r-u3	AGQ-j-t-u3

Figure 6.3: Optimized geometries of the calculated conformers of compound AJP.

	
AJP-m-r-u1	AJP-m-s-u1
	
AJP-m-q-u1	AJP-k-q-u1
	
AJP-k-r-u1	AJP-k-s-u1
	
AJP-m-r-u2	AJP-m-s-u2

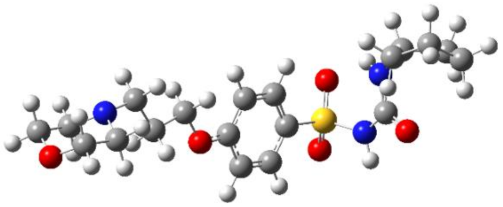
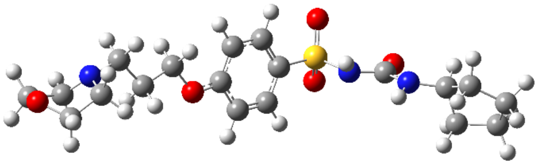
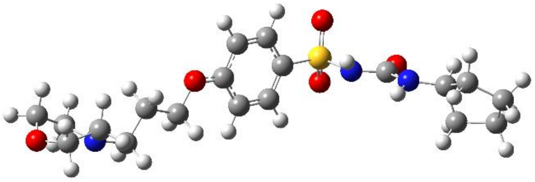
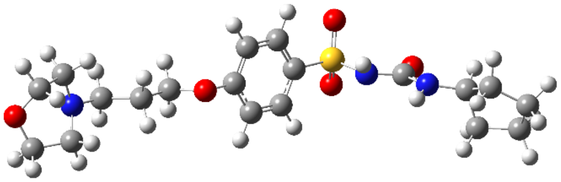
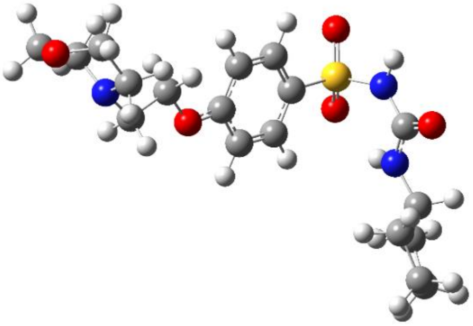
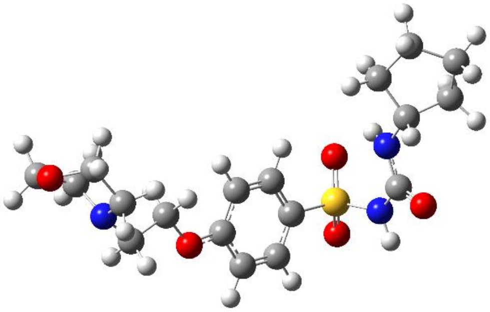
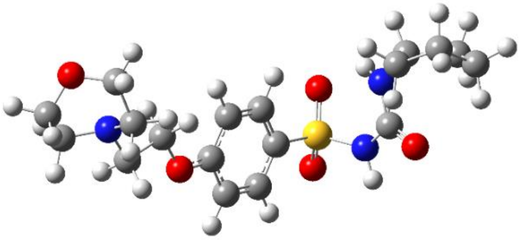
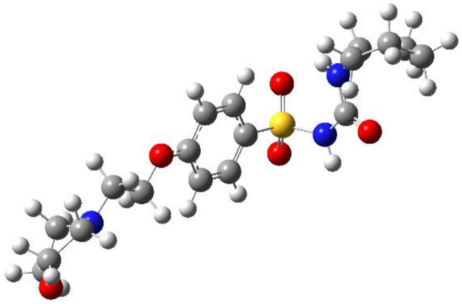
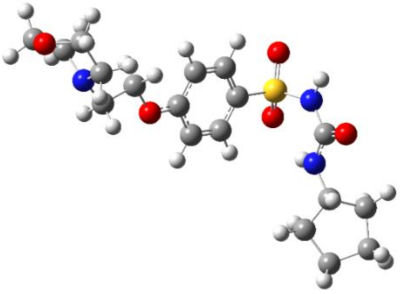
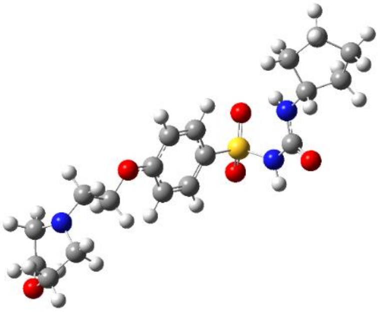
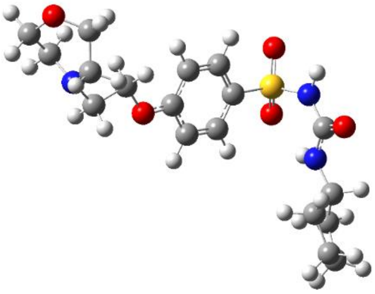
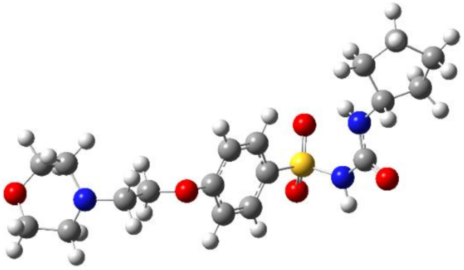
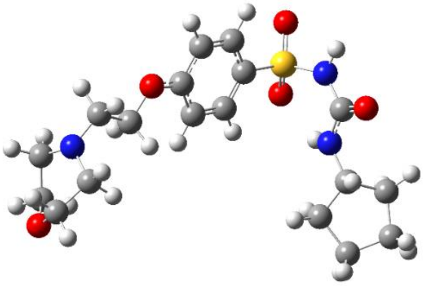
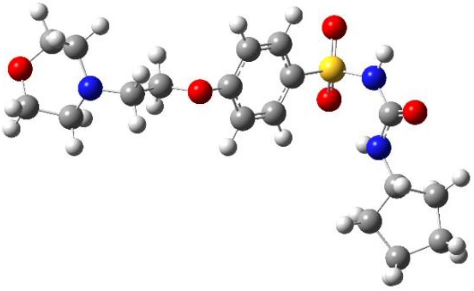
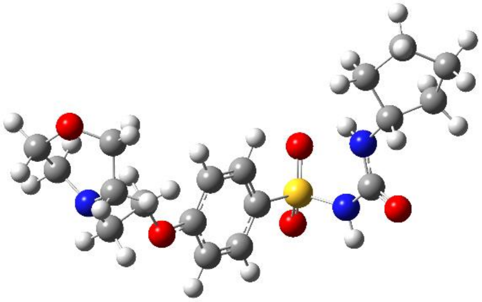
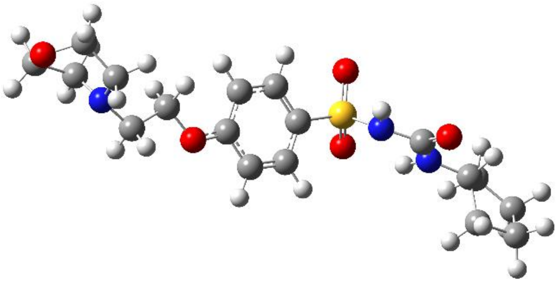
	
AJP-m-q-u2	AJP-j-q-u3
	
AJP-j-r-u3	AJP-j-s-u3

Figure 6.4: Optimized geometries of the calculated conformers of compound AJQ.

	
AJQ-p-q-u5	AJQ-m-q-u1
	
AJQ-m-q-u2	AJQ-m-r-u2

	
AJQ-p-q-u3	AJQ-m-r-u1
	
AJQ-p-q-u5	AJQ-m-s-u1
	
AJQ-p-r-u3	AJQ-p-s-u3
	
AJQ-m-q-u1	AJQ-k-q-u1

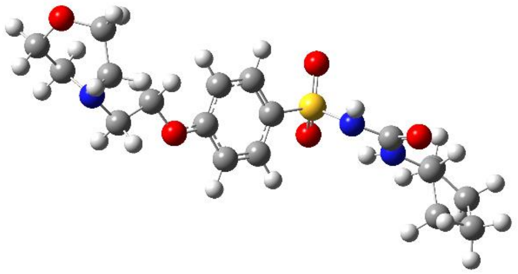
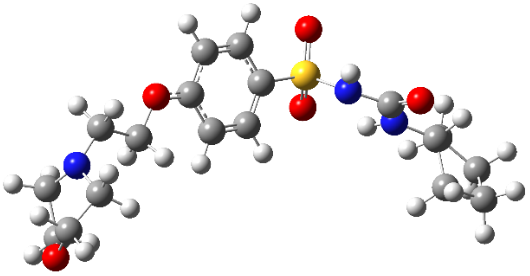
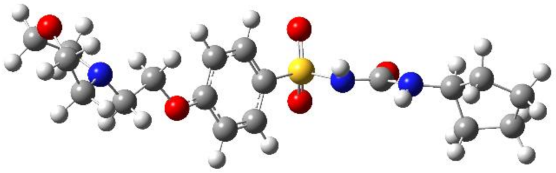
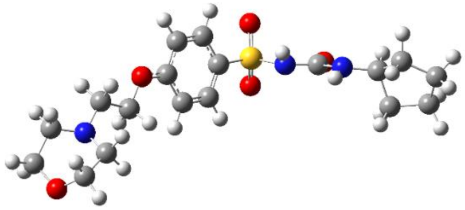
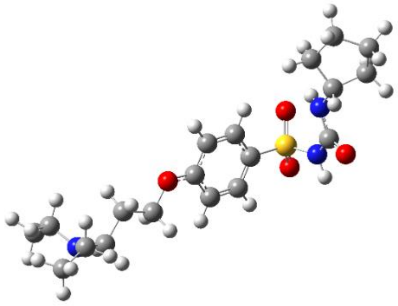
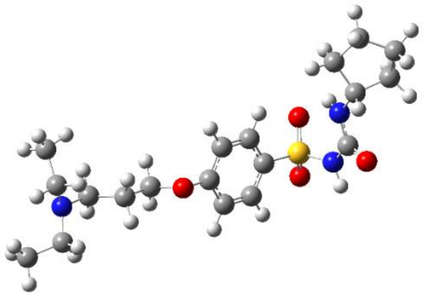
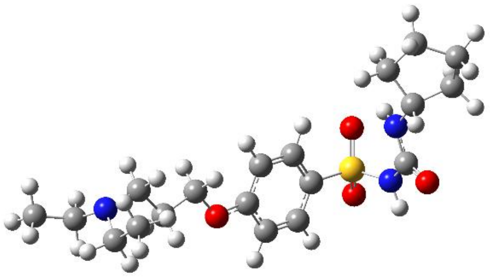
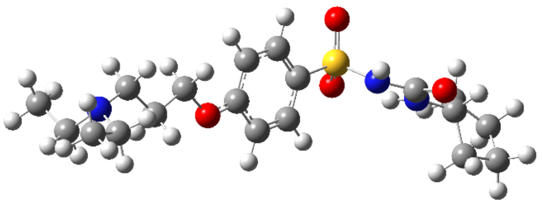
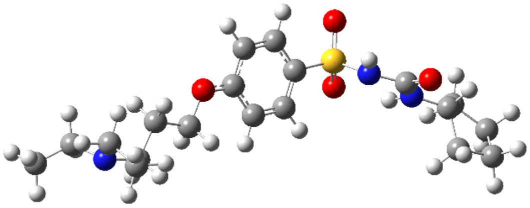
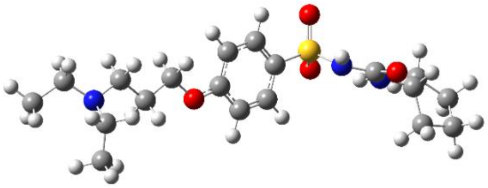
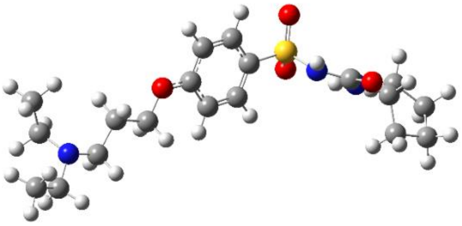
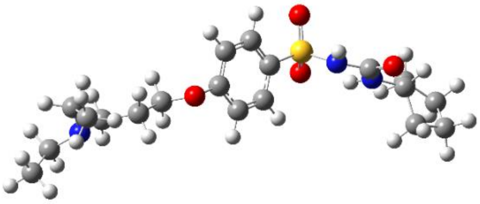
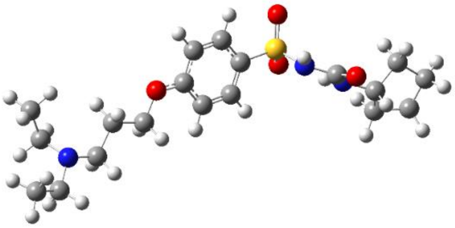
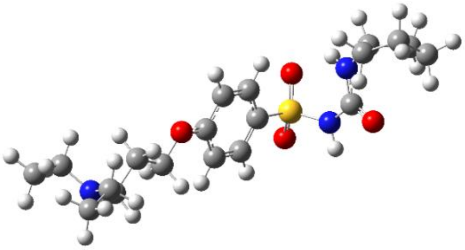
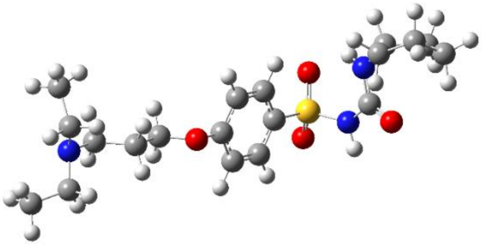
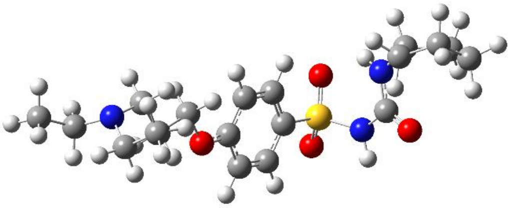
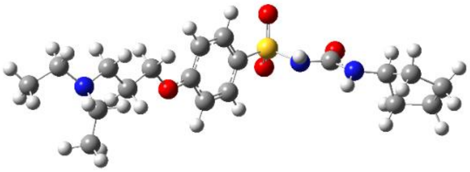
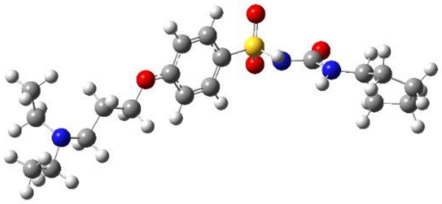
	
AJQ-k-q-u1	AJQ-r-u1
	
AJQ-j-q-u1	AJQ-j-r-u1

Figure 6.5: Optimized geometries of the calculated conformers of compound ALP.

	
ALP-m-r-u1	ALP-m-s-u1
	
ALP-m-q-u1	ALP-k-q-u1

	
ALP-k-r-u1	ALP-k-q-u1′
	
ALP-k-r-u1′	ALP-k-s-u1
	
ALP-k-r-u3	ALP-m-r-u2
	
ALP-m-s-u2	ALP-m-q-u2
	
ALP-j-q-u3	ALP-j-r-u3

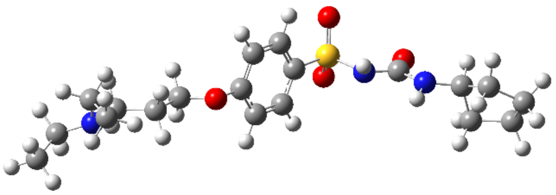
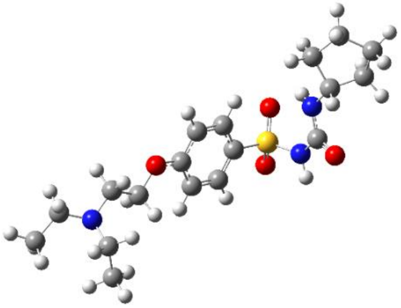
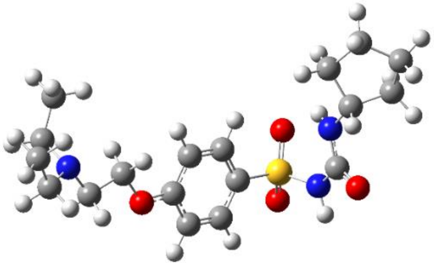
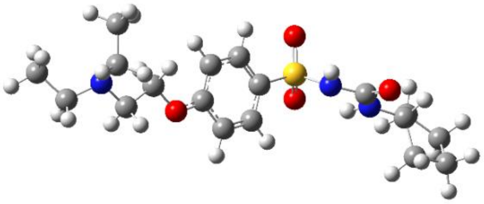
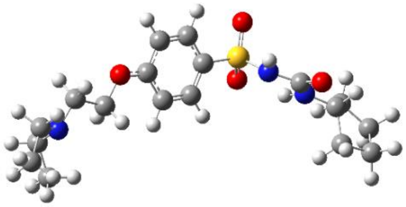
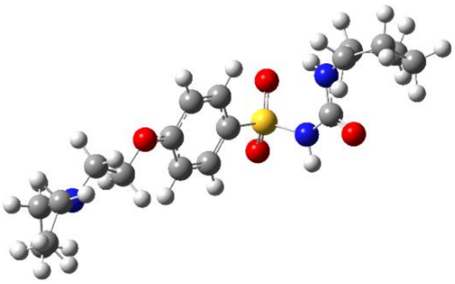
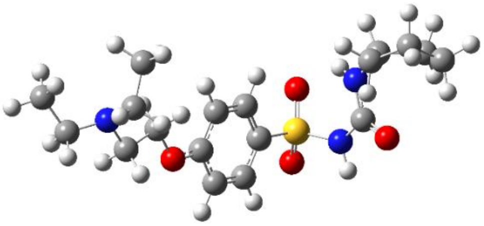
	
ALP-j-s-u3	

Figure 6.6: Optimized geometries of the calculated conformers of compound ALQ.

	
ALQ-m-r-u1	ALQ-m-q-u1
	
ALQ-k-q-u1	ALQ-k-r-u1
	
ALQ-m-r-u2	ALQ-m-q-u2

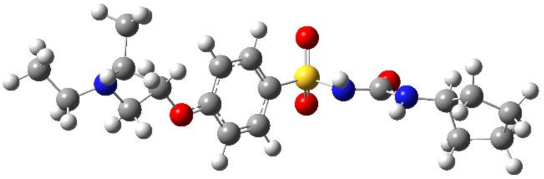
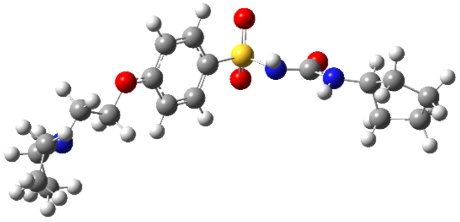
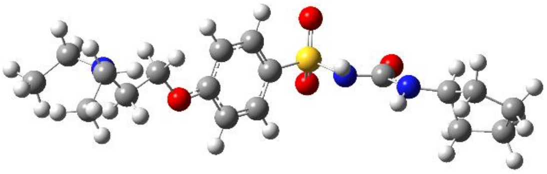
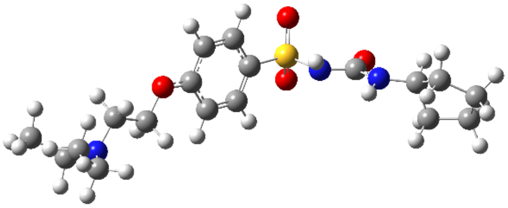
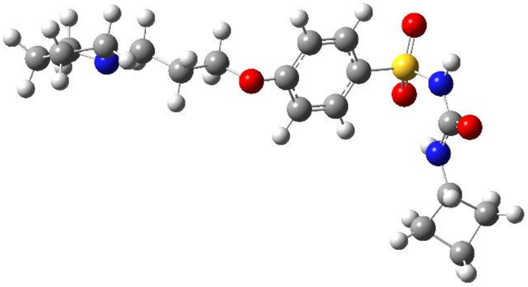
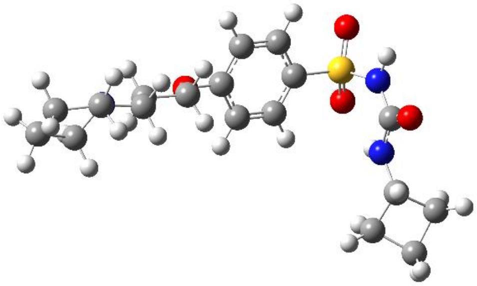
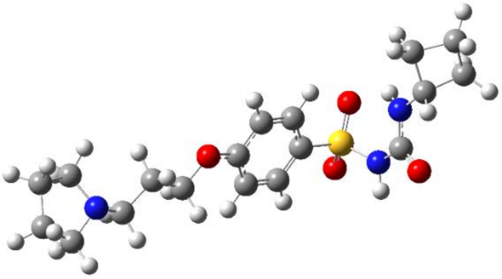
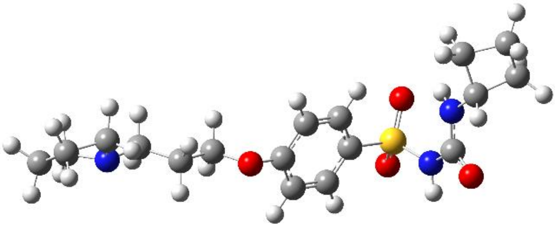
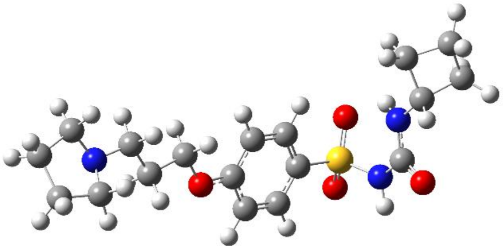
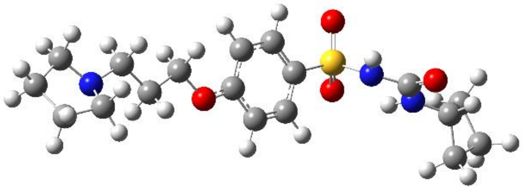
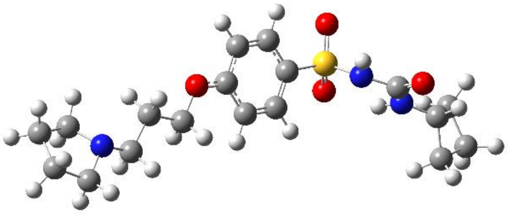
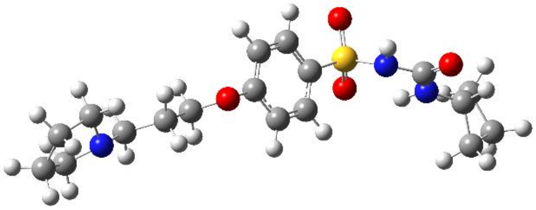
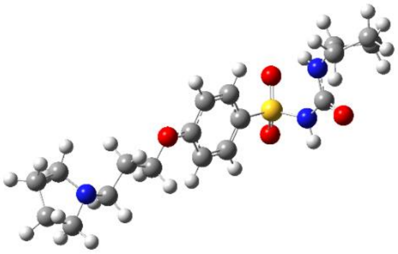
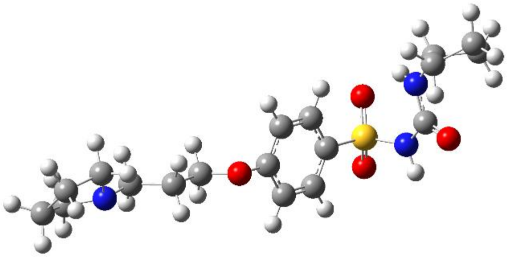
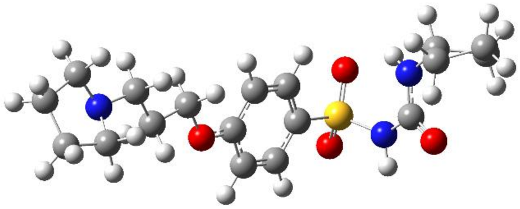
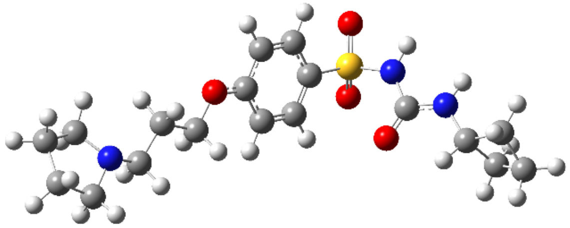
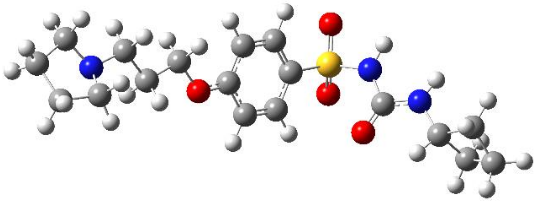
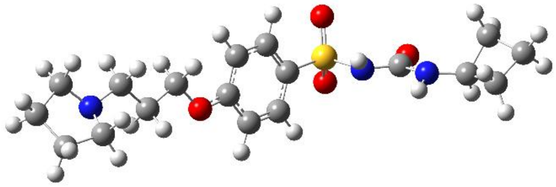
	
ALQ-j-q-u3	ALQ-j-r-u3
	
ALQ-j-q-u3	ALQ-j-r-u3′

Figure 6.7: Optimized geometries of the calculated conformers of compound BGP.

	
BGP-p-s-v3	BGP-p-t-v3
	
BGP-m-r-v1	BGP-m-s-v1

	
BGP-m-q-v1	BGP-k-q-v3
	
BGP-k-r-v3	BGP-k-s-v3
	
BGP-m-r-v2	BGP-m-s-v2
	
BGP-m-q-v2	BGP-g-r-v1
	
BGP-g-q-v1	BGP-j-q-v5

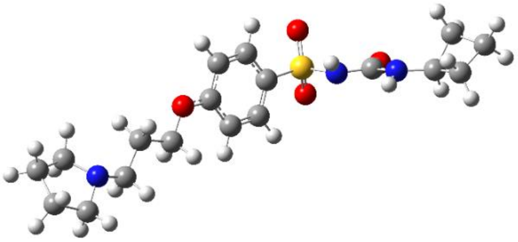
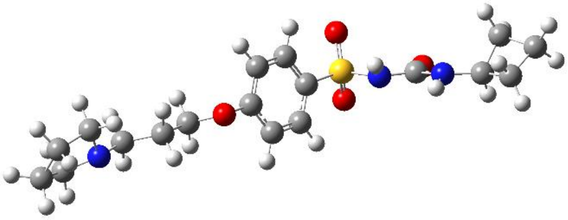
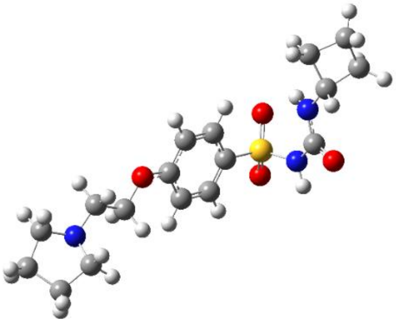
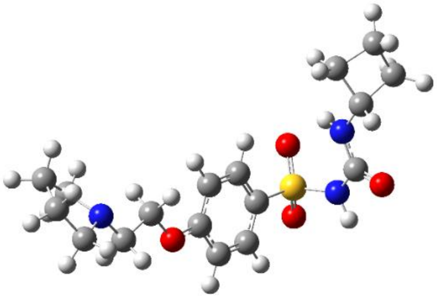
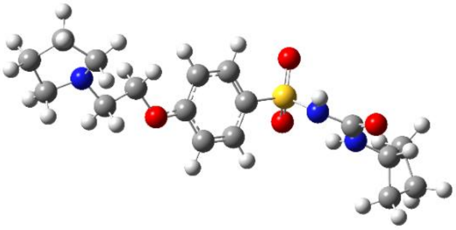
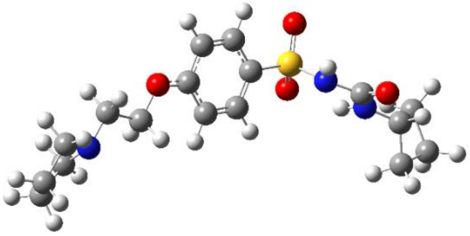
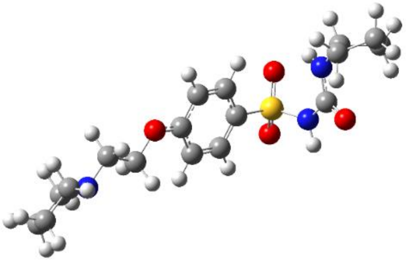
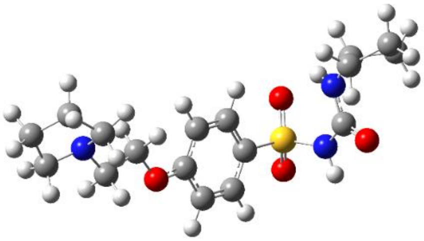
	
BGP-j-r-v5	BGP-j-r-v5

Figure 6.8: Optimized geometries of the calculated conformers of compound BGQ.

	
BGQ-m-r-v1	BGQ-m-q-v1
	
BGQ-k-q-v1	BGQ-k-r-v1
	
BGQ-m-r-v2	BGQ-m-q-v2

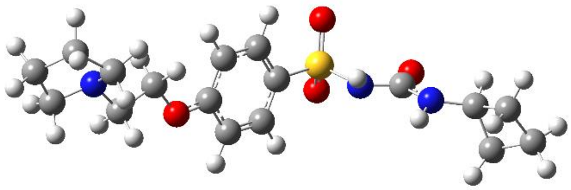
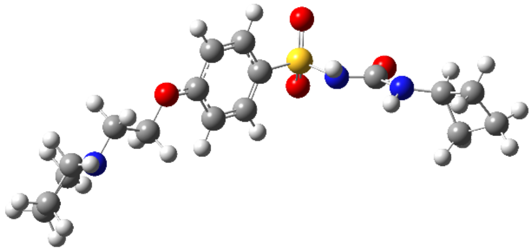
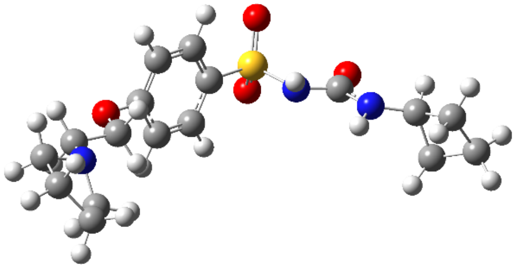
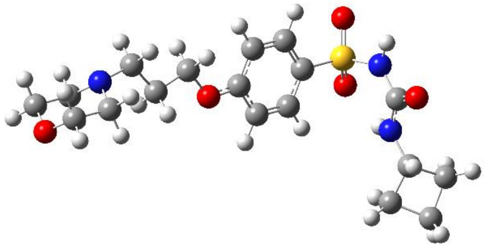
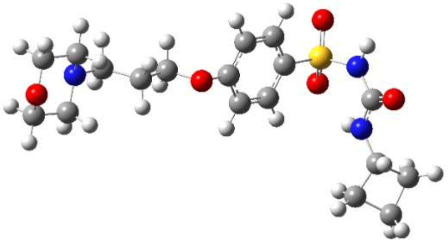
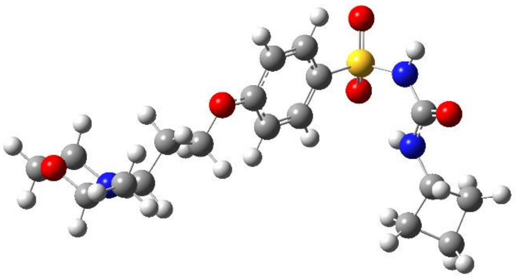
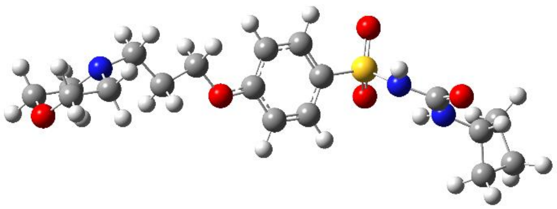
	
BGQ-j-q-v3	BGQ-j-r-v3
	
BGQ-j-t-v3	

Figure 6.9: Optimized geometries of the calculated conformers of compound BJP.

	
BJP-p-q-v3	BJP-p-s-v3
	
BJP-p-r-v3	BJP-k-q-v1

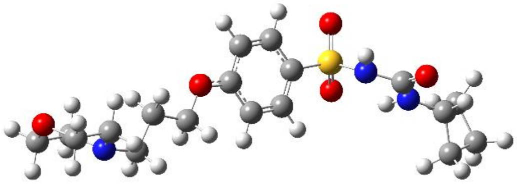
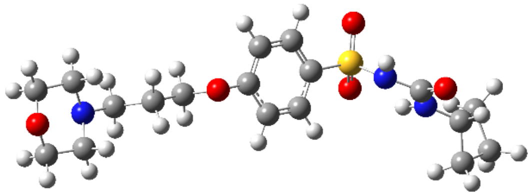
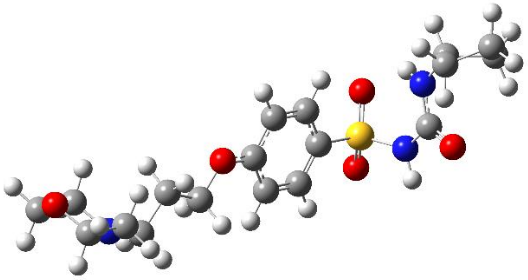
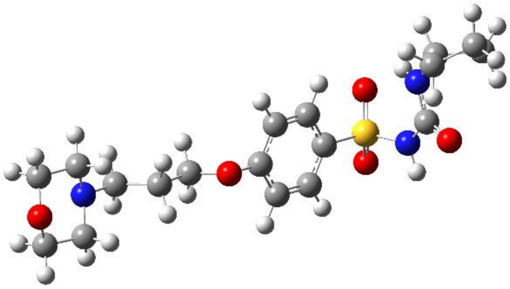
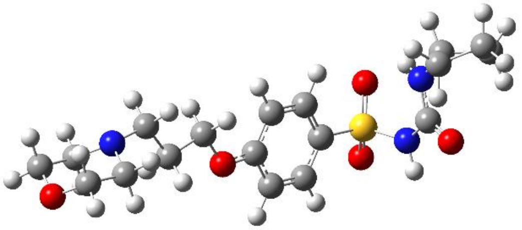
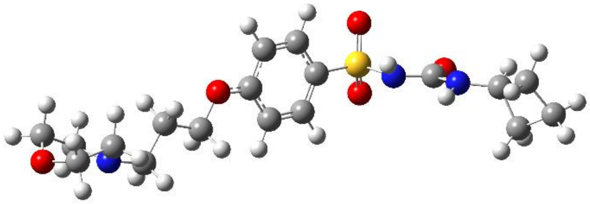
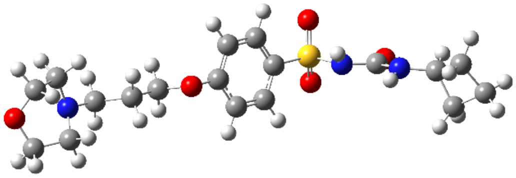
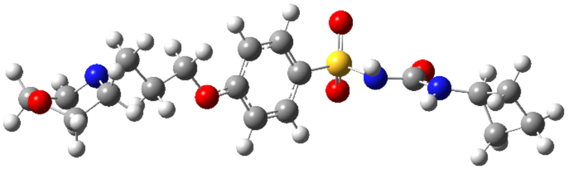
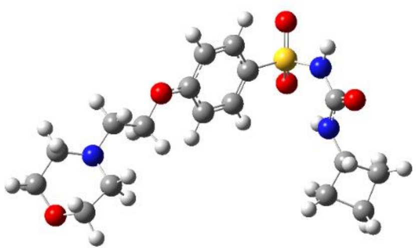
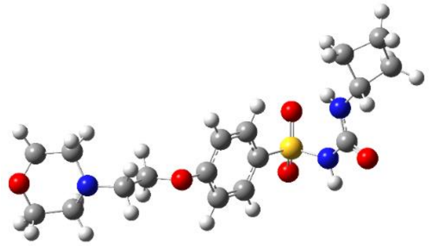
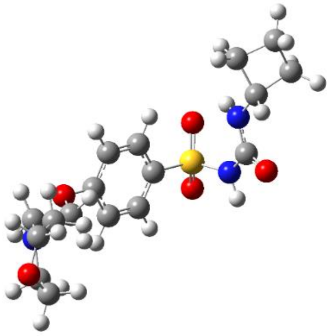
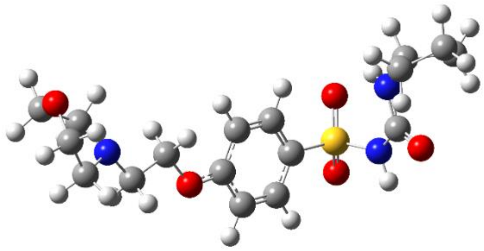
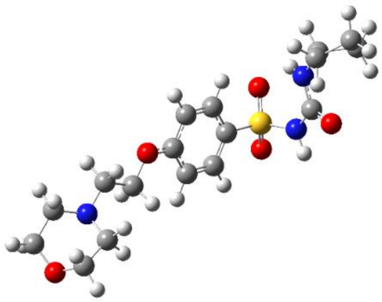
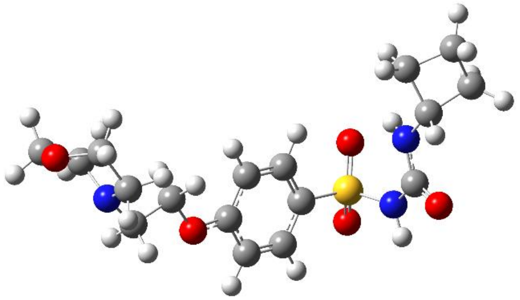
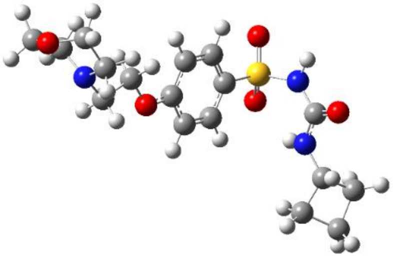
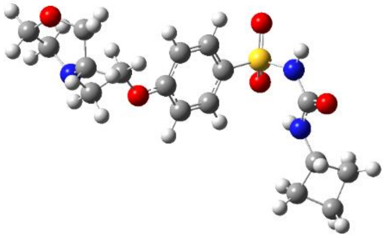
	
BJP-k-r-v1	BJP-k-s-v1
	
BJP-m-r-v2	BJP-m-s-v2
	
BJP-m-q-v2	BJP-j-r-v3
	
BJP-j-s-v3	BJP-j-q-v3

Figure 6.10: Optimized geometries of the calculated conformers of compound BJQ.

	
BJQ-p-r-v3	BJQ-m-s-v1
	
BJQ-m-t-v1	BJQ-m-q-v2
	
BJQ-m-r-v2	BJQ-m-q-v1
	
BJQ-p-q-v3	BJQ-p-q-v3

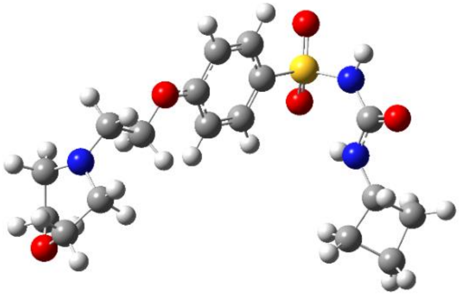
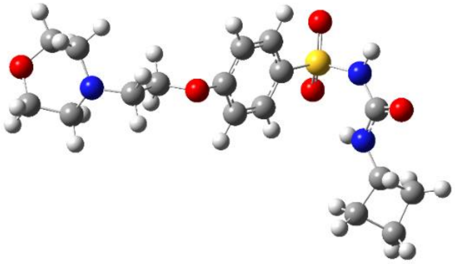
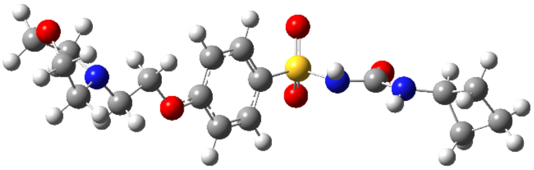
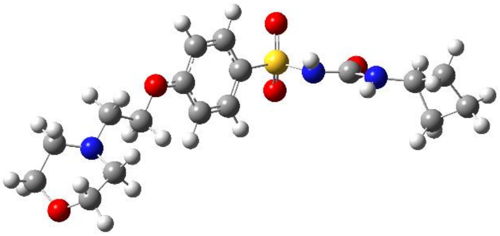
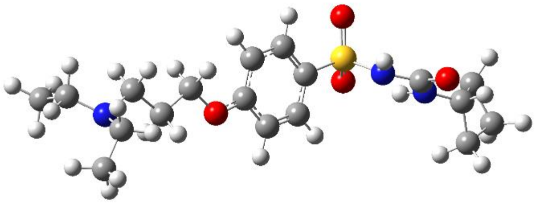
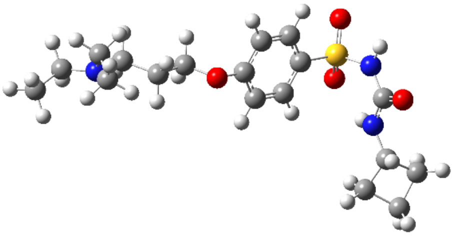
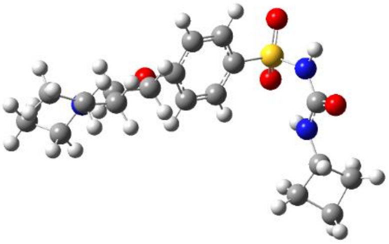
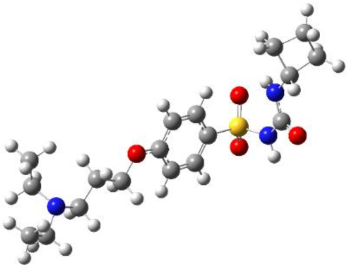
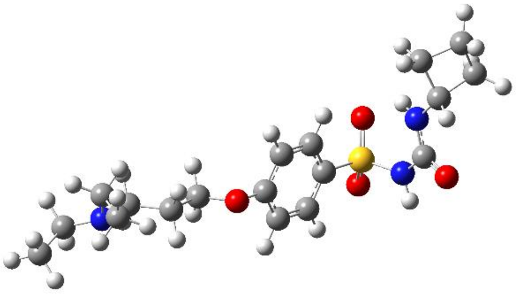
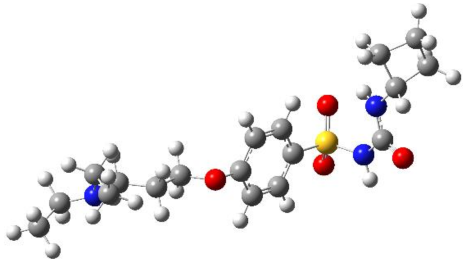
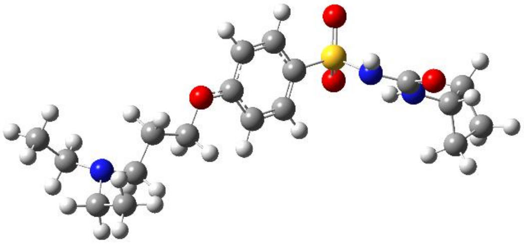
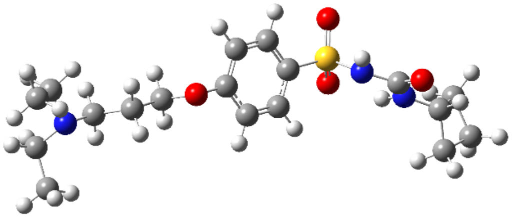
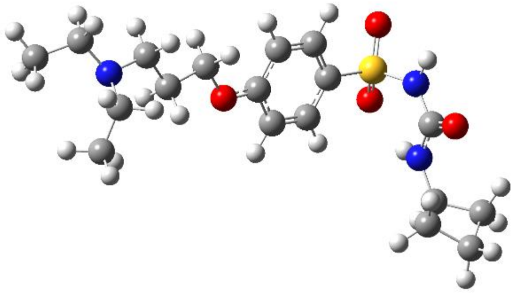
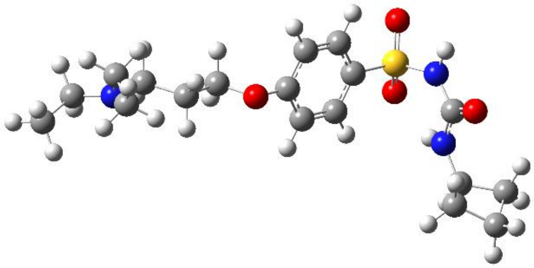
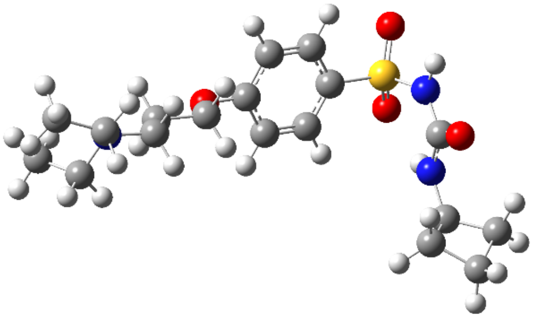
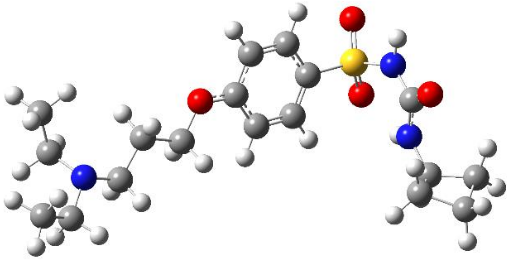
	
BJQ-p-r-v3	BJQ-p-s-v3
	
BJQ-j-q-v3	BJQ-j-r-v3

Figure 6.11: Optimized geometries of the calculated conformers of compound BLP.

	
BLP-k-q-v1	BLP-p-s-v3
	
BLP-p-t-v3	BLP-m-r-v1

	
BLP-m-s-v1	BLP-m-r-v1′
	
BLP-k-r-v1	BLP-k-s-v1
	
BLP-p-q-v4	BLP-p-s-v4
	
BLP-p-t-v4	BLP-p-r-v4

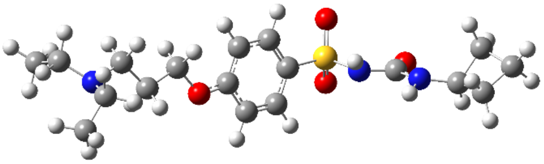
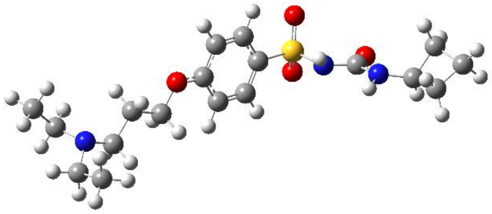
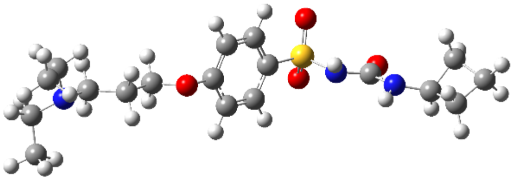
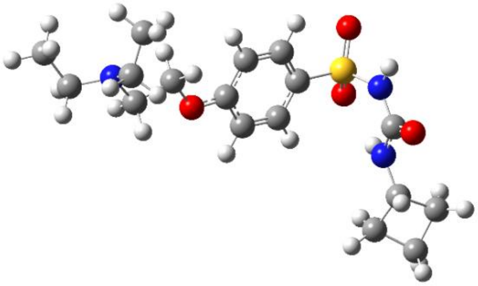
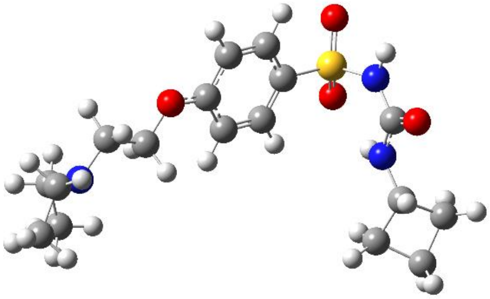
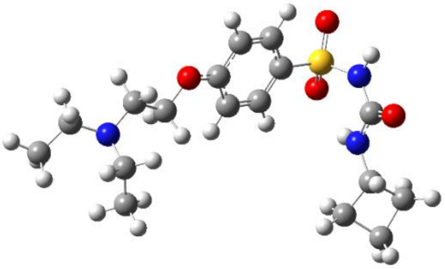
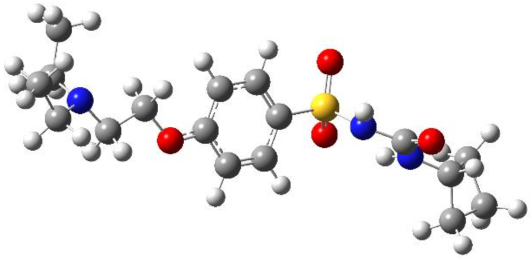
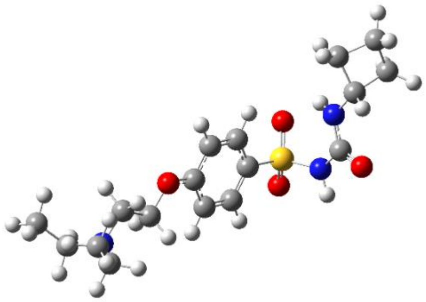
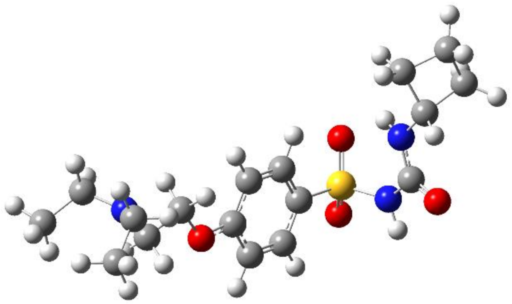
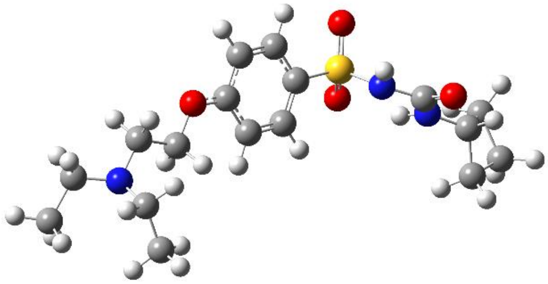
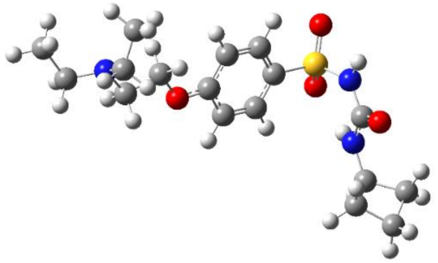
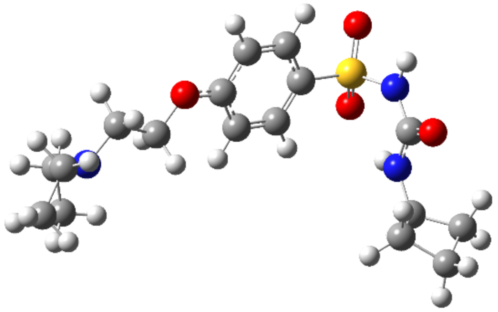
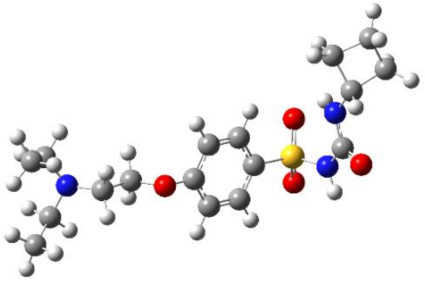
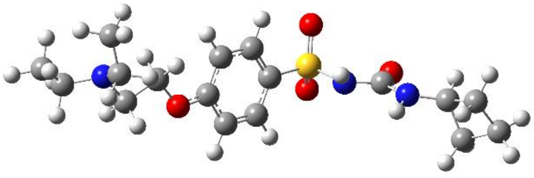
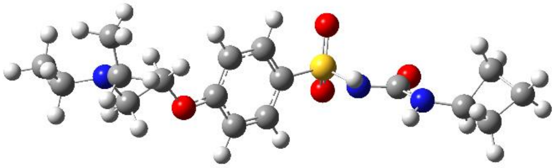
	
BLP-j-q-v5	BLP-j-r-v5
	
BLP-j-s-v5	

Figure 6.12: Optimized geometries of the calculated conformers of compound BLQ.

	
BLQ-p-q-v3	BLQ-p-r-v3
	
BLQ-p-r-v3′	BLQ-k-q-v1

	
BLQ-m-r-v1	BLQ-m-q-v1
	
BLQ-k-r-v1	BLQ-p-q-v4
	
BLQ-p-r-v4	BLQ-m-s-v1
	
BLQ-j-q-v3	BLQ-j-q-v5

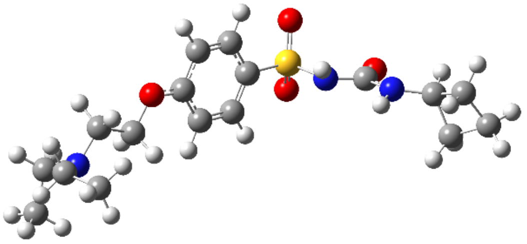
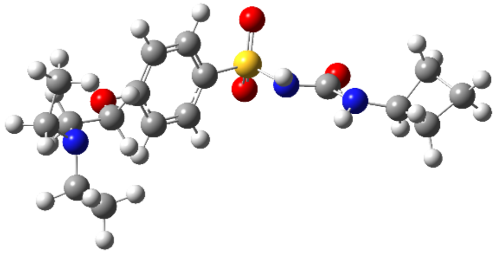
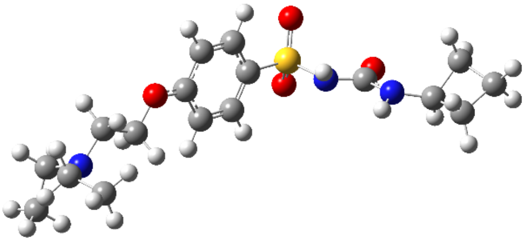
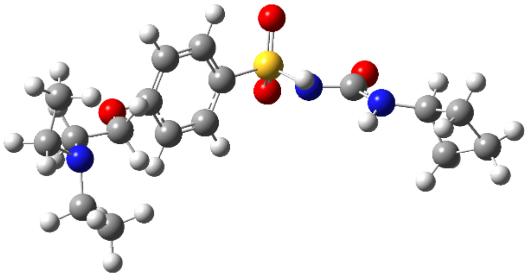
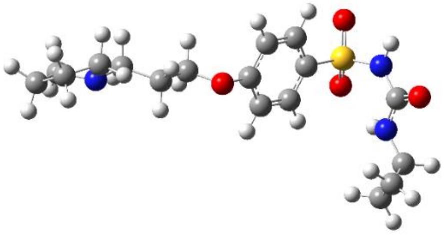
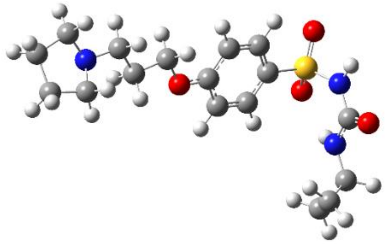
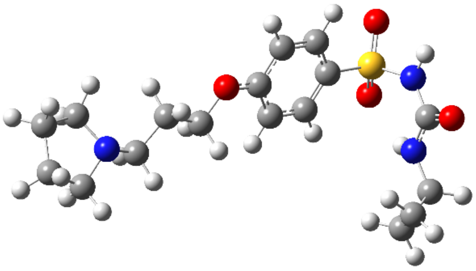
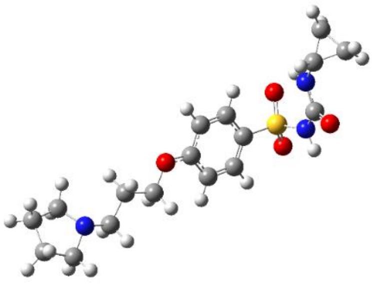
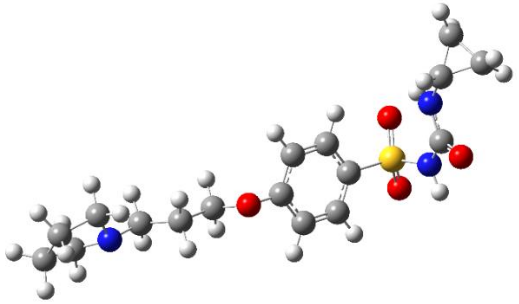
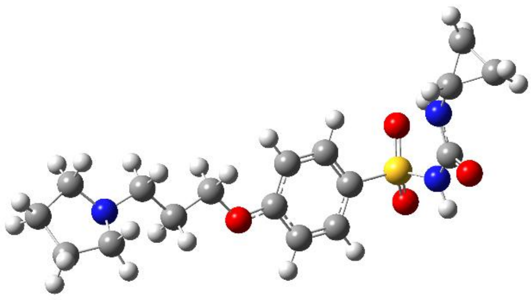
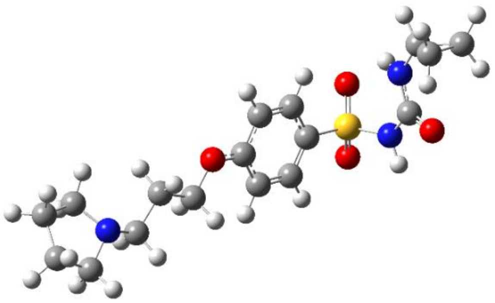
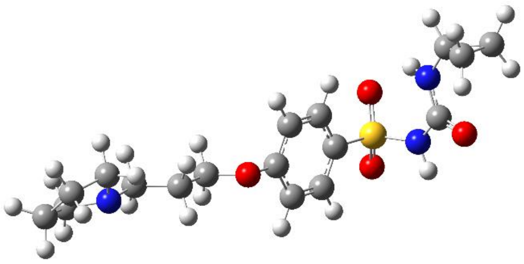
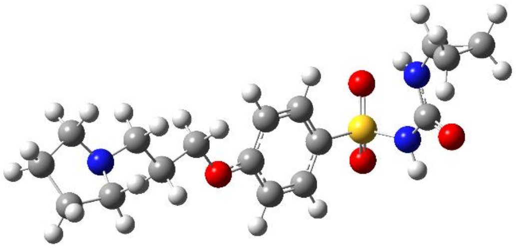
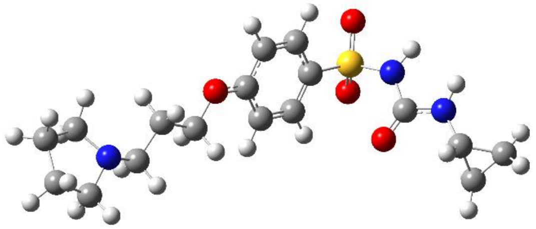
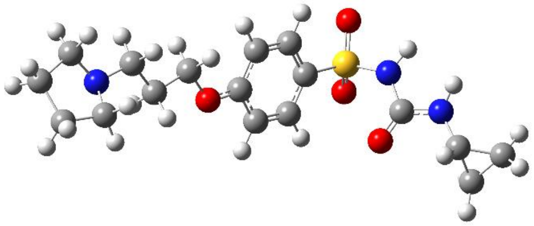
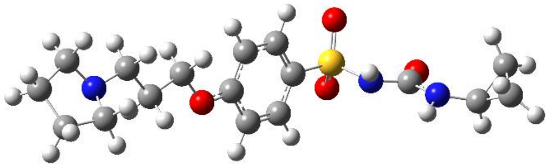
	
BLQ-j-r-v3	BLQ-j-t-v5
	
BLQ-j-r-v5	BLQ-j-t-v3

Figure 6.13: Optimized geometries of the calculated conformers of compound CGP.

	
CGP-p-s-w5	CGP-p-q-w5
	
CGP-p-r-w5	CGP-m-r-w1

	
CGP-m-s-w1	CGP-m-q-w1
	
CGP-m-r-w2	CGP-m-s-w2
	
CGP-m-q-w2	CGP-g-r-w5
	
CGP-g-q-w5	CGP-j-q-w5

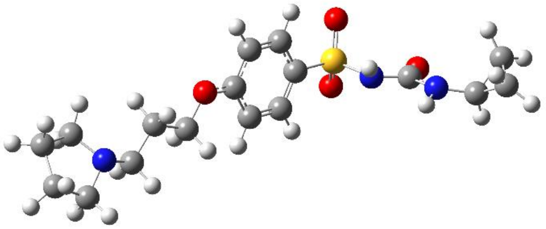
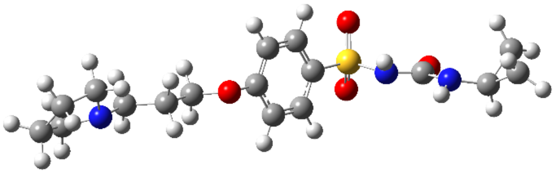
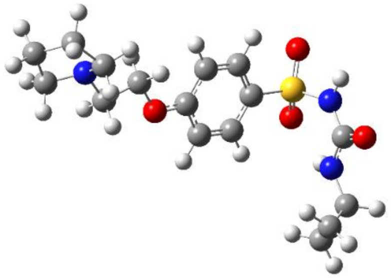
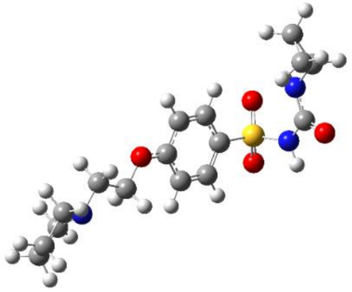
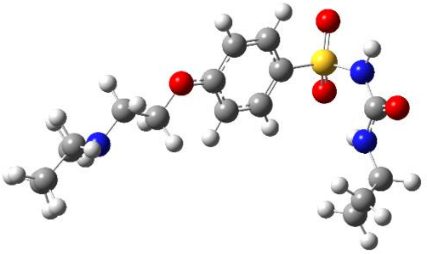
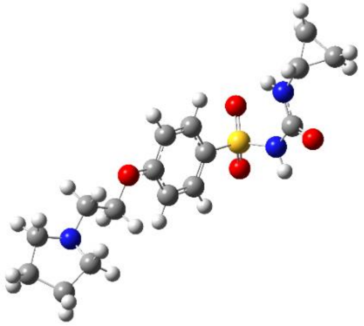
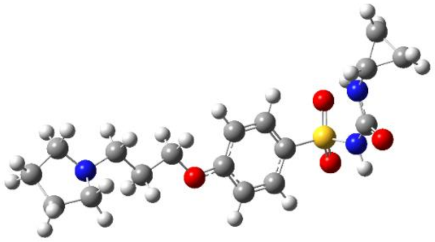
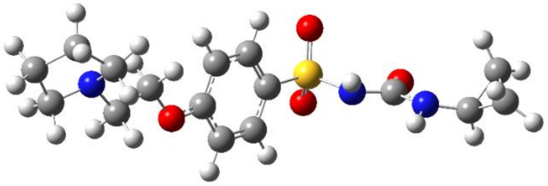
	
CGP-j-r-w5	CGP-j-s-w5

Figure 6.14: Optimized geometries of the calculated conformers of compound CGQ.

	
CGQ-p-q-w5	CGQ-m-q-w3
	
CGQ-p-r-w5	CGQ-m-r-w1
	
CGQ-m-q-w1	CGQ-j-q-w5

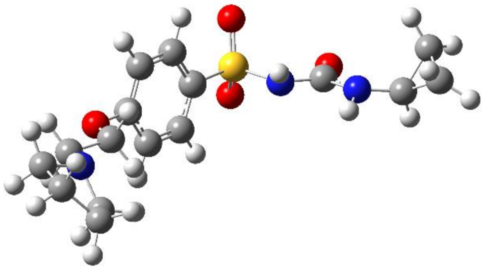
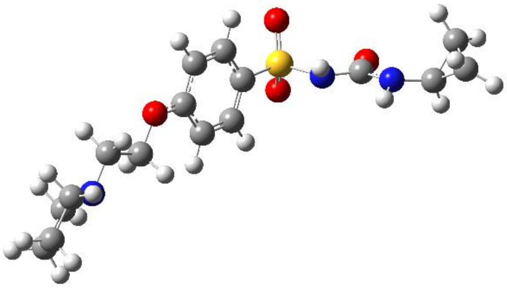
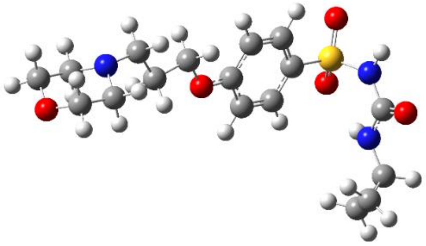
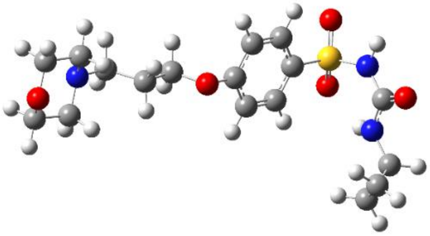
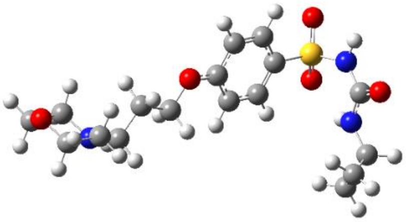
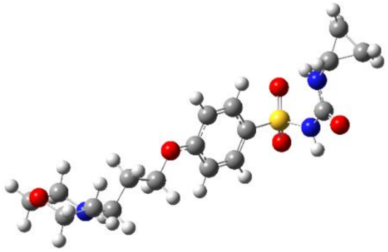
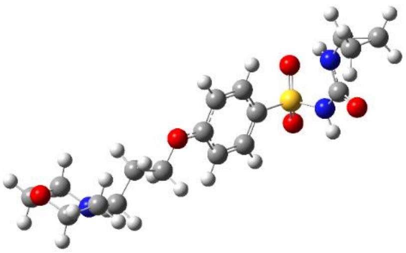
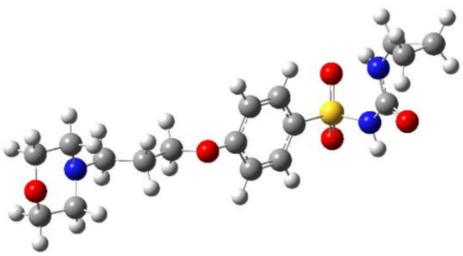
	
CGQ-j-t-w5	CGQ-j-r-w5

Figure 6.15: Optimized geometries of the calculated conformers of compound CJP.

	
CJP-p-q-w3	CJP-p-s-w3
	
CJP-p- r-w3	CJP-m-r-w1
	
CJP-m-r-w2	CJP-m-s-w2

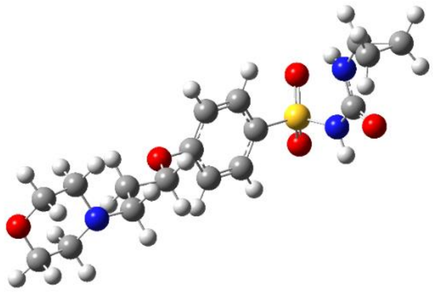
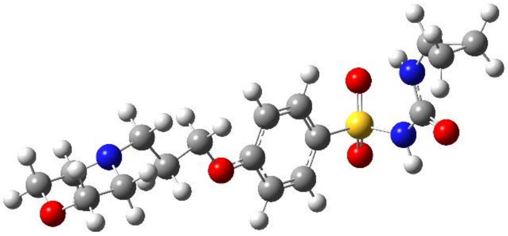
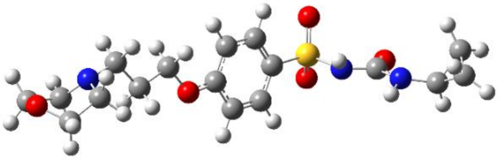
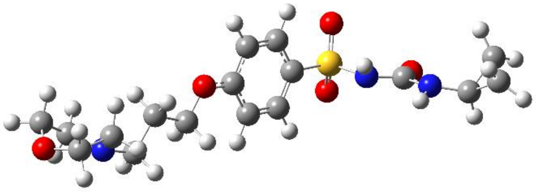
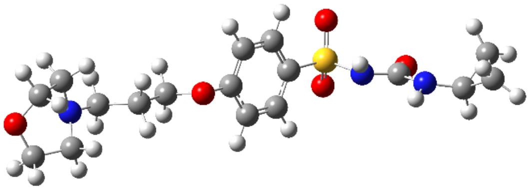
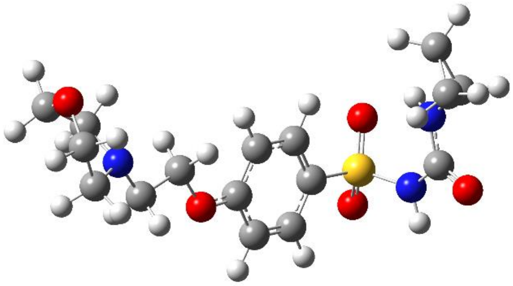
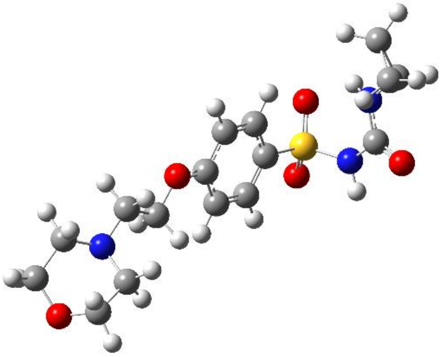
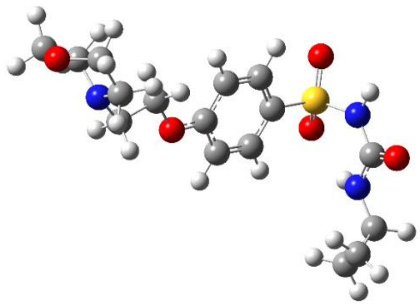
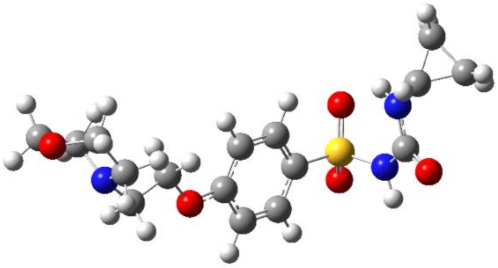
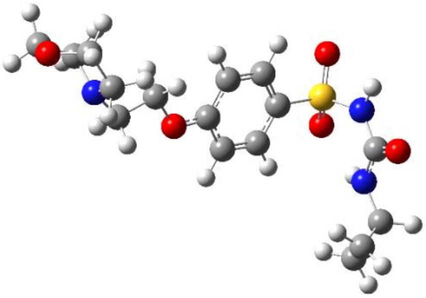
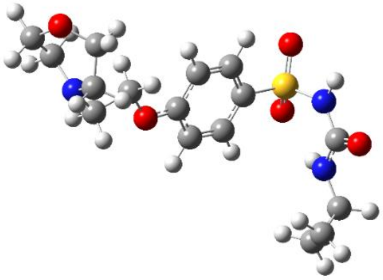
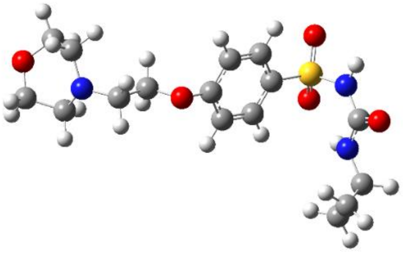
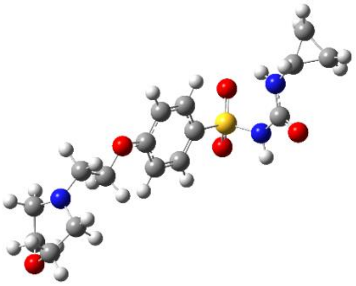
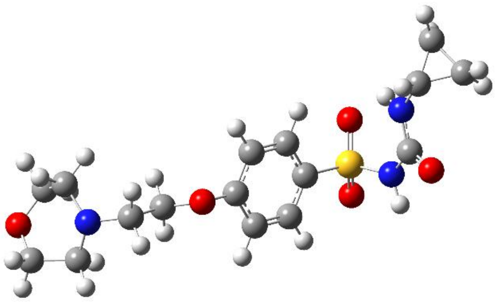
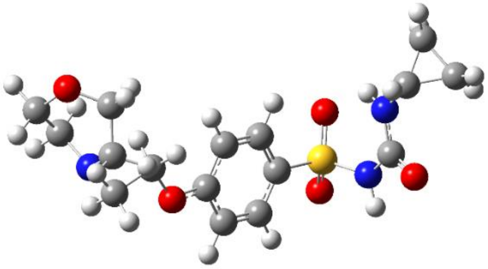
	
CJP-m-t-w2	CJP-m-q-w2
	
CJP-j-q-w1	CJP-j-r-w1
	
CJP-j-s-w1	

Figure 6.16: Optimized geometries of the calculated conformers of compound CJQ.

	
CJQ-m-q-w6	CJQ-m-r-w6

	
CJQ-p-q-w5	CJQ-m-q-w1
	
CJQ-p-q-w5	CJQ-p-q-w5′
	
CJQ-p-s-w5	CJQ-m-r-w1
	
CJQ-m-s-w1	CJQ-m-q-w1′

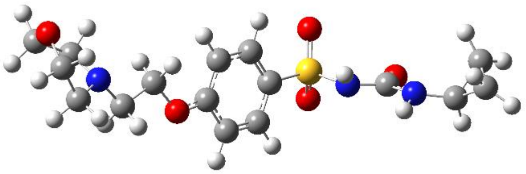
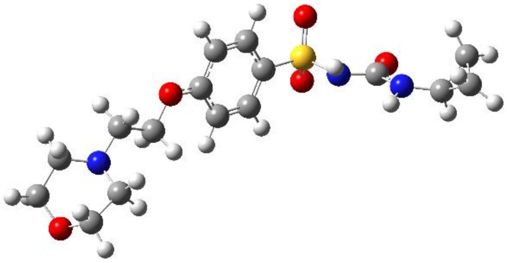
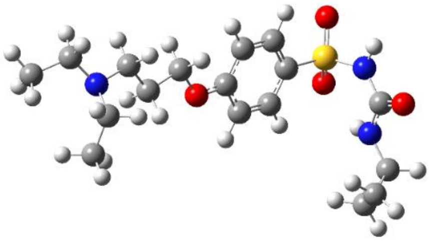
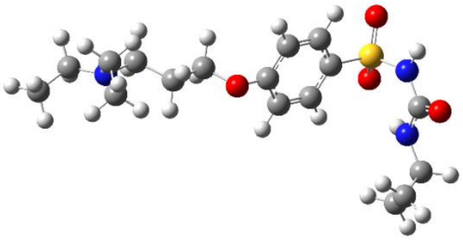
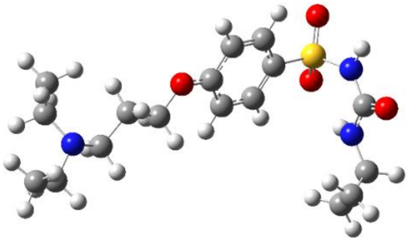
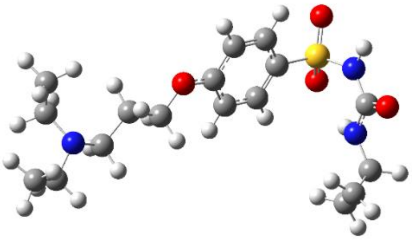
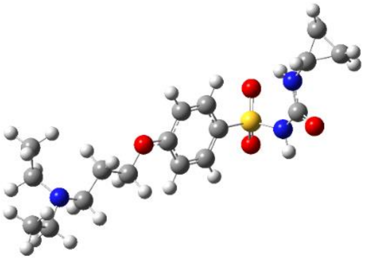
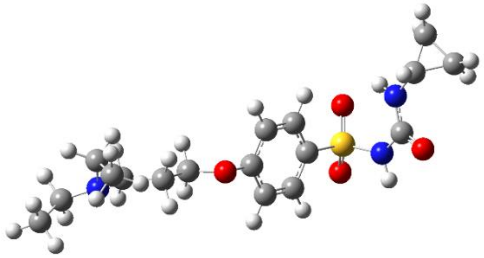
	
CJQ-j-q-w5	CJQ-j-r-w5

Figure 6.17: Optimized geometries of the calculated conformers of compound CLP.

	
CLP-p-q-w5	CLP-p-s-w5
	
CLP-p-r-w5	CLP-p-r-w5′
	
CLP-m-r-w1	CLP-m-s-w1

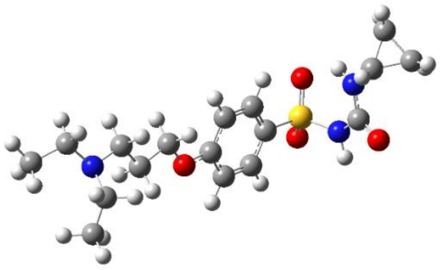
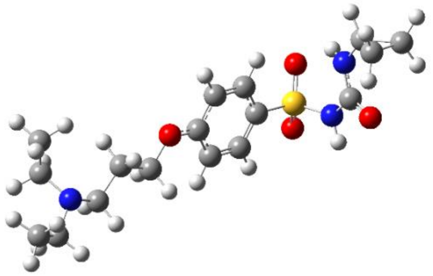
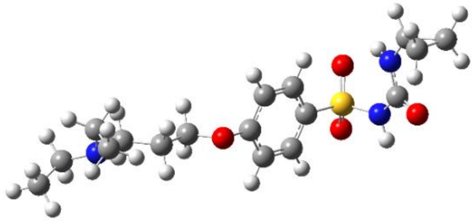
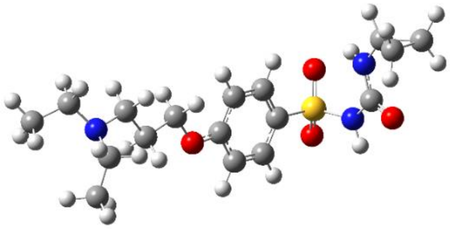
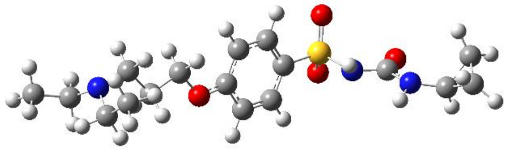
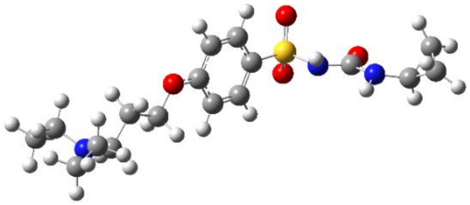
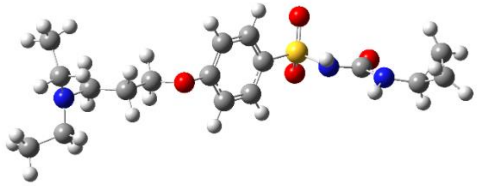
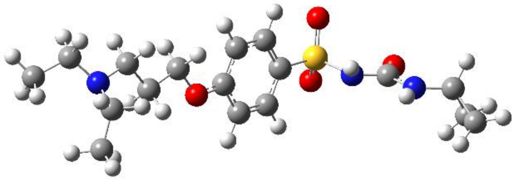
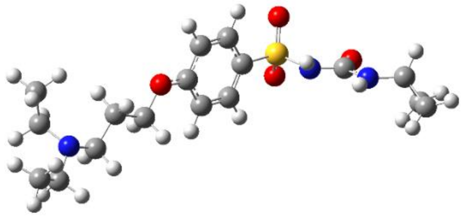
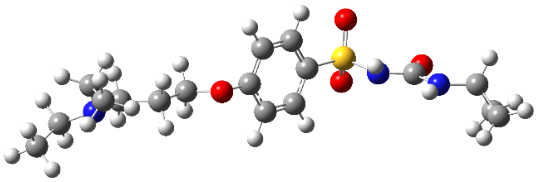
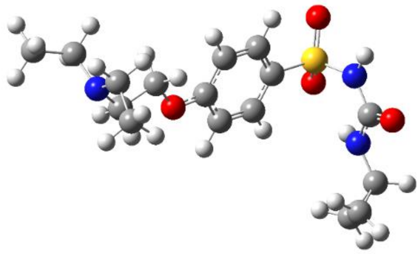
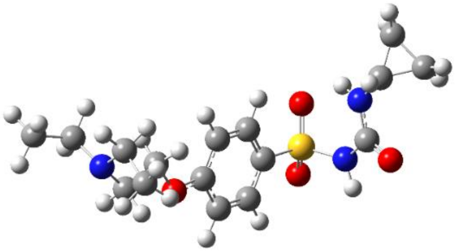
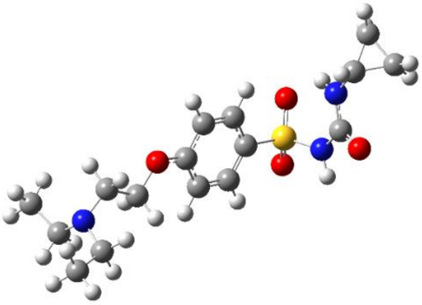
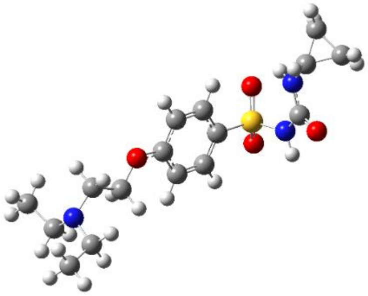
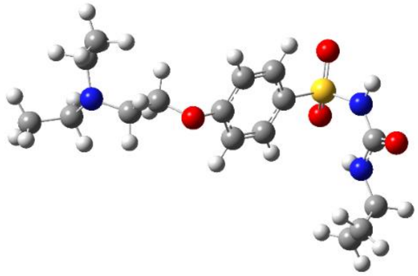
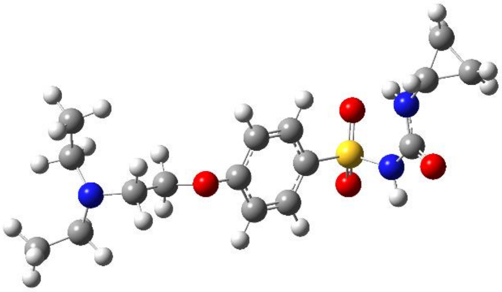
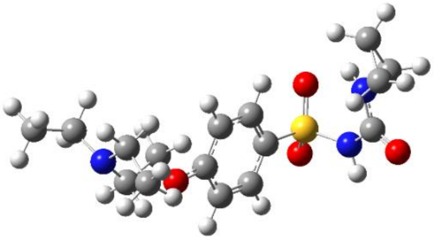
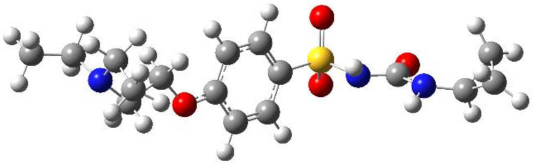
	
CLP-m-q-w1	CLP-m-q-w2
	
CLP-m-s-w2	CLP-m-q-w2
	
CLP-j-q-w5	CLP-j-r-w5
	
CLP-j-s-w5	CLP-j-q-w6
	
CLP-j-r-w6	CLP-j-s-w6

Figure 6.18: Optimized geometries of the calculated conformers of compound CLQ.

	
CLQ-p-q-w5	CLQ-p-s-w5
	
CLQ-m-q-w1	CLQ-m-q-w1′
	
CLQ-m-r-w1	CLQ-m-r-w1′
	
CLQ-m-s-w1	CLQ-j-q-w5

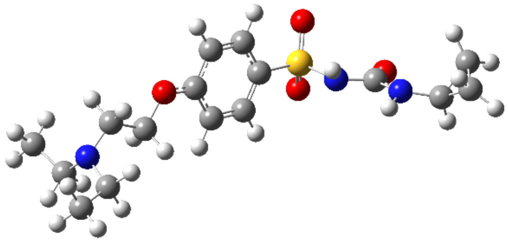
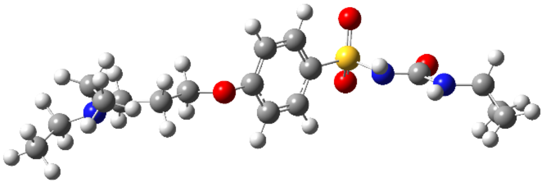
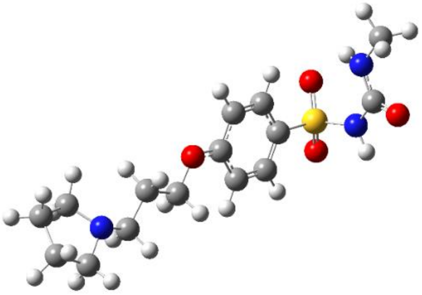
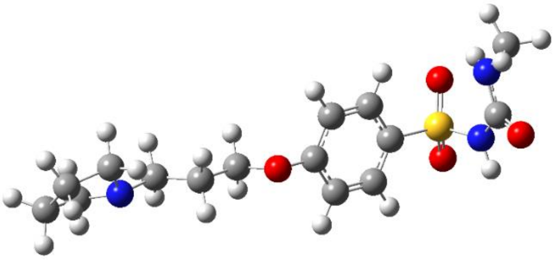
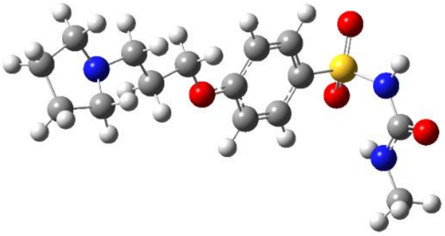
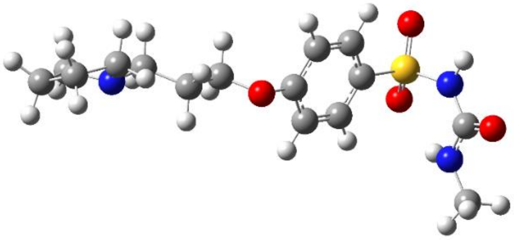
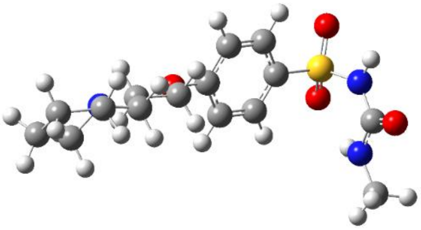
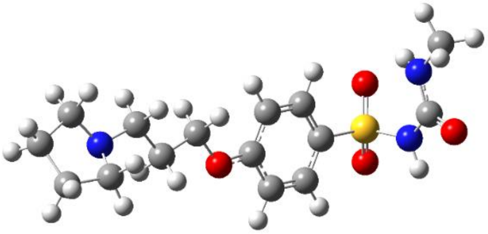
	
CLQ-j-r-w5	CLQ-j-s-w6

Figure 6.19: Optimized geometries of the calculated conformers of compound DGP.

	
DGP-m-r	DGP-m-s
	
DGP-p-q	DGP-p-s
	
DGP-p-t	DGP-m-q

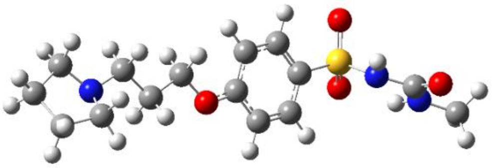
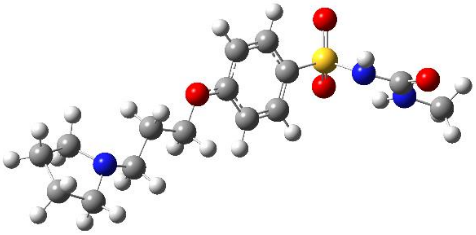
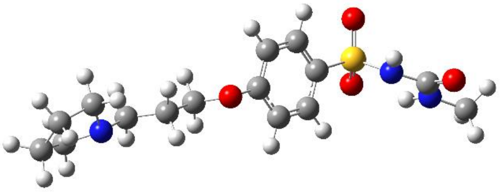
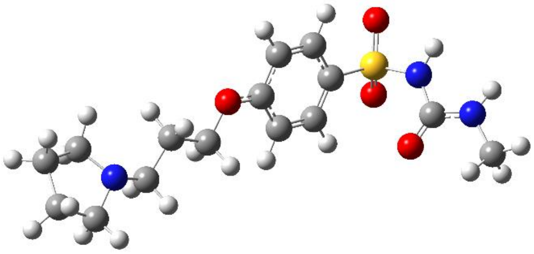
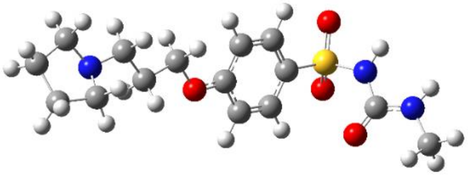
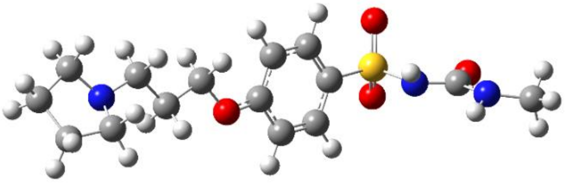
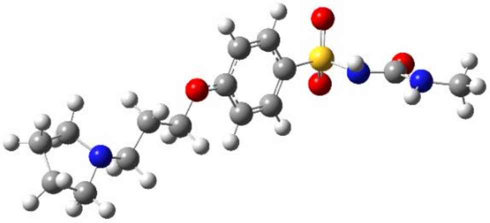
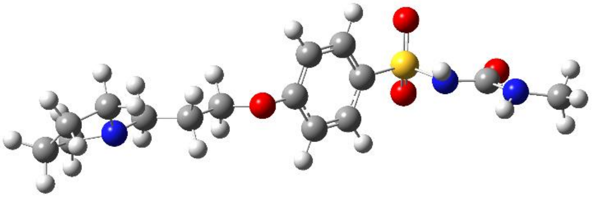
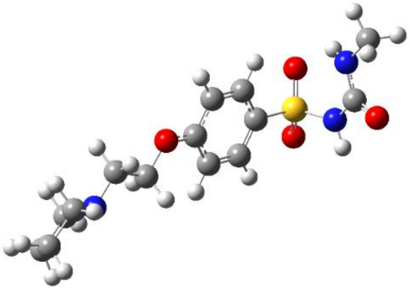
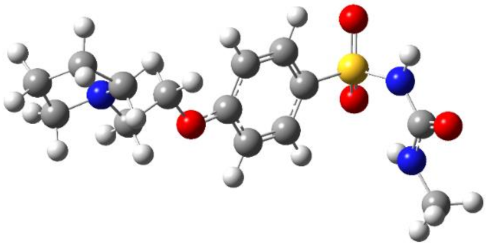
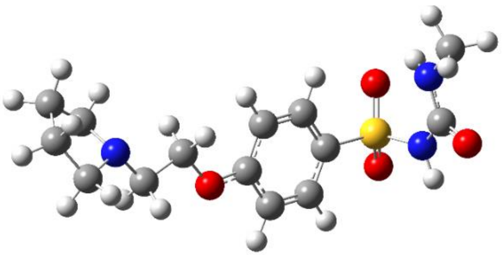
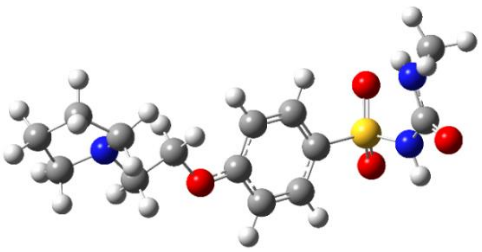
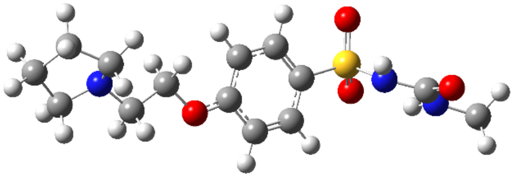
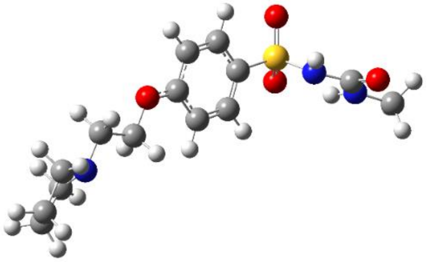
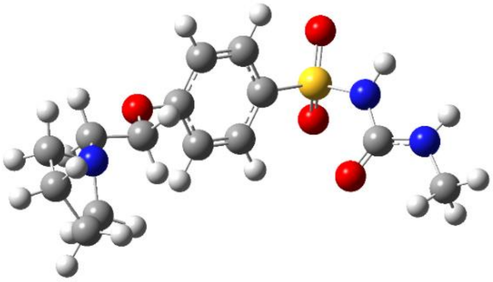
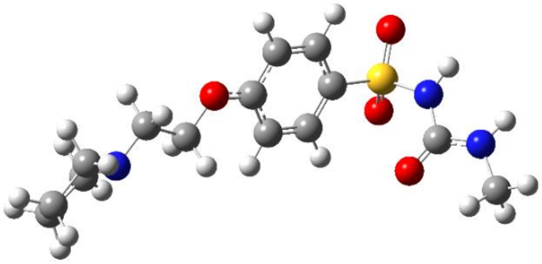
	
DGP-k-q	DGP-k-r
	
DGP-k-s	DGP-g-r
	
DGP-g-q	DGP-j-q
	
DGP-j-r	DGP-j-s

Figure 6.20: Optimized geometries of the calculated conformers of compound DGQ.

	
DGQ-m-r	DGQ-p-q
	
DGQ-m-q	DGQ-m-q′
	
DGQ-k-q	DGQ-k-r
	
DGQ-g-t	DGQ-g-r

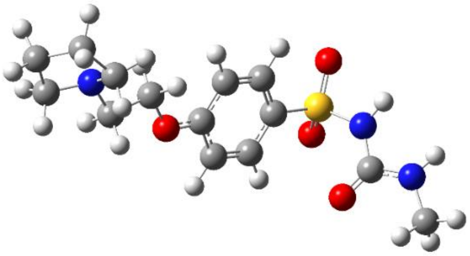
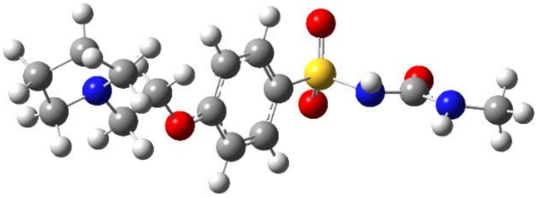
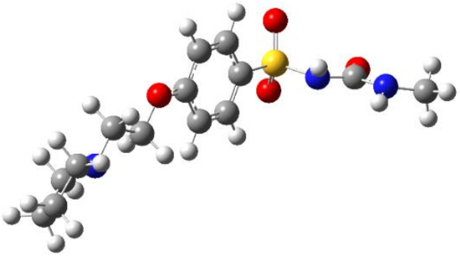
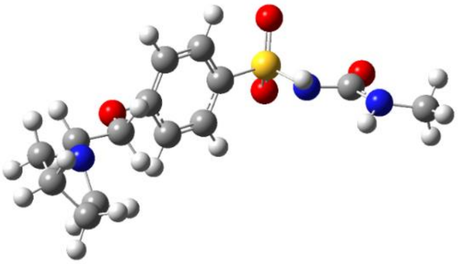
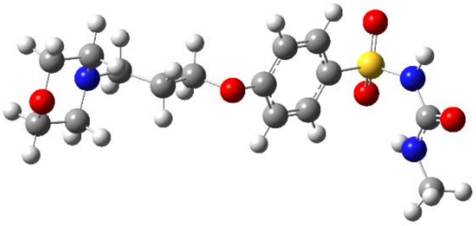
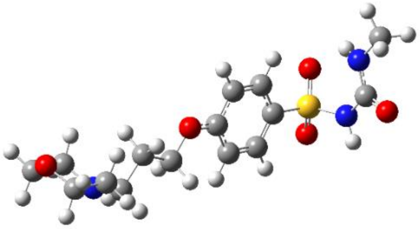
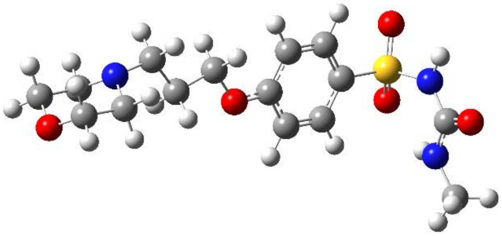
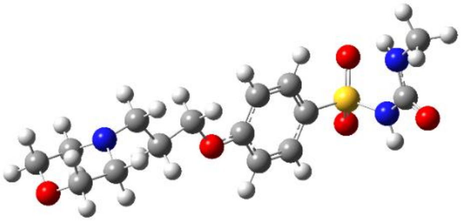
	
DGQ-g-q	DGQ-j-q
	
DGQ-j-r	DGQ-j-t

Figure 6.21: Optimized geometries of the calculated conformers of compound DJP.

	
DJP-p-s	DJP-m-r
	
DJP-p-q	DJP-m-q

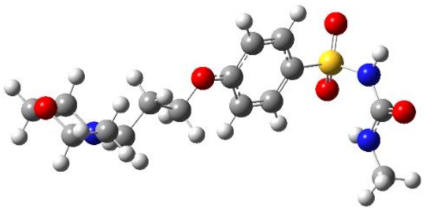
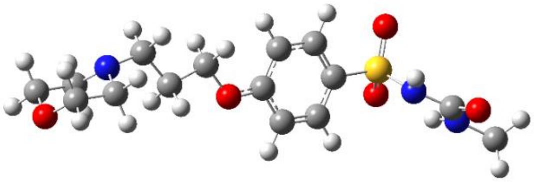
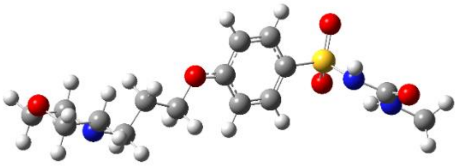
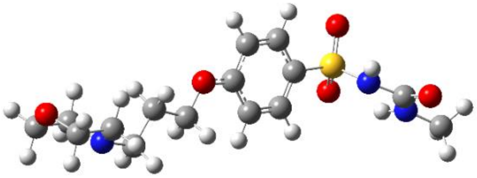
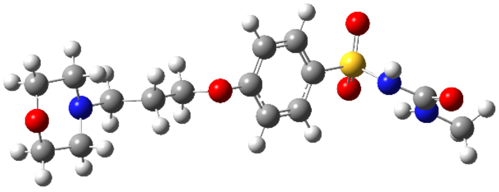
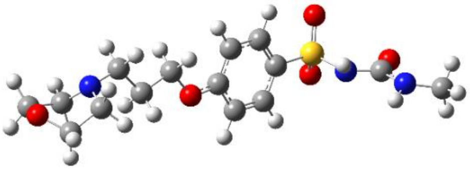
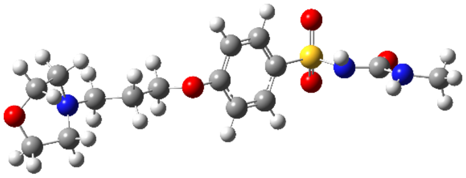
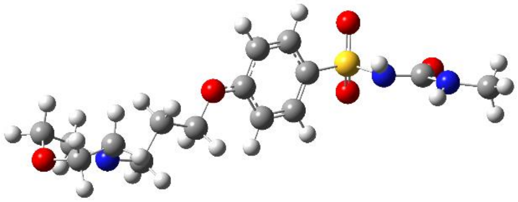
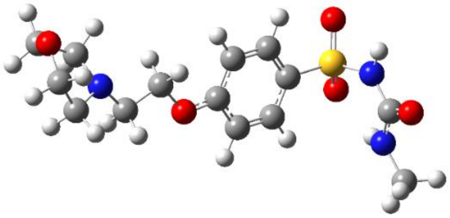
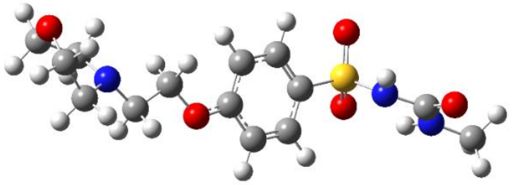
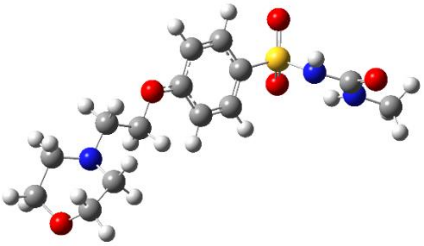
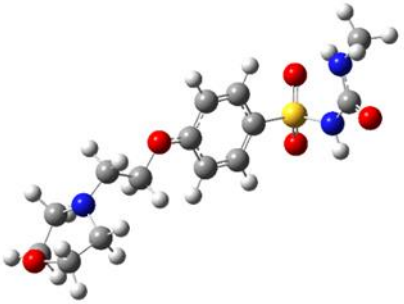
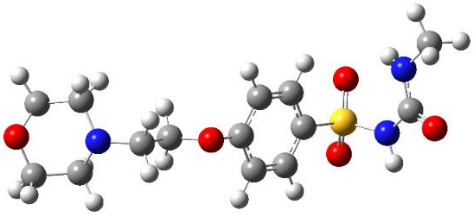
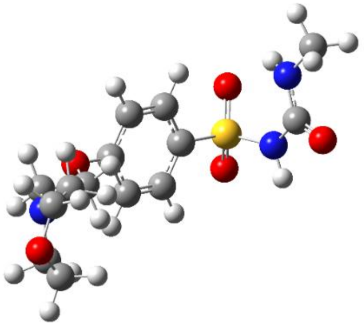
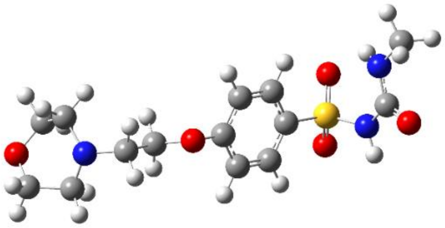
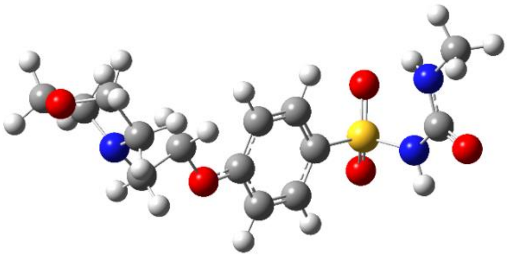
	
DJP-p-r	DJP-k-q
	
DJP-k-r	DJP-k-r′
	
DJP-k-s	DJP-j-q
	
DJP-j-s	DJP-j-r

Figure 6.22: Optimized geometries of the calculated conformers of compound DJQ.

	
DJQ-m-q	DJQ-k-q
	
DJQ-k-r	DJQ-m-r
	
DJQ-m-s	DJQ-m-t
	
DJQ-m-s′	DJQ-m-q

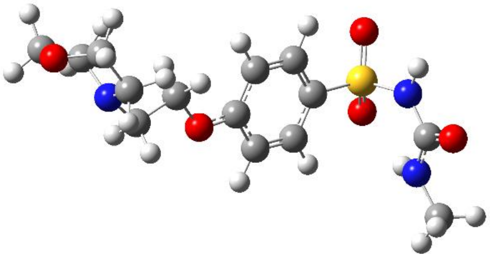
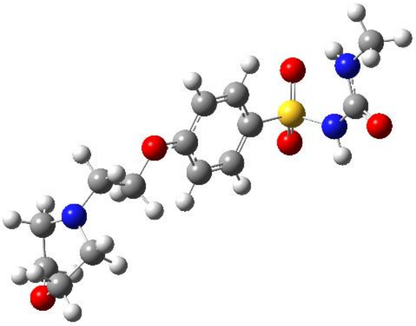
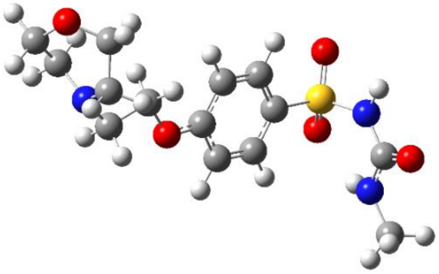
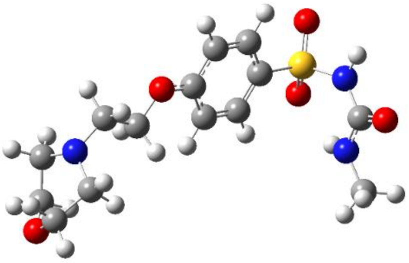
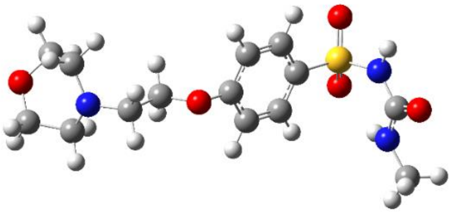
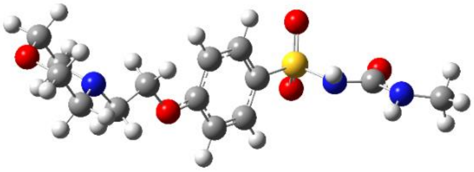
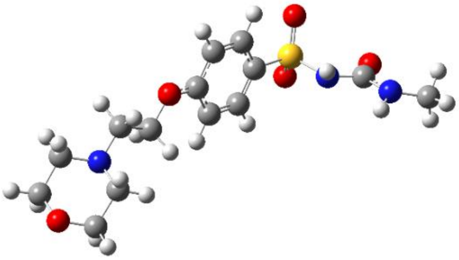
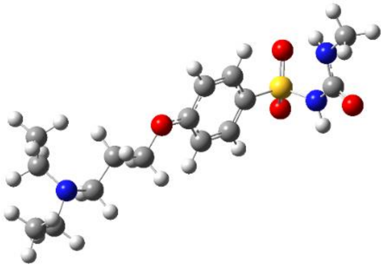
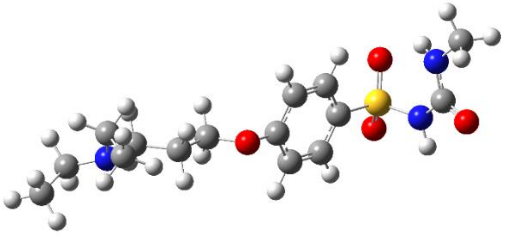
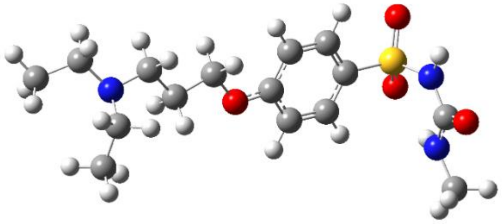
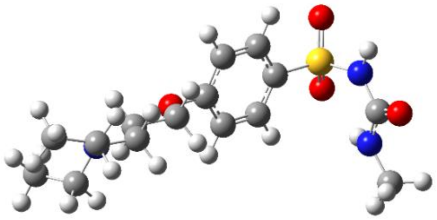
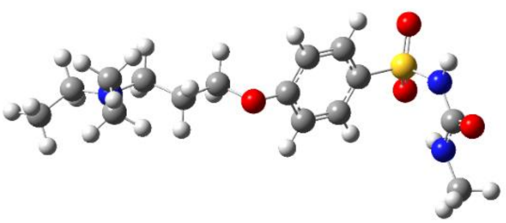
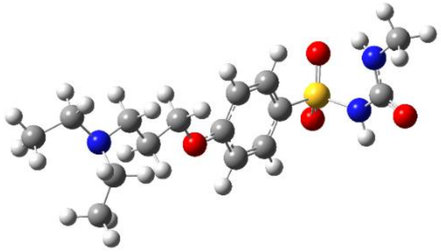
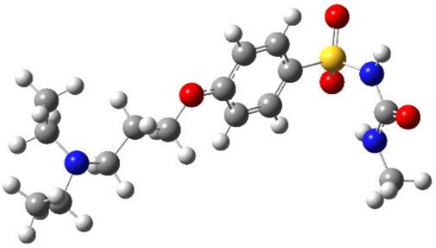
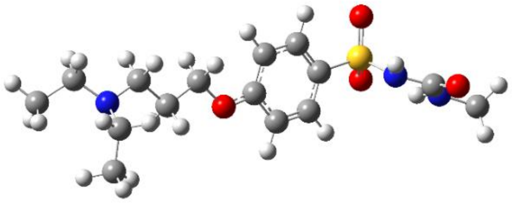
	
DJQ-p-q	DJQ-m-r′
	
DJQ-p-q′	DJQ-p-r
	
DJQ-m-q′	DJQ-j-q
	
DJQ-j-r	

Figure 6.23: Optimized geometries of the calculated conformers of compound DLP.

	
DLP-m-r	DLP-m-s
	
DLP-p-q	DLP-p-t
	
DLP-p-s	DLP-m-q
	
DLP-p-r	DLP-k-q

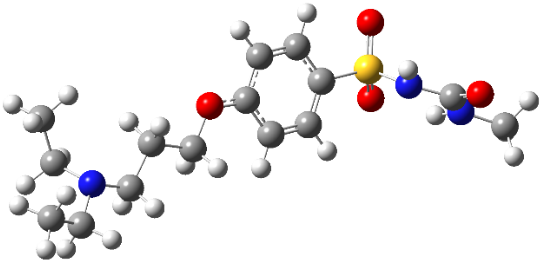
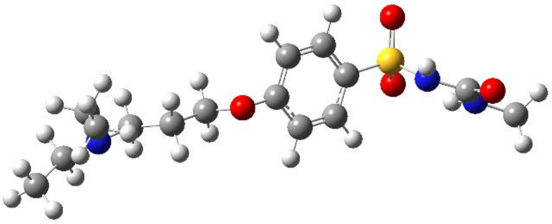
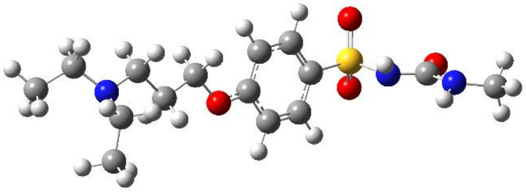
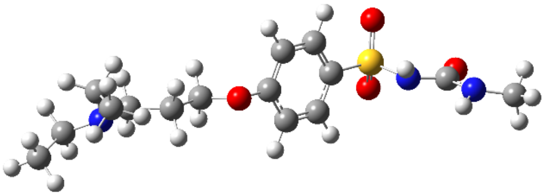
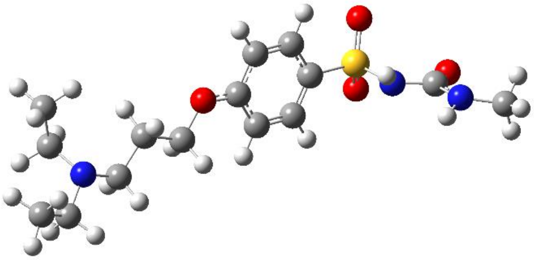
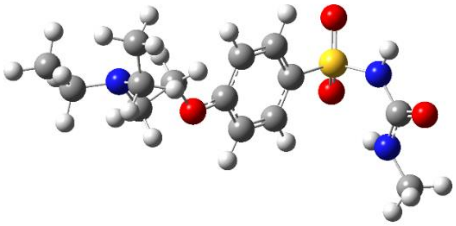
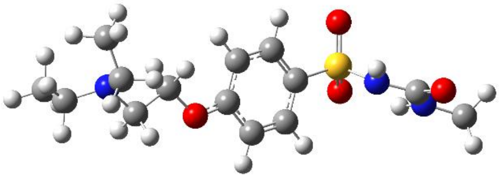
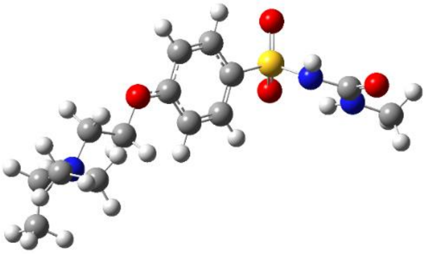
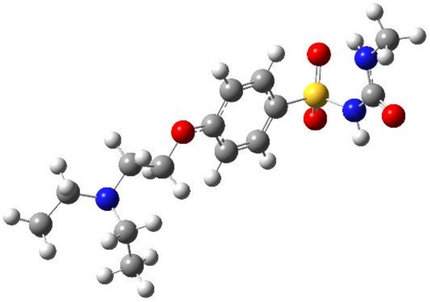
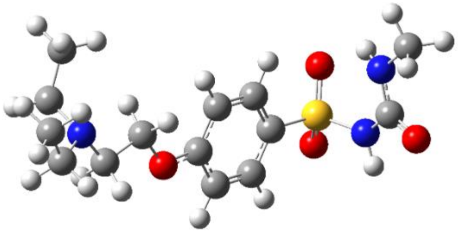
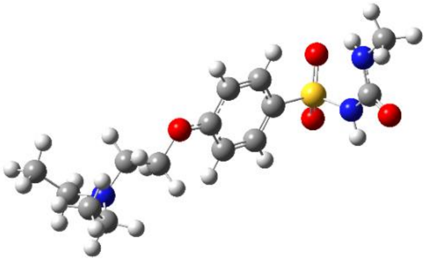
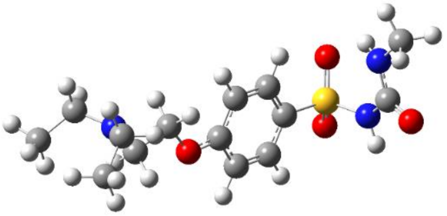
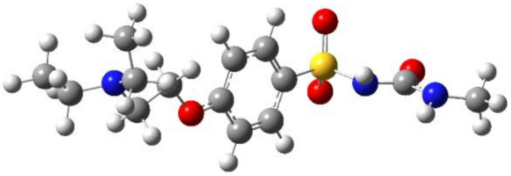
	
DLP-k-r	DLP-k-s
	
DLP-j-q	DLP-j-s
	
DLP-j-r	

Figure 6.24: Optimized geometries of the calculated conformers of compound DLQ.

	
DLQ-p-q	DLQ-k-q
	
DLQ-k-r	DLQ-m--r
	
DLQ-m-q	DLQ-m-r′
	
DLQ-m-q′	DLQ-j-q

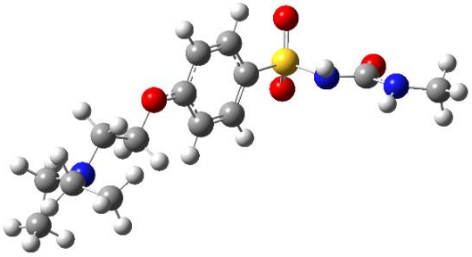
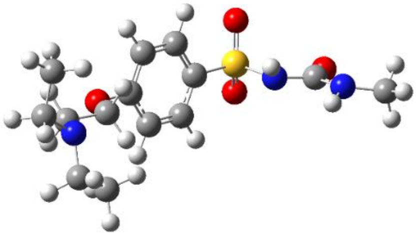
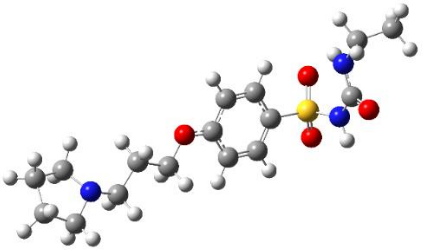
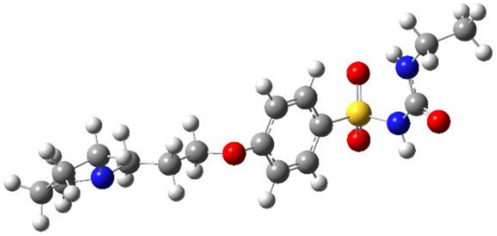
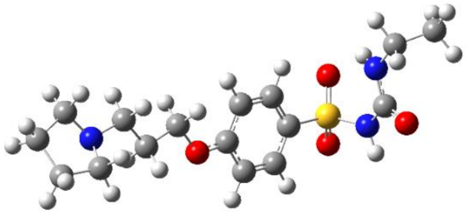
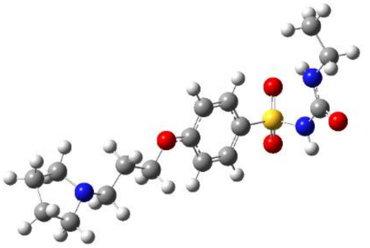
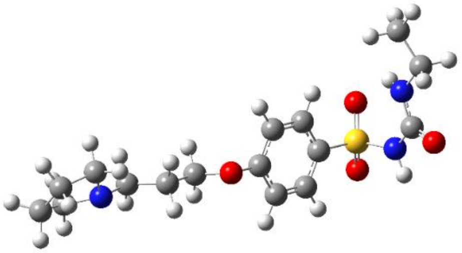
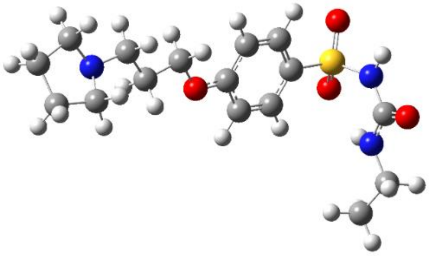
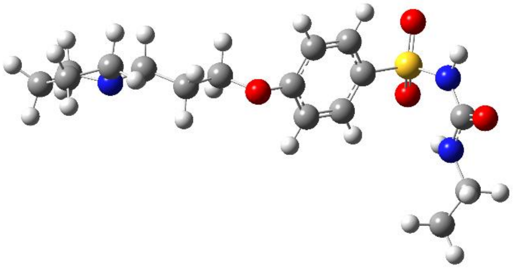
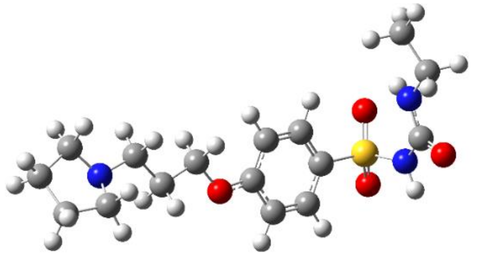
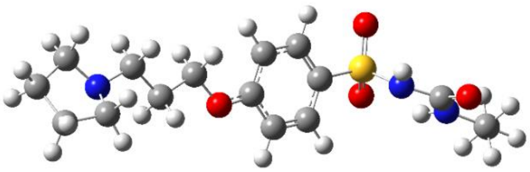
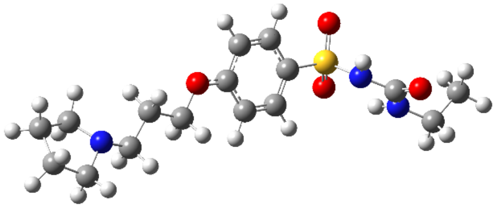
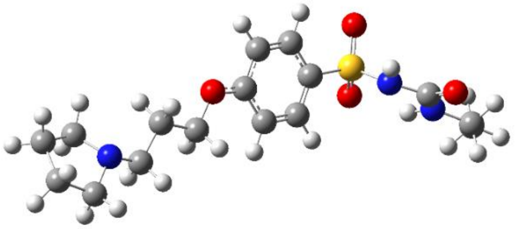
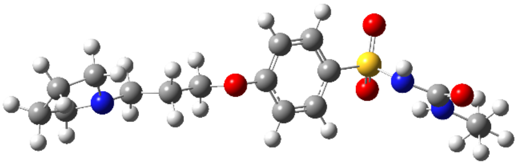
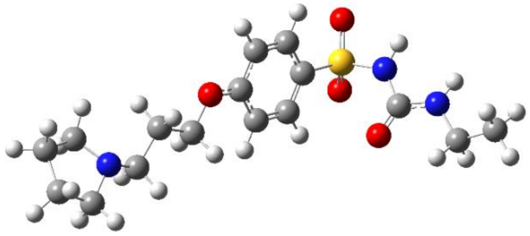
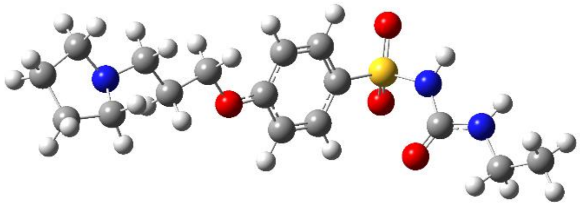
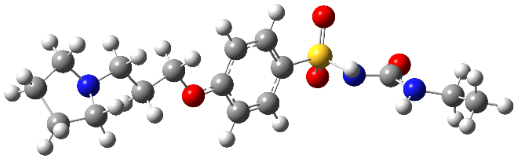
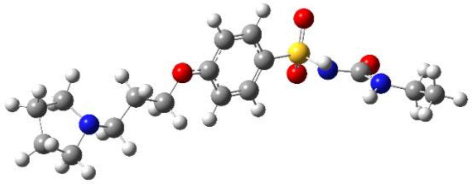
	
DLQ-j-r	DLQ-j-t

Figure 6.25: Optimized geometries of the calculated conformers of compound EGP.

	
EGP-m-r-x4	EGP-m-s-x4
	
EGP-m-q-x4	EGP-m-r-x1
	
EGP-m-s-x1	EGP-p-q-x3

	
EGP-p-s-x3	EGP-m-q-x1
	
EGP-k-q-x1	EGP-k-r-x2
	
EGP-k-q-x1′	EGP-k-s-x1
	
EGP-g-r-x1	EGP-g-q-x1
	
EGP-j-q-x3	EGP-j-r-x3

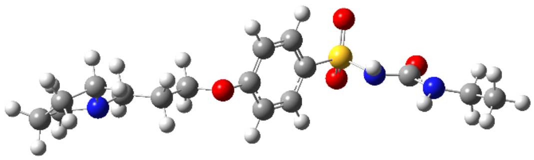
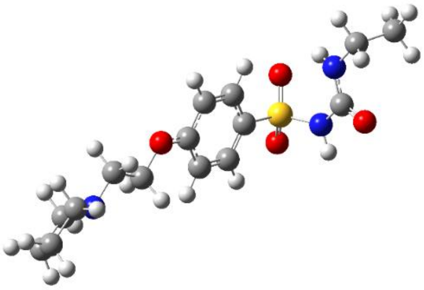
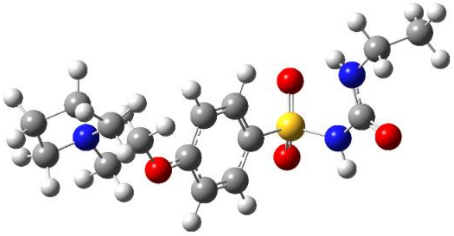
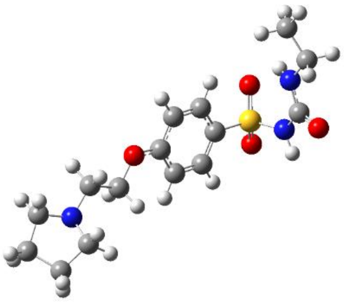
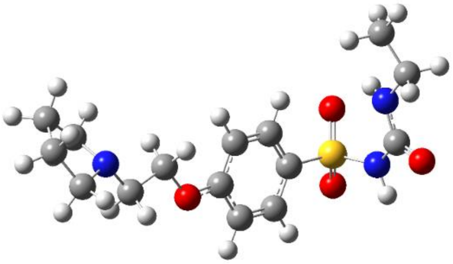
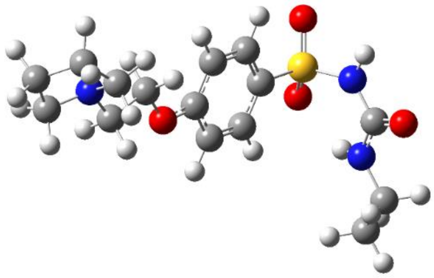
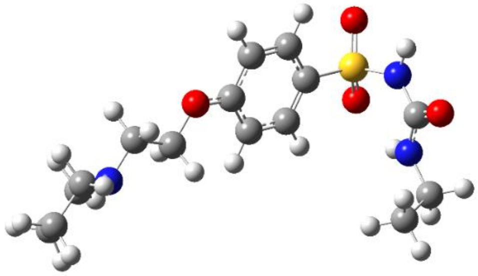
	
EGP-j-s-x3	

Figure 6.26: Optimized geometries of the calculated conformers of compound EGQ.

	
EGQ-m-r-x4	EGQ-m-q-x4
	
EGQ-m-r-x1	EGQ-m-q-x1
	
EGQ-p-q-x3	EGQ-p-r-x3

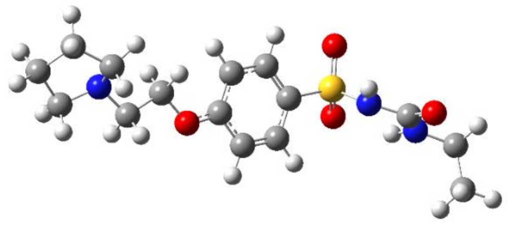
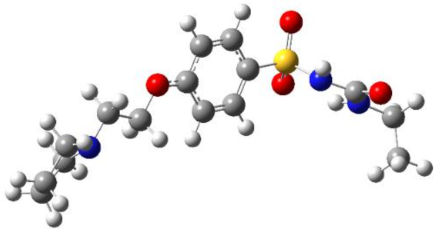
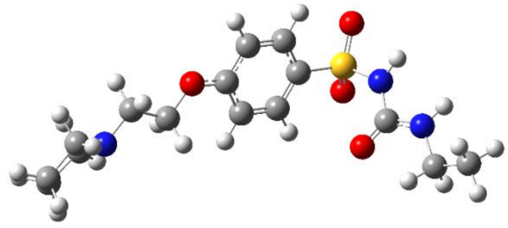
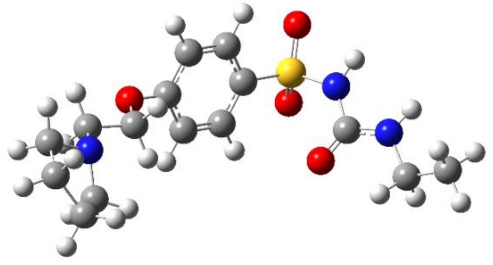
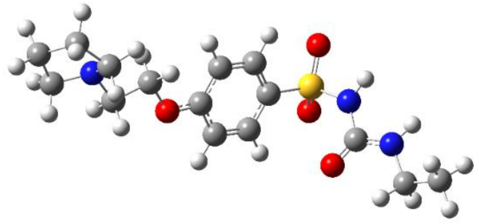
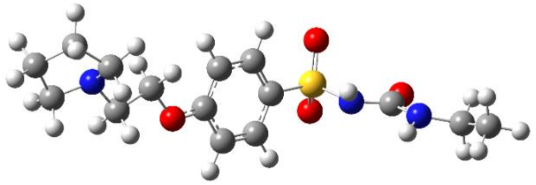
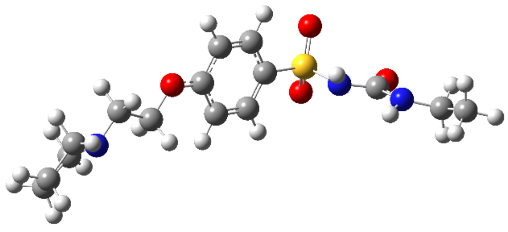
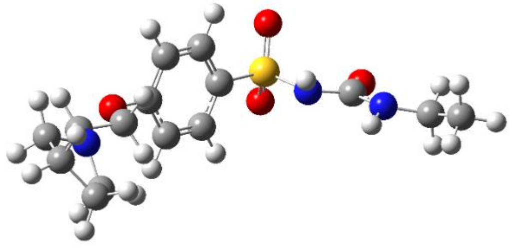
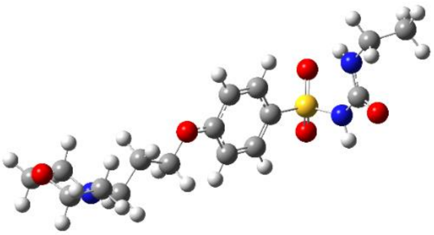
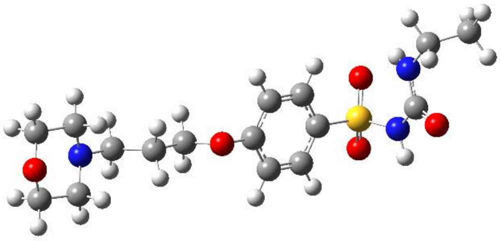
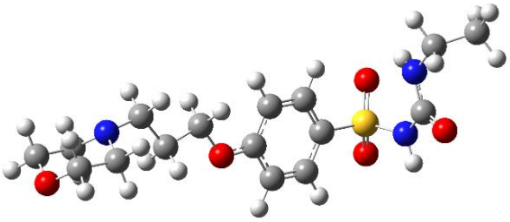
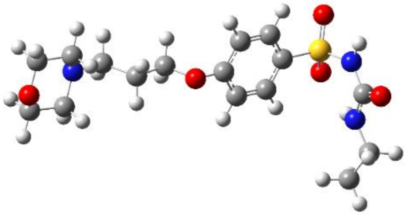
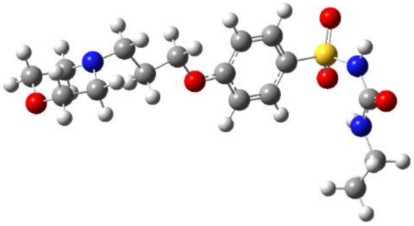
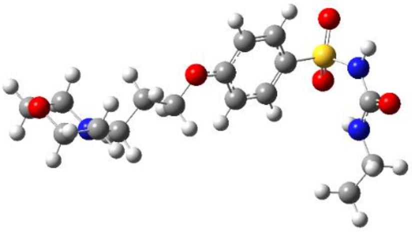
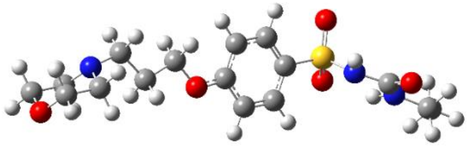
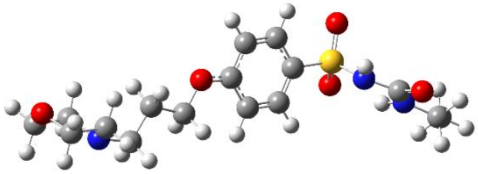
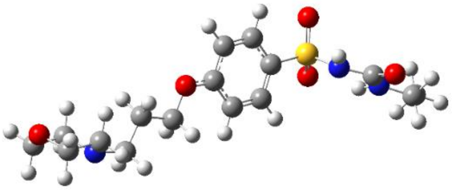
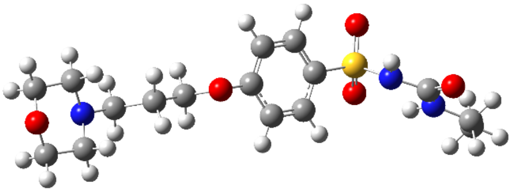
	
EGQ-k-q-x4	EGQ-k-r-x4
	
EGQ-g-r-x1	EGQ-g-t-x1
	
EGQ-g-q-x1	EGQ-j-q-x3
	
EGQ-j-r-x3	EGQ-j-t-x3

Figure 6.27: Optimized geometries of the calculated conformers of compound EJP.

	
EJP-m-r-x4	EJP-m-s-x4
	
EJP-m-q-x4	EJP-p-s-x4
	
EJP-p-q-x4	EJP-p-r-x4
	
EJP-k-q-x1	EJP-k-r-x1
	
EJP-k-r-x1′	EJP-k-s-x1

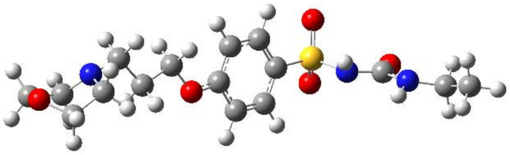
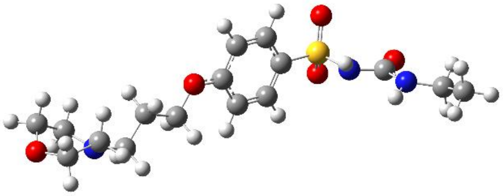
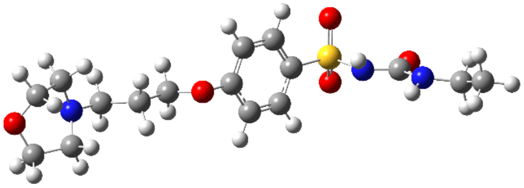
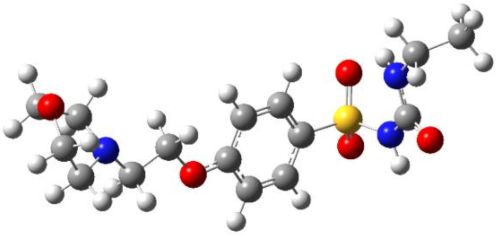
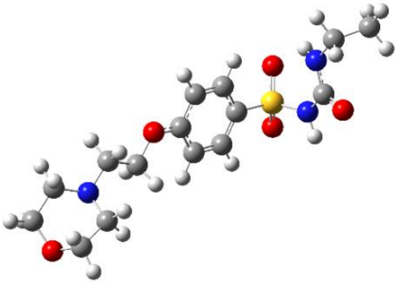
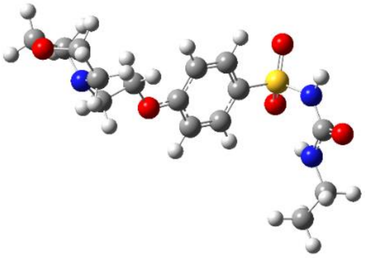
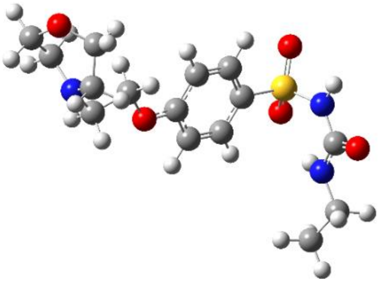
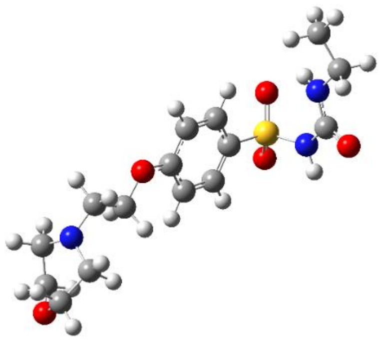
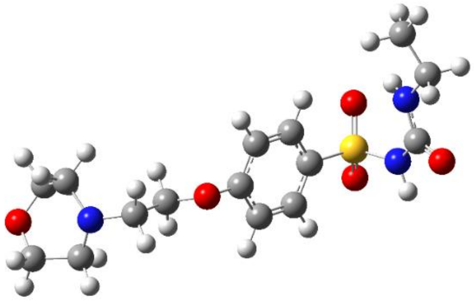
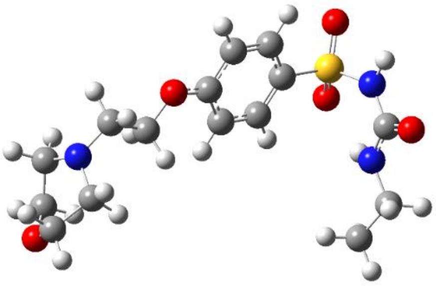
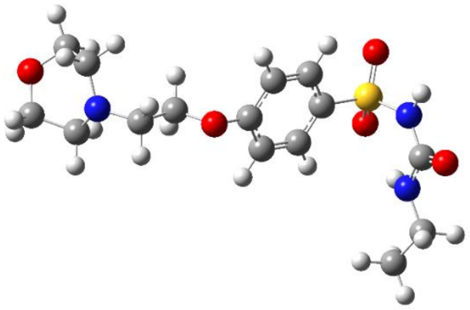
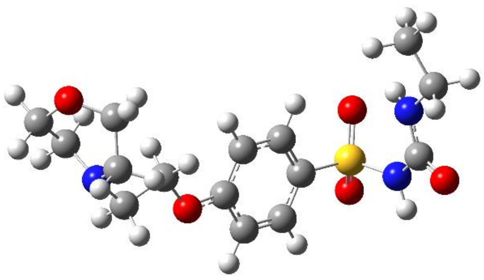
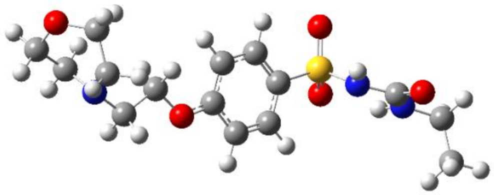
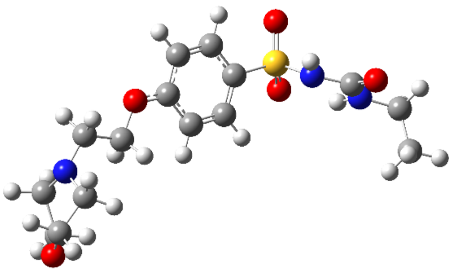
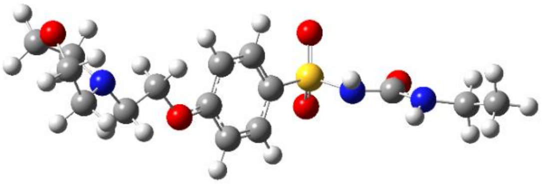
	
EJP-j-q-x3	EJP-j-r-x3
	
EJP-j-s-x3	

Figure 6.28: Optimized geometries of the calculated conformers of compound EJQ.

	
EJQ-m-q-x4	EJQ-m-r-x4
	
EJQ-p-q-x4	EJQ-p-q-x4′

	
EJQ-m-r-x1	EJQ-m-s-x1
	
EJQ-p-r-x4	EJQ-p-s-x4
	
EJQ-m-q-x1	EJQ-k-q-x4
	
EJQ-k-r-x4	EJQ-j-q-x3

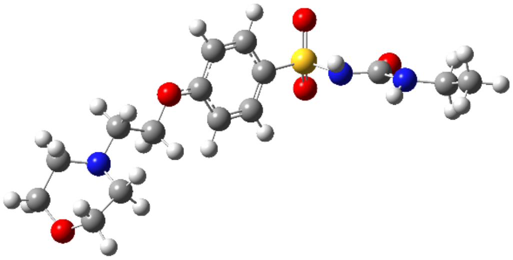
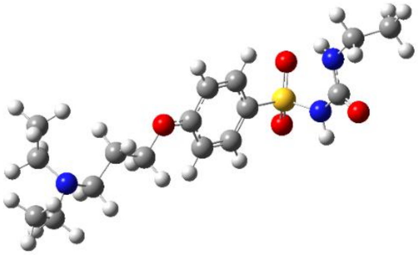
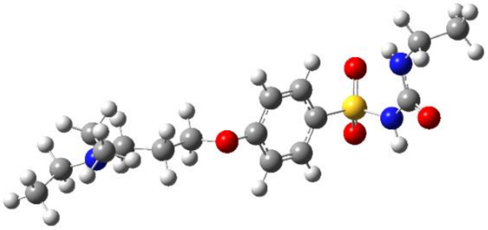
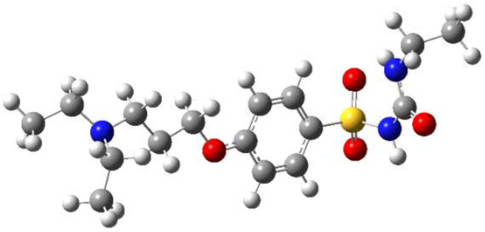
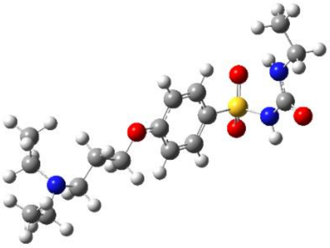
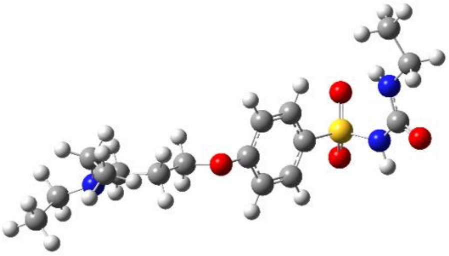
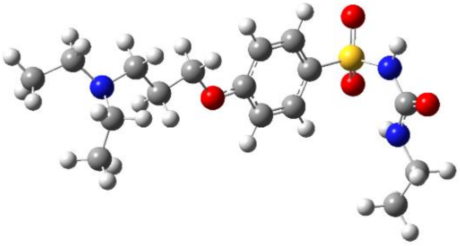
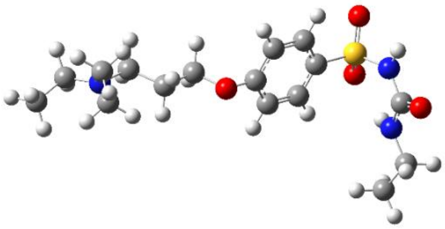
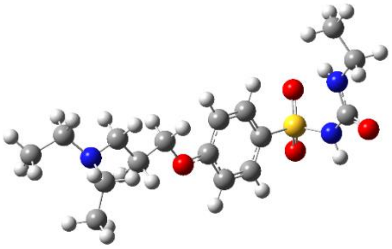
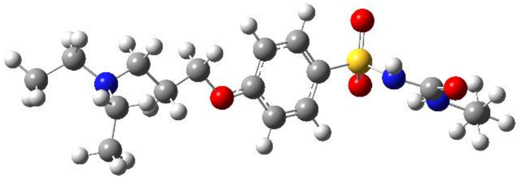
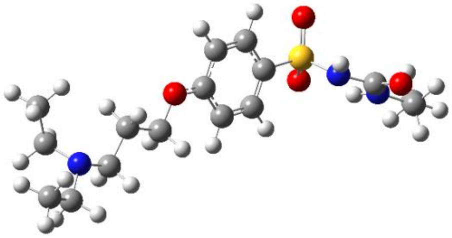
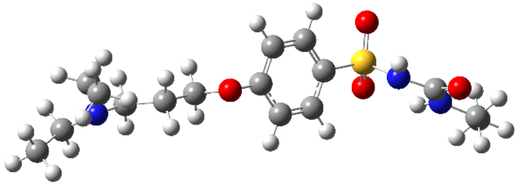
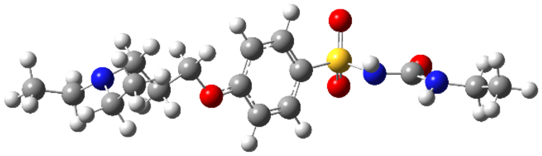
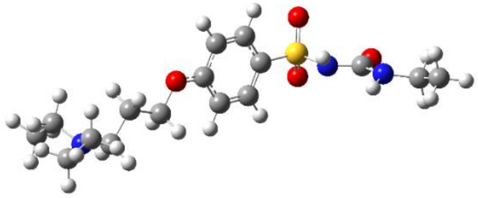
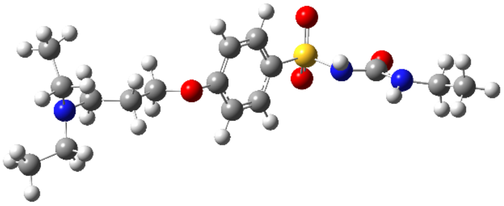
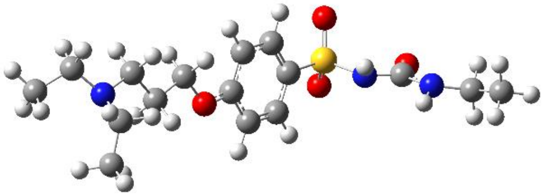
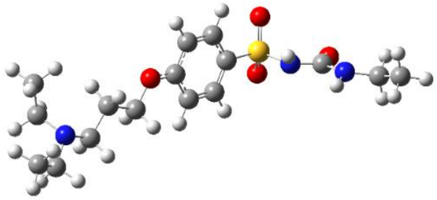
	
EJQ-j-r-x3	

Figure 6.29: Optimized geometries of the calculated conformers of compound ELP.

	
ELP-m-q-x4	ELP-m-s-x4
	
ELP-m-q-x4	ELP-m-r-x1
	
ELP-m-s-x1	ELP-p-s-x4

	
ELP-p-s-x4′	ELP-m-q-x1
	
ELP-k-q-x1	ELP-k-r-x1
	
ELP-k-s-x1	ELP-j-q-x3
	
ELP-j-r-x3	ELP-j-s-x3
	
ELP-j-q-x3′	ELP-j-r-x3′

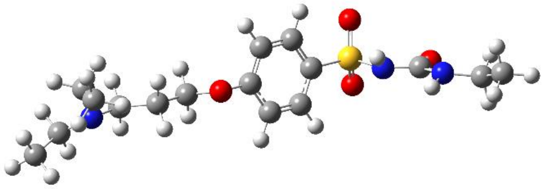
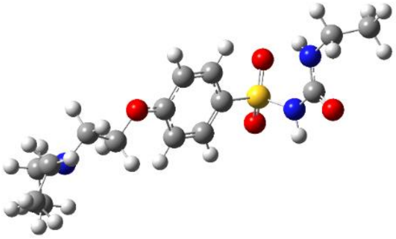
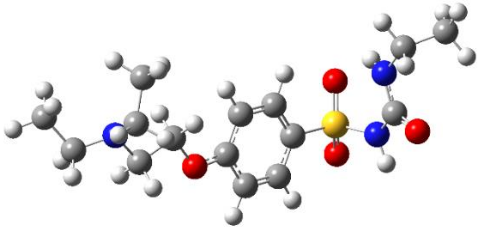
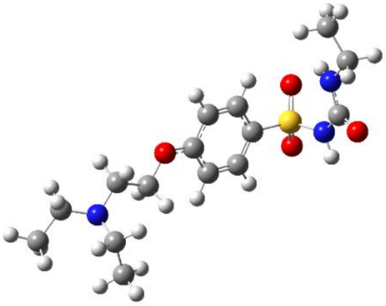
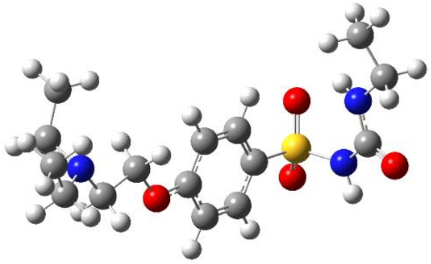
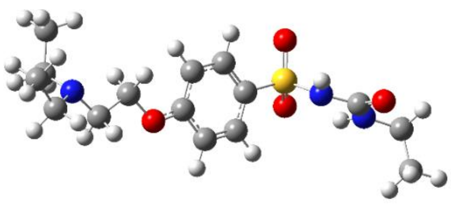
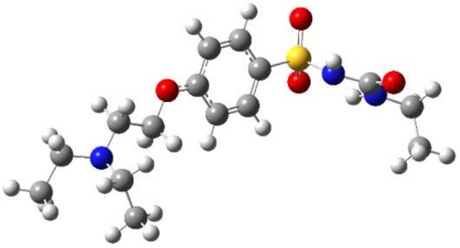
	
ELP-j-s-x3′	

Figure 6.30: Optimized geometries of the calculated conformers of compound ELQ.

	
ELQ-m-r-x4	ELQ-m-q-x4
	
ELQ-m-r-x1	ELQ-m-q-x1
	
ELQ-k-q-x4	ELQ-k-r-x4

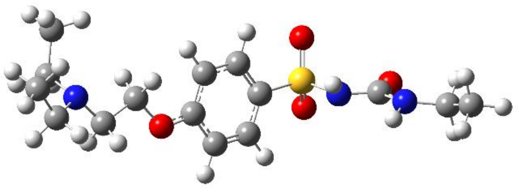
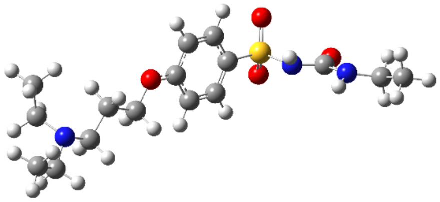
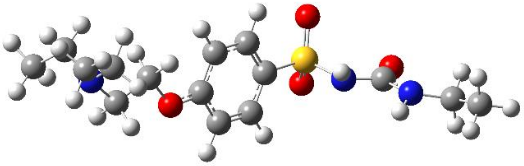
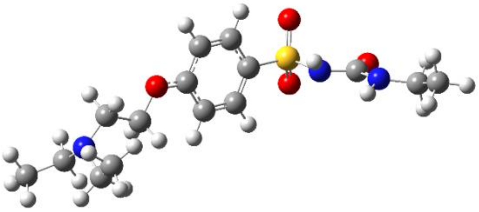
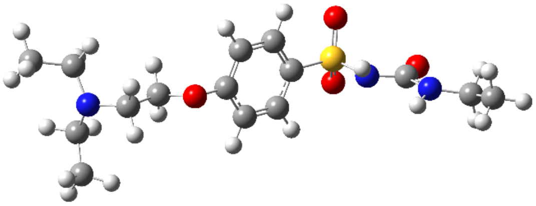
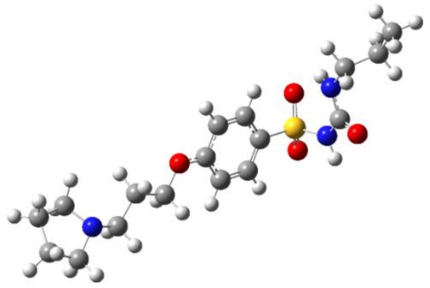
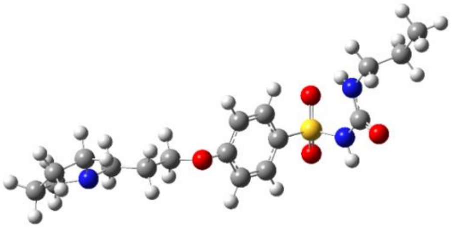
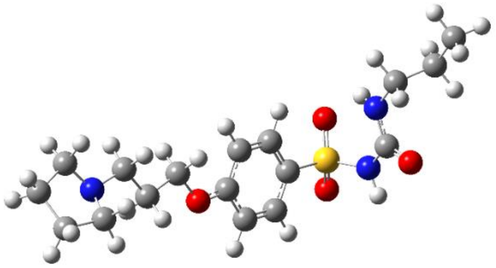
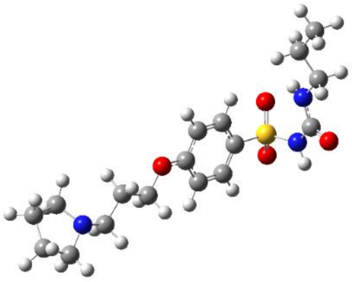
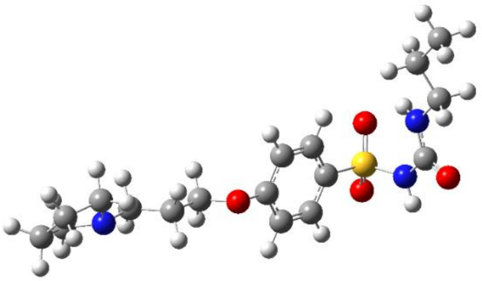
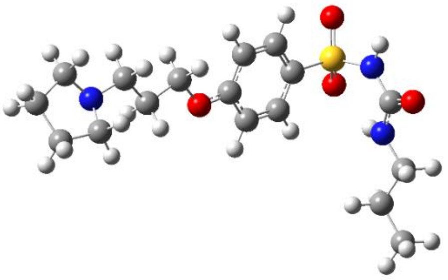
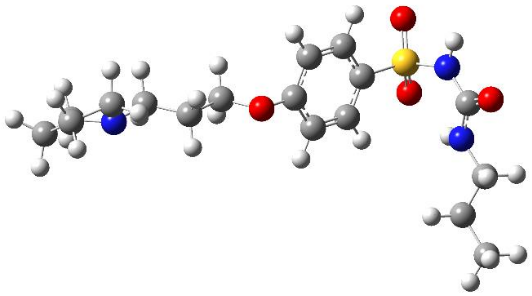
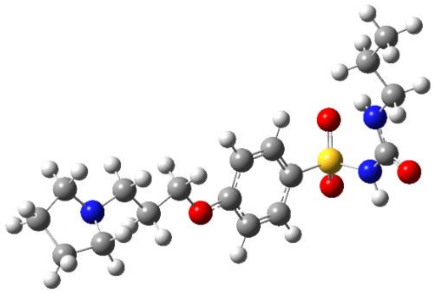
	
ELQ-j-q-x3	ELQ-j-r-x3
	
ELQ-j-q-x3′	ELQ-j-r-x3′
	
ELQ-j-s-x3	

Figure 6.31: Optimized geometries of the calculated conformers of compound FGP.

	
FGP-m-r-x4	FGP-m-s-x4
	
FGP-m-q-x4	FGP-m-r-x1
	
FGP-m-s-x1	FGP-p-q-x4
	
FGP-p-s-x4	FGP-m-q-x1

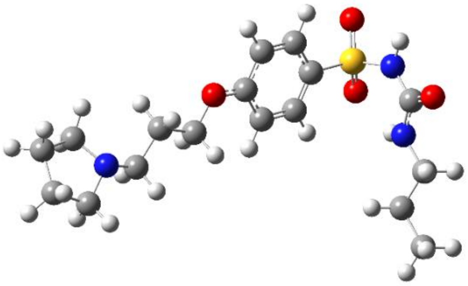
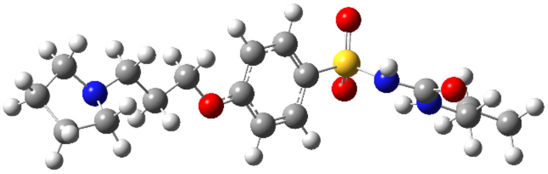
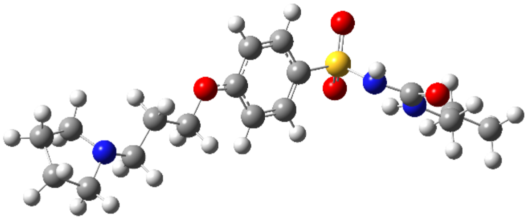
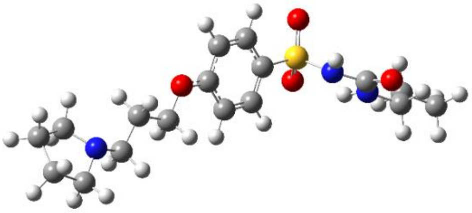
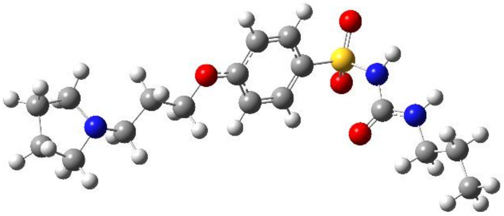
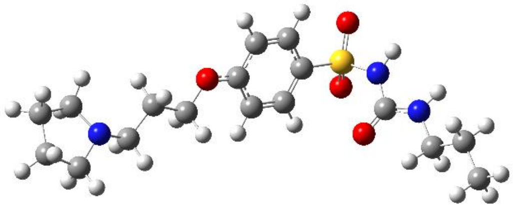
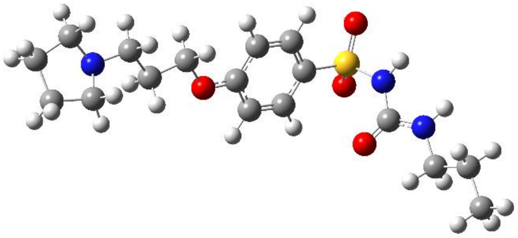
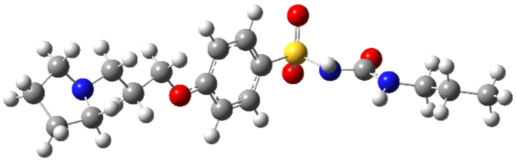
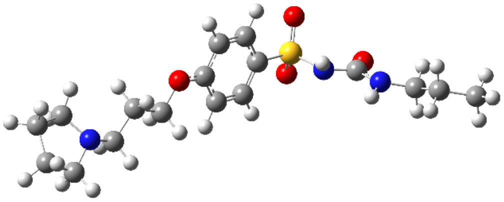
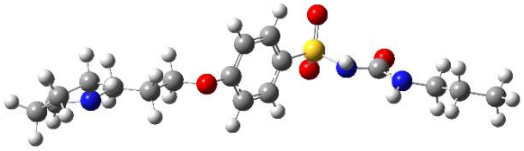
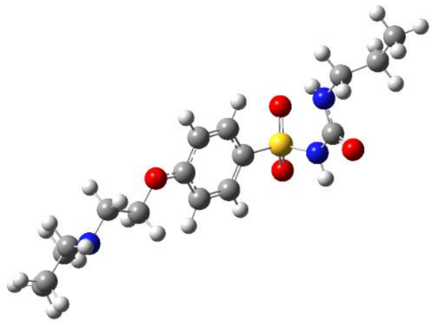
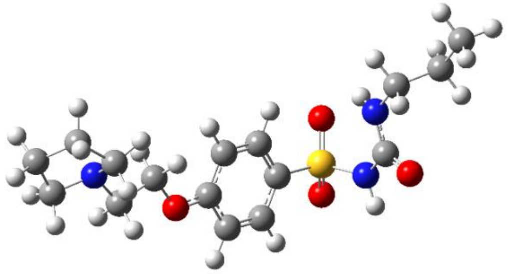
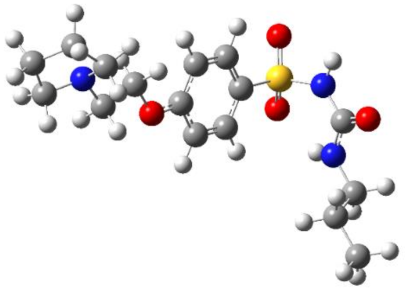
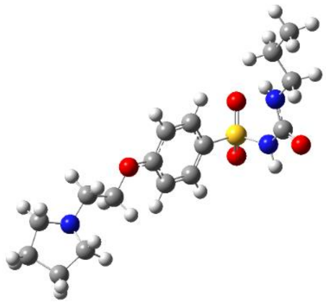
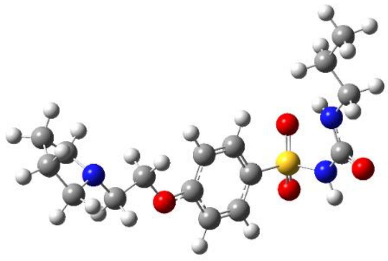
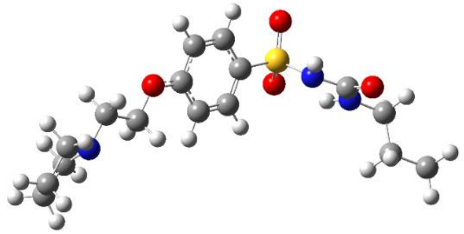
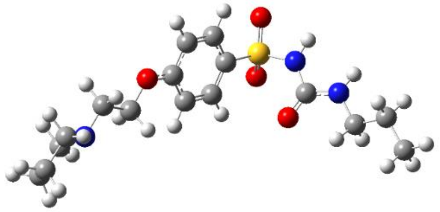
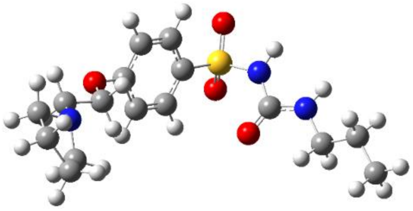
	
FGP-p-r-x4	FGP-k-q-x1
	
FGP-k-r-x1	FGP-k-r-x1
	
FGP-g-r-x1	FGP-g-r-x1
	
FGP-g-q-x1	FGP-j-q-x3
	
FGP-j-r-x3	FGP-j-s-x3

Figure 6.32: Optimized geometries of the calculated conformers of compound FGQ.

	
FGQ-m-r-x4	FGQ-m-q-x4
	
FGQ-p-q-x4	FGQ-m-r-x1
	
FGQ-m-q-x1	FGQ-k-r-x4
	
FGQ-g-r-x1	FGQ-g-t-x1

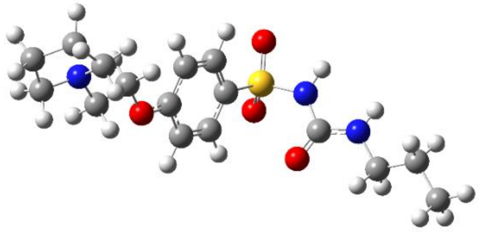
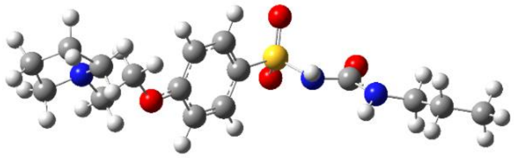
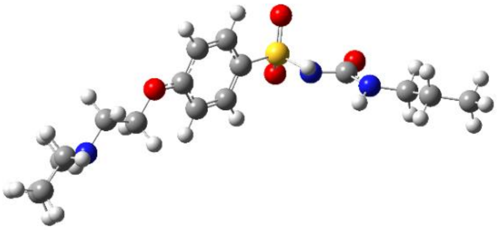
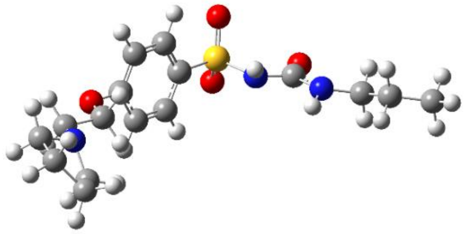
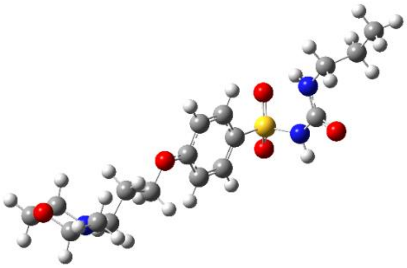
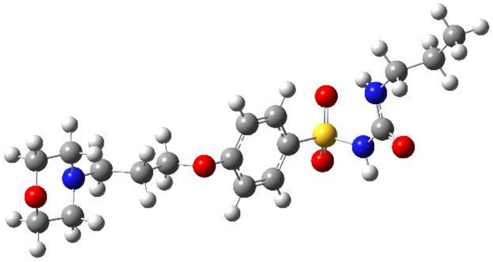
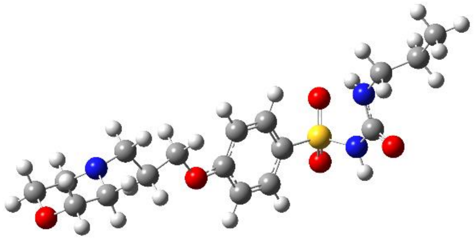
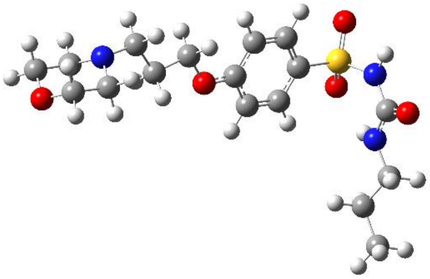
	
FGQ-g-q-x1	FGQ-j-q-x3
	
FGQ-j-r-x3	FGQ-j-t-x3

Figure 6.33: Optimized geometries of the calculated conformers of compound FJP.

	
FJP-m-r-x4	FJP-m-s-x4
	
FJP-m-q-x4	FJP-p-q-x4

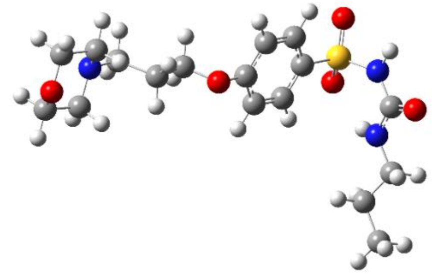
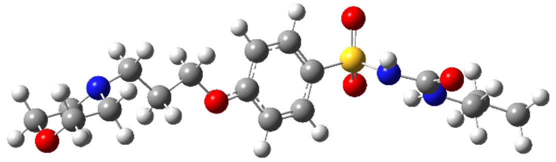
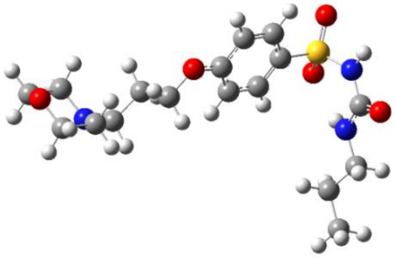
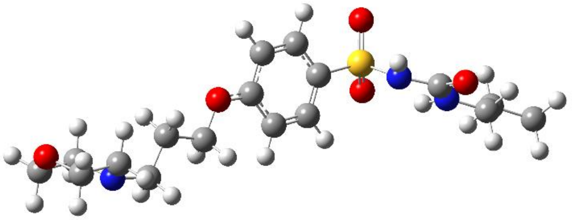
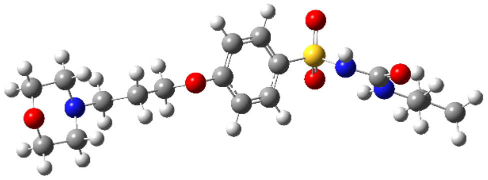
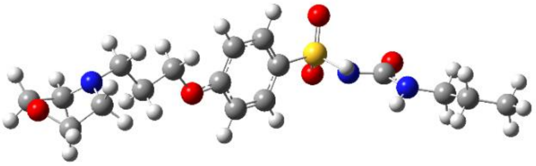
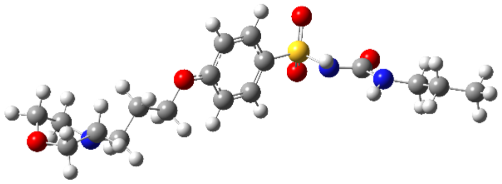
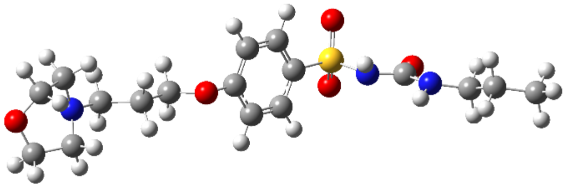
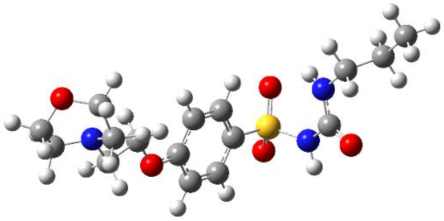
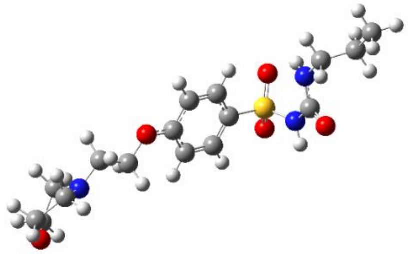
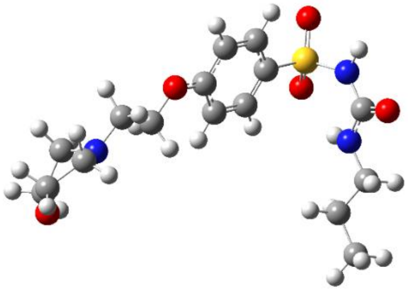
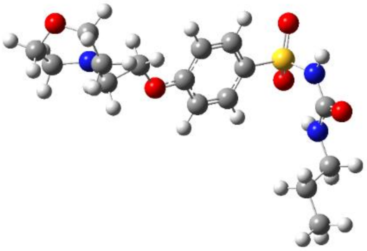
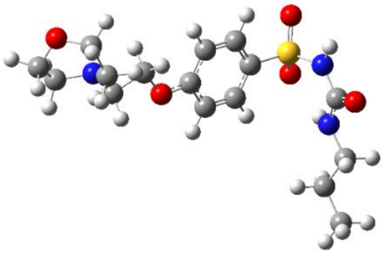
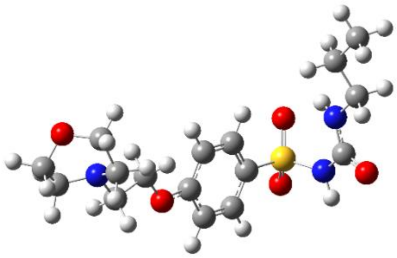
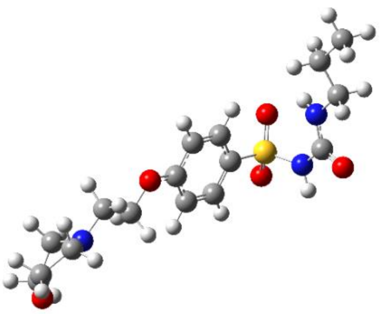
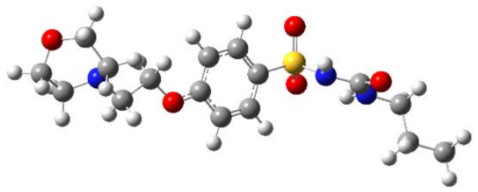
	
FJP-p-s-x4	FJP-k-q-x1
	
FJP-p-r-x1	FJP-k-r-x1
	
FJP-k-s-x1	FJP-j-q-x3
	
FJP-j-r-x3	FJP-j-s-x3

Figure 6.34: Optimized geometries of the calculated conformers of compound FJQ.

	
FJQ-m-q-x4	FJQ-m-r-x4
	
FJQ-p-r-x4	FJQ-p-q-x4
	
FJQ-p-q-x4′	FJQ-m-q-x1
	
FJQ-m-r-x1	FJQ-k-q-x4

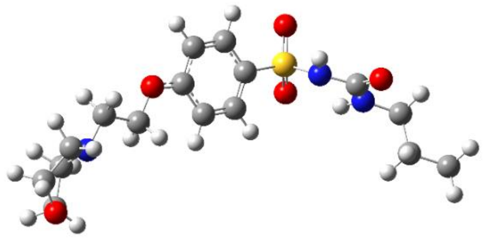
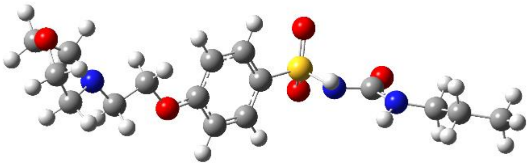
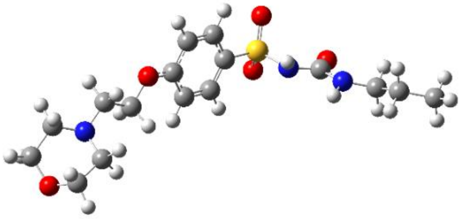
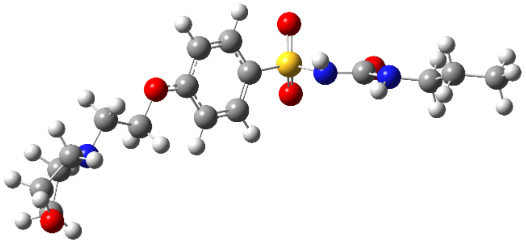
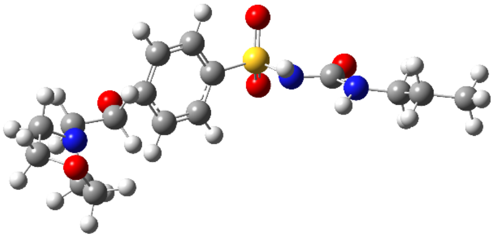
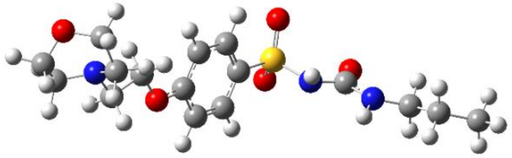
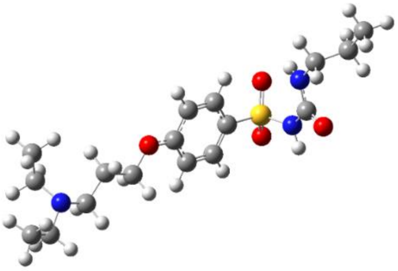
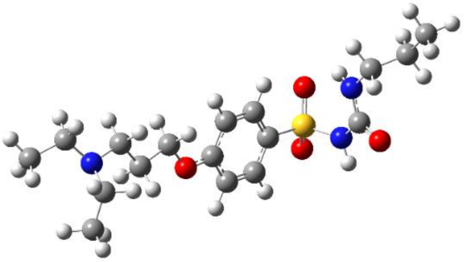
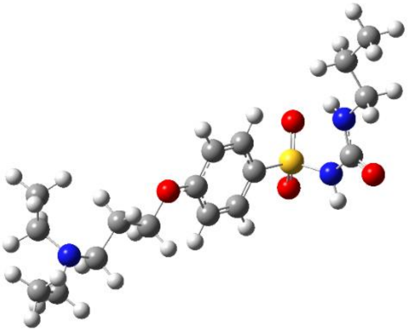
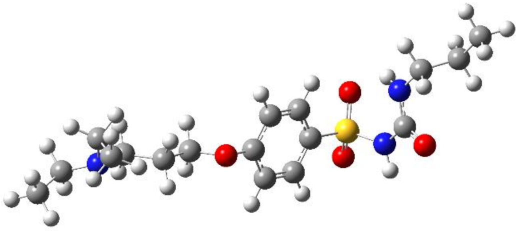
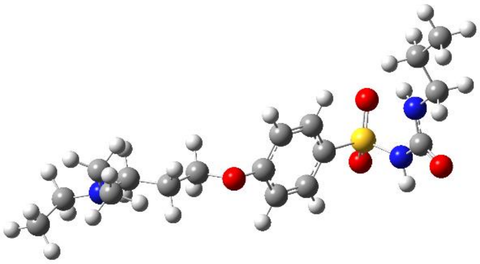
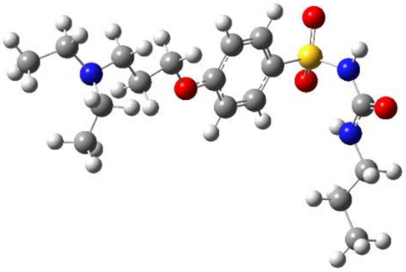
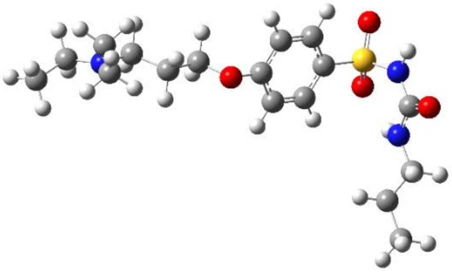
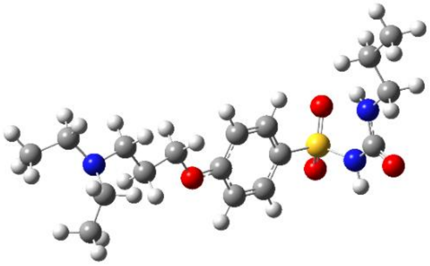
	
FJQ-k-r-x4	FJQ-j-q-x3
	
FJQ-j-r-x3	FJQ-j-r-x3′
	
FJQ-j-t-x3	FJQ-j-q-x3′

Figure 6.35: Optimized geometries of the calculated conformers of compound FLP.

	
FLP-m-r-x4	FLP-m-q-x4
	
FLP-m-r-x1	FLP-m-s-x4
	
FLP-m-s-x1	FLP-p-q-x4
	
FLP-p-s-x4	FLP-m-q-x1

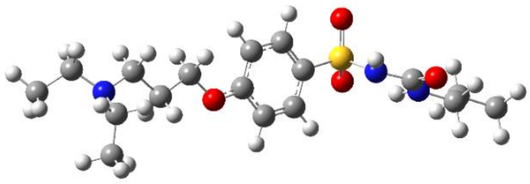
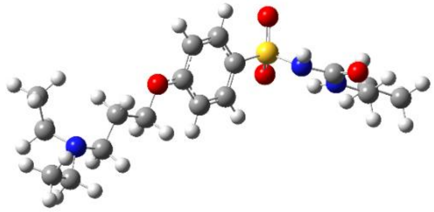
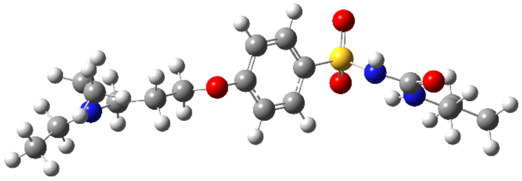
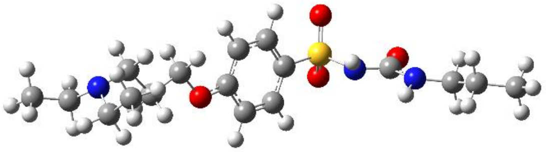
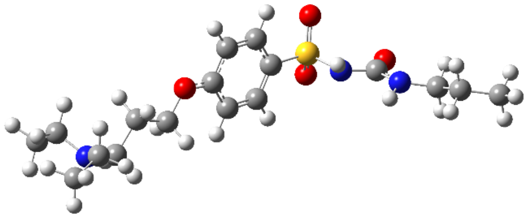
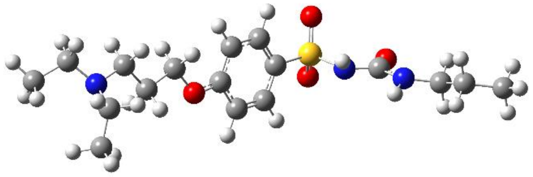
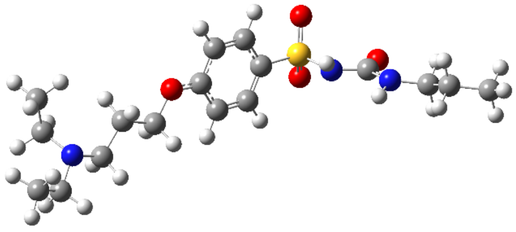
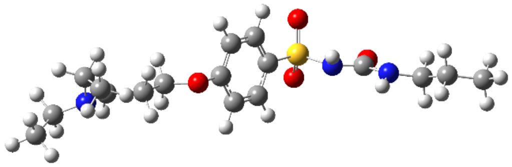
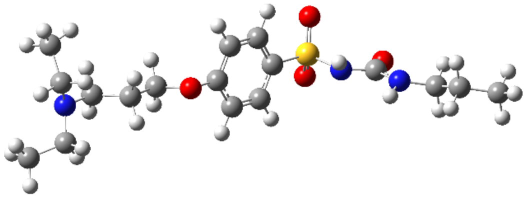
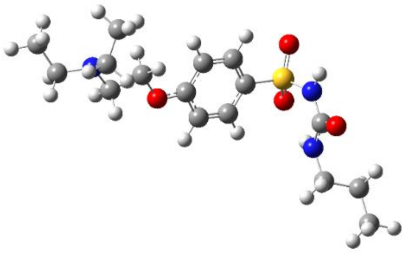
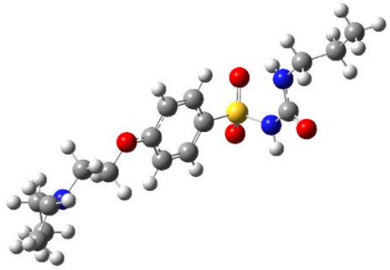
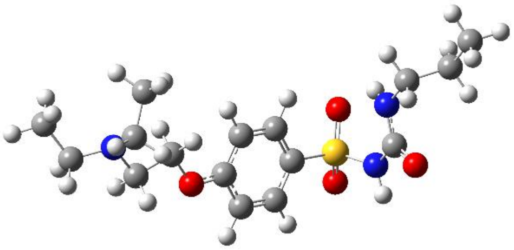
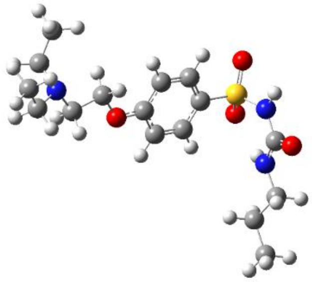
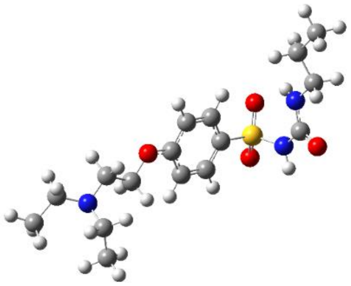
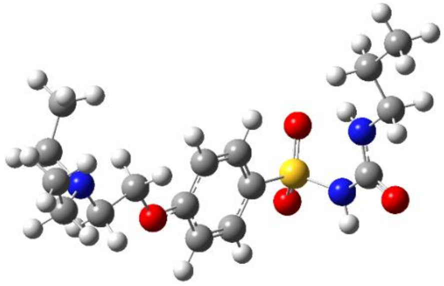
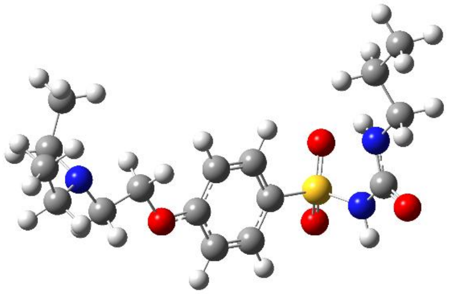
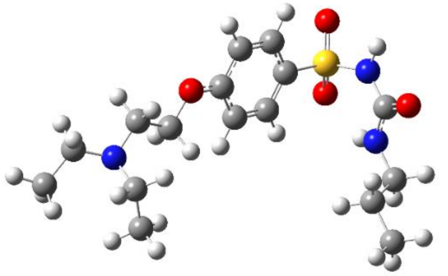
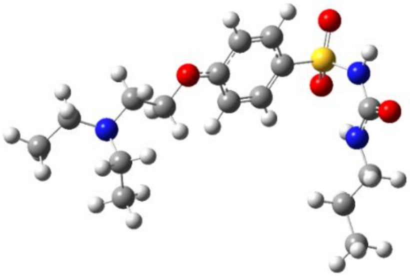
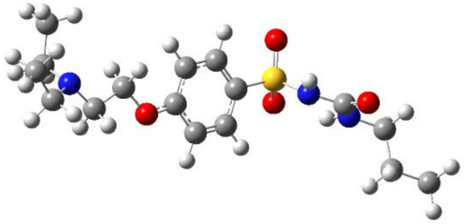
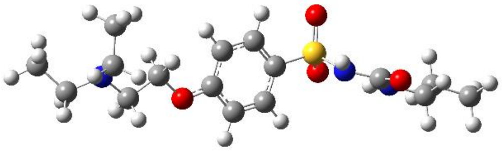
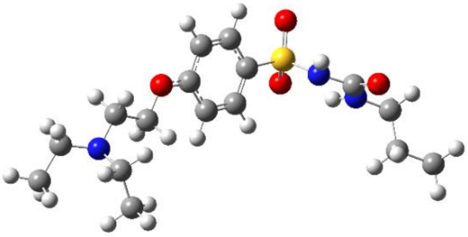
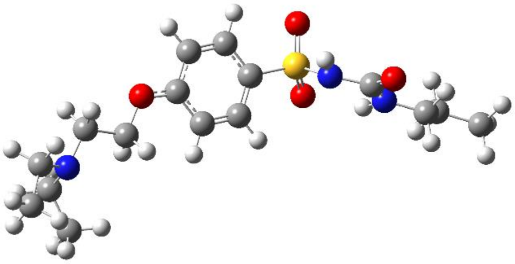
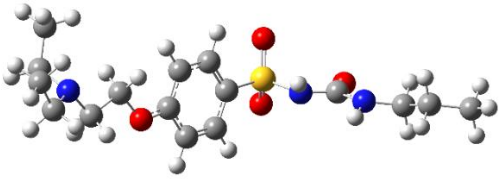
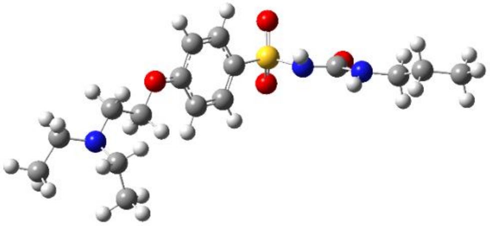
	
FLP-k-q-x1	FLP-k-r-x1
	
FLP-k-s-x1	FLP-j-q-x3
	
FLP-j-r-x3	FLP-j-q-x3′
	
FLP-j-r-x3′	FLP-j-s-x3
	
FLP-j-s-x3′	

Figure 6.36: Optimized geometries of the calculated conformers of compound FLQ.

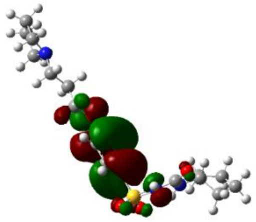
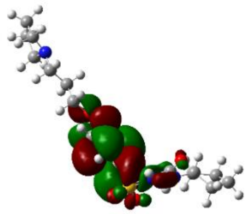
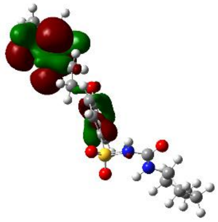
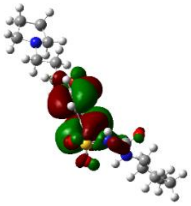
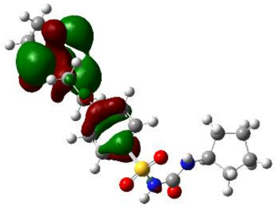
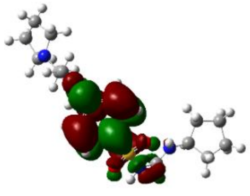
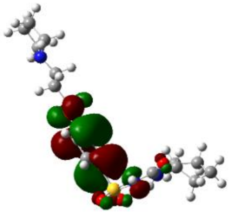
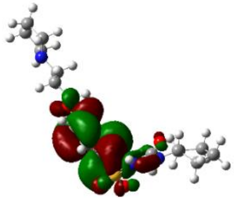
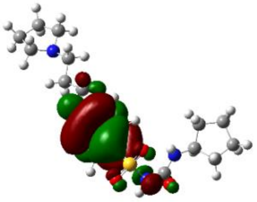
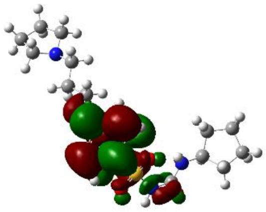
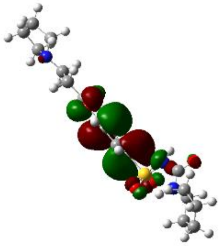
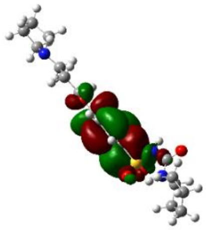
	
FLQ-p-q-x2	FLQ-m-r-x4
	
FLQ-m-q-x4	FLQ-p-q-x4
	
FLQ-m-r-x1	FLQ-m-q-x1
	
FLQ-m-q-x1′	FLQ-p-r-x4

	
FLQ-p-r-x4′	FLQ-k-q-x4
	
FLQ-k-q-x1	FLQ-k-r-x4
	
FLQ-k-r-x1	FLQ-j-q-x3
	
FLQ-j-r-x3	

6.2.2. Shapes of the frontier molecular orbitals (HOMO and LUMO) of the calculated conformers of the compounds considered.

This section presents the shapes of the HOMO and LUMO for the calculated conformers of each of the compounds considered. The shapes are from the HF results (for the same reasons explained in section 6.2.1). HOMO and LUMO is indicated next to the names of each of the conformers in all the tables.

Figure 6.37: Shapes of HOMO and LUMO for the calculated conformers of compound AGP.

			
AGP-m-r-u1 HOMO	AGP-m-r-u1 LUMO	AGP-m-s-u1 HOMO	AGP-m-s-u1 LUMO
			
AGP-p-t-u3 HOMO	AGP-p-t-u3 LUMO	AGP-m-q-u1 HOMO	AGP-m-q-u1 LUMO
			
AGP-p-r-u3 HOMO	AGP-p-r-u3 LUMO	AGP-k-q-u1 HOMO	AGP-k-q-u1 LUMO

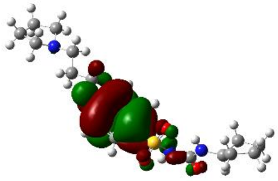
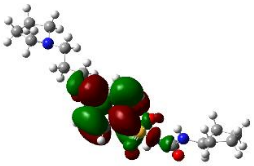
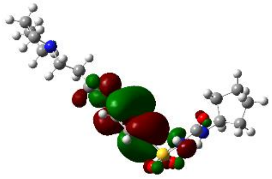
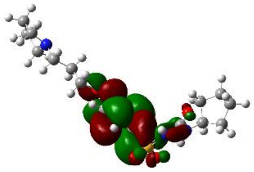
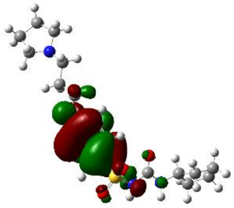
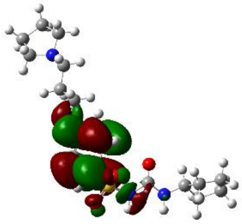
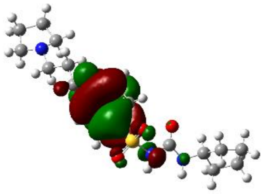
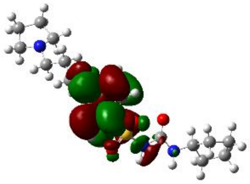
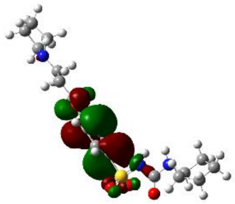
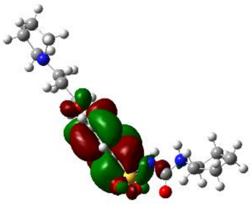
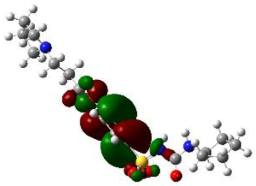
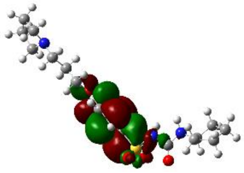
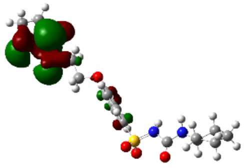
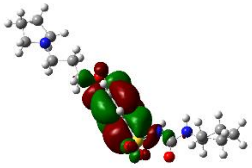
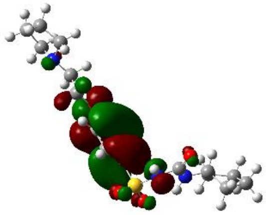
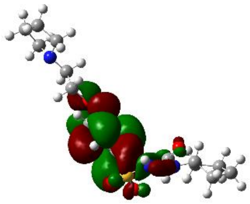
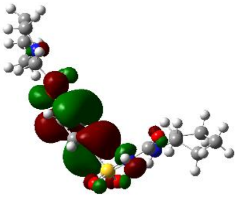
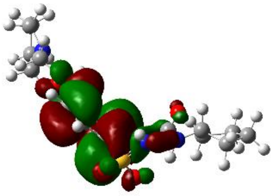
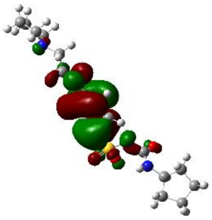
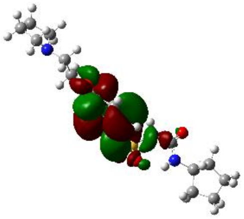
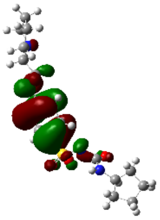
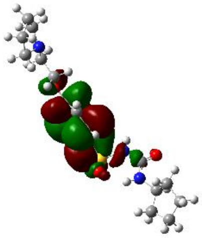
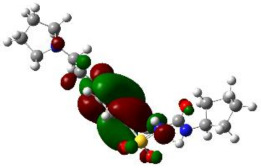
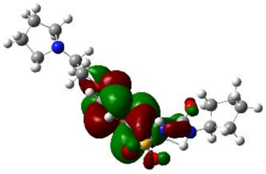
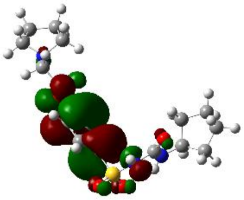
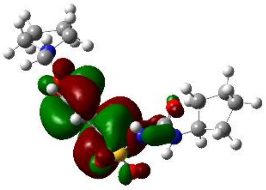
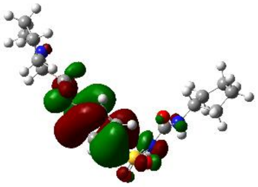
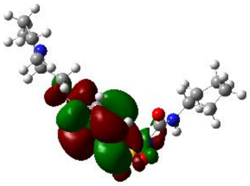
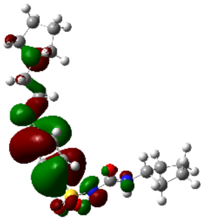
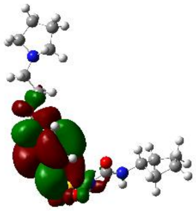
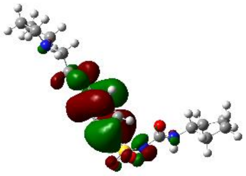
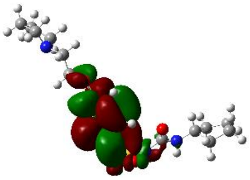
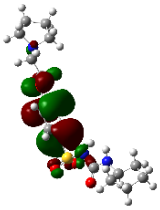
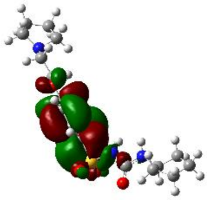
			
AGP-k-r-u1 HOMO	AGP-k-r-u1 LUMO	AGP.m-r-u2 HOMO	AGP.m-r-u2 LUMO
			
AGP-g-r-u3 HOMO	AGP-g-r-u3 LUMO	AGP-g-q-u3 HOMO	AGP-g-q-u3 LUMO
			
AGP-j-q-u3 HOMO	AGP-j-q-u3 LUMO	AGP-j-r-u3 HOMO	AGP-j-r-u3 LUMO
			
AGP-j-s-u3 HOMO	AGP-j-s-u3 LUMO		

Figure 6.38: Shapes of HOMO and LUMO for the calculated conformers of compound AGQ.

			
AGQ-m-r-u1 HOMO	AGQ-m-r-u1 LUMO	AGQ-m-q-u1 HOMO	AGQ-m-q-u1 LUMO
			
AGQ-k-q-u1 HOMO	AGQ-k-q-u1 LUMO	AGQ-k-r-u1 HOMO	AGQ-k-r-u1 LUMO
			
AGQ-m-r-u2 HOMO	AGQ-m-r-u2 LUMO	AGQ-m-q-u2 HOMO	AGQ-m-q-u2 LUMO
			
AGQ-g-r-u3 HOMO	AGQ-g-r-u3 LUMO	AGQ-g-t-u3 HOMO	AGQ-g-t-u3 LUMO
			
AGQ-g-q-u3 HOMO	AGQ-g-q-u3 LUMO	AGQ-j-q-u3 HOMO	AGQ-j-q-u3 LUMO

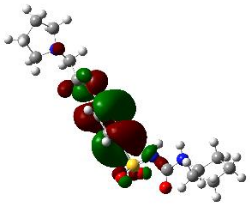
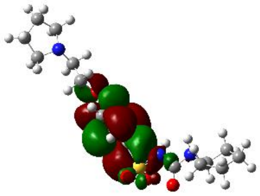
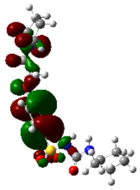
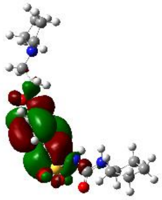
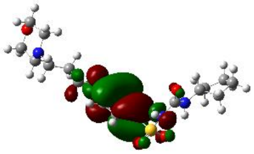
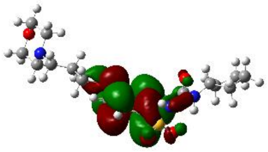
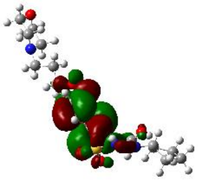
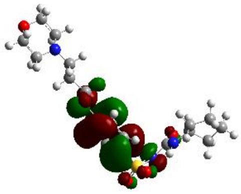
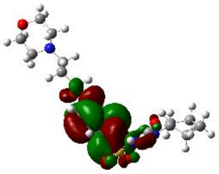
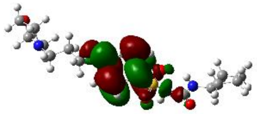
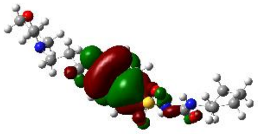
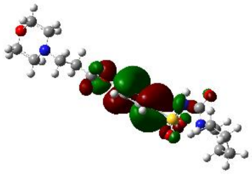
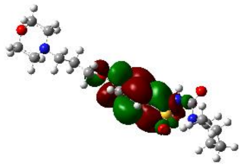
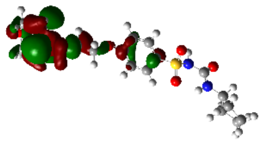
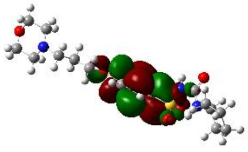
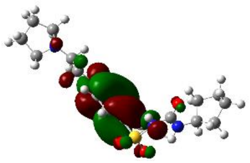
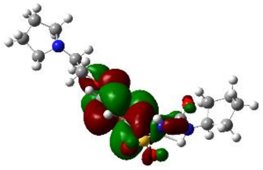
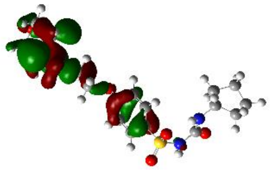
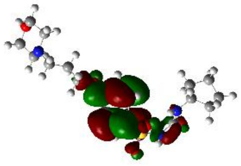
			
AGQ-j-r-u3 HOMO	AGQ-j-r-u3 LUMO	AGQ-j-t-u3 HOMO	AGQ-j-t-u3 LUMO

Figure 6.39: Shapes of HOMO and LUMO for the calculated conformers of compound AJP.

			
AJP-m-r-u1 HOMO	AJP-m-r-u1 LUMO	AJP-m-s-u1 HOMO	AJP-m-s-u1 LUMO
			
AJP-m-q-u1 HOMO	AJP-m-q-u1 LUMO	AJP-k-q-u1 HOMO	AJP-k-q-u1 LUMO
			
AJP-k-r-u1 HOMO	AJP-k-r-u1 LUMO	AJP-k-s-u1 HOMO	AJP-k-s-u1 LUMO
			
AJP-m-r-u2 HOMO	AJP-m-r-u2 LUMO	AJP-m-s-u2 HOMO	AJP-m-s-u2 LUMO

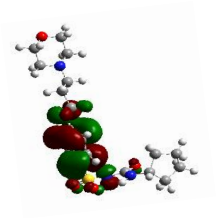
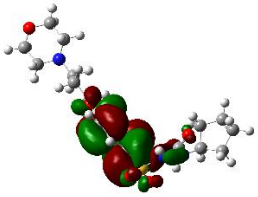
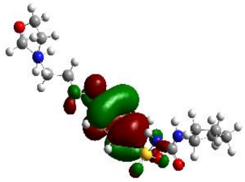
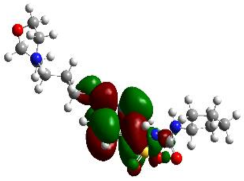
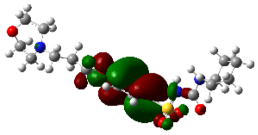
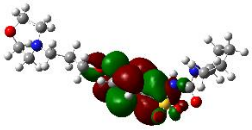
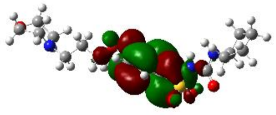
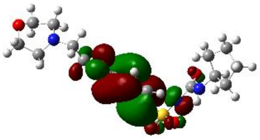
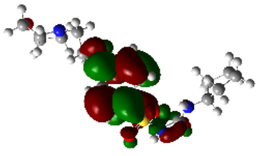
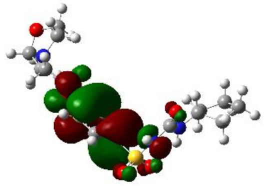
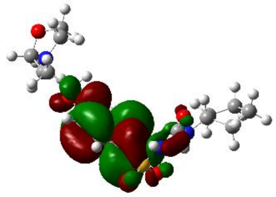
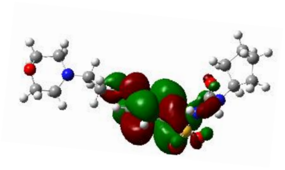
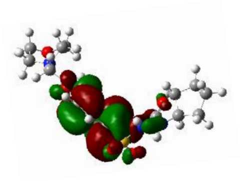
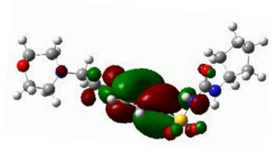
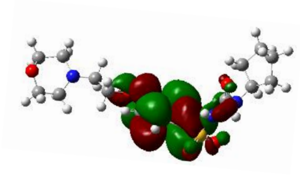
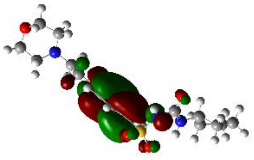
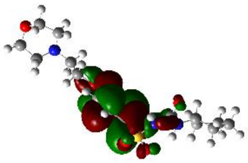
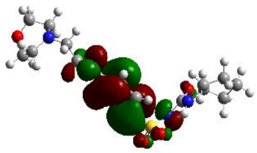
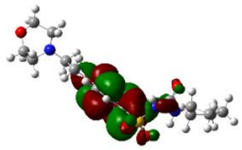
			
AJP-m-q-u2 HOMO	AJP-m-q-u2 LUMO	AJP-j-q-u3 HOMO	AJP-j-q-u3 LUMO
			
AJP-j-r-u3 HOMO	AJP-j-r-u3 LUMO	AJP-j-s-u3 HOMO	AJP-j-s-u3 LUMO

Figure 6.40: Shapes of HOMO and LUMO for the calculated conformers of compound AJQ.

			
AJQ-p-q-u5 HOMO	AJQ-p-q-u5 LUMO	AJQ-m-q-u1 HOMO	AJQ-m-q-u1 LUMO
			
AJQ-m-q-u2 HOMO	AJQ-m-q-u2 LUMO	AJQ-m-r-u2 HOMO	AJQ-m-r-u2 LUMO
			
AJQ-p-q-u3 HOMO	AJQ-p-q-u3 LUMO	AJQ-m-r-u1 HOMO	AJQ-m-r-u1 LUMO

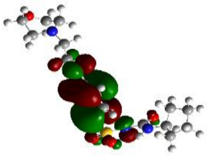
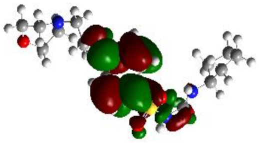
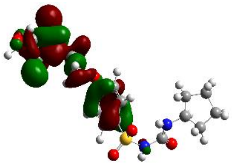
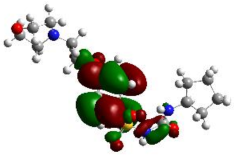
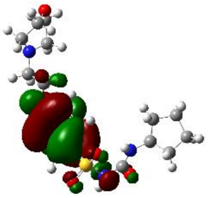
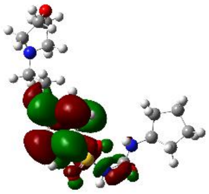
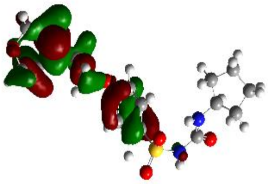
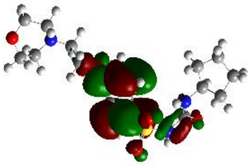
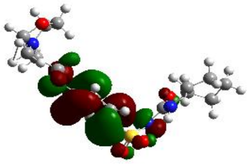
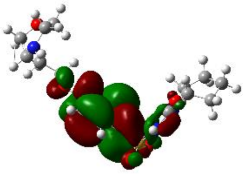
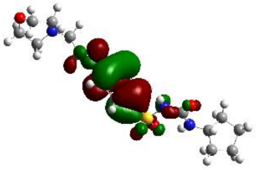
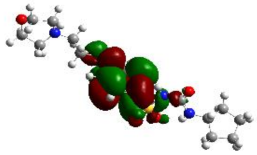
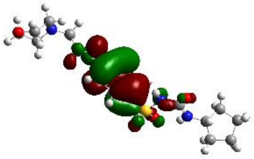
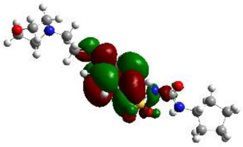
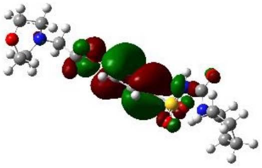
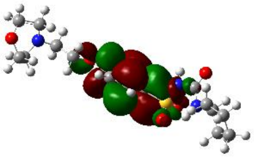
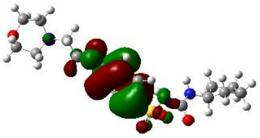
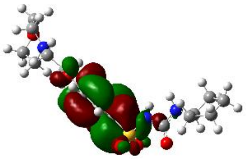
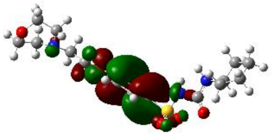
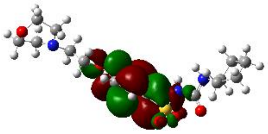
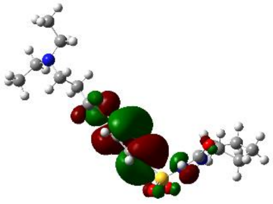
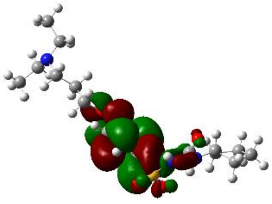
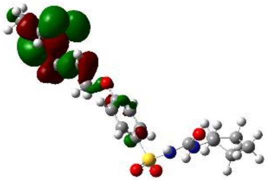
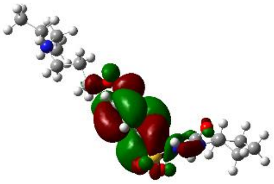
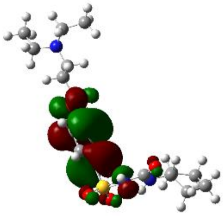
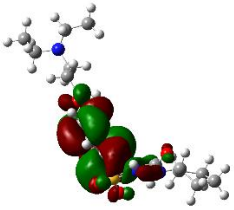
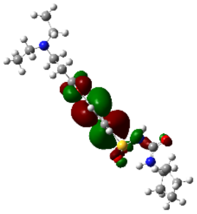
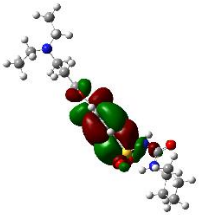
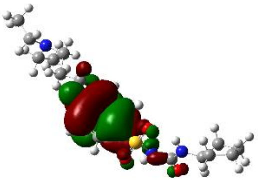
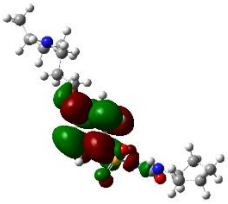
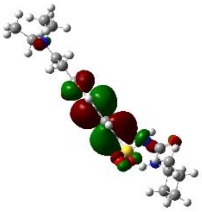
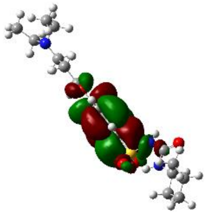
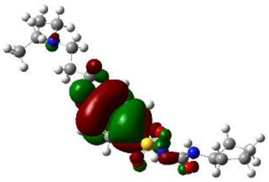
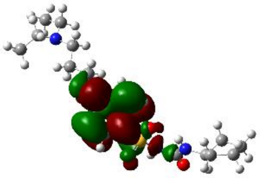
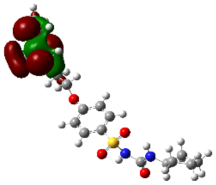
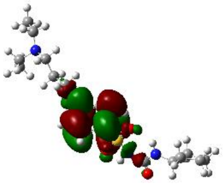
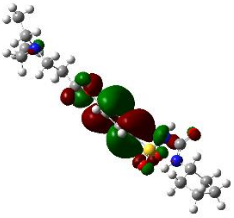
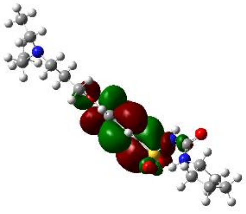
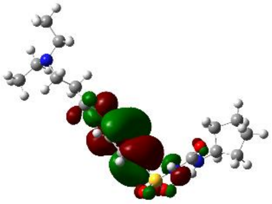
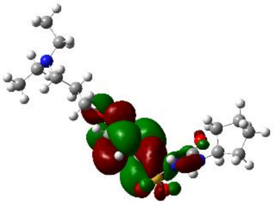
			
AJQ-p-q-u5 HOMO	AJQ-p-q-u5 LUMO	AJQ-m-s-u1 HOMO	AJQ-m-s-u1 LUMO
			
AJQ-p-r-u3 HOMO	AJQ-p-r-u3 LUMO	AJQ-p-s-u3 HOMO	AJQ-p-s-u3 LUMO
			
AJQ-m-q-u1 HOMO	AJQ-m-q-u1 LUMO	AJQ-k-q-u1 HOMO	AJQ-k-q-u1 LUMO
			
AJQ-k-q-u1 HOMO	AJQ-k-q-u1 LUMO	AJQ-k-r-u1 HOMO	AJQ-k-r-u1 LUMO
			
AJQ-j-q-u1 HOMO	AJQ-j-q-u1 LUMO	AJQ-j-r-u1 HOMO	AJQ-j-r-u1 LUMO

Figure 6.41: Shapes of HOMO and LUMO for the calculated conformers of compound ALP.

			
ALP-m-r-u1 HOMO	ALP-m-r-u1 LUMO	ALP-m-s-u1 HOMO	ALP-m-s-u1 LUMO
			
ALP-m-q-u1 HOMO	ALP-m-q-u1 LUMO	ALP-k-q-u1 HOMO	ALP-k-q-u1 LUMO
			
ALP-k-r-u1 HOMO	ALP-k-r-u1 LUMO	ALP-k-q-u1′ HOMO	ALP-k-q-u1′ LUMO
			
ALP-k-r-u1′ HOMO	ALP-k-r-u1′ LUMO	ALP-k-s-u1 HOMO	ALP-k-s-u1 LUMO
			

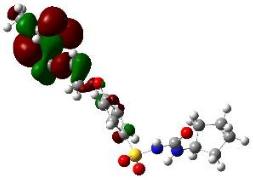
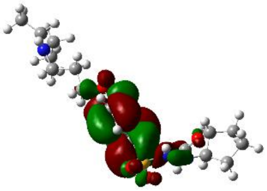
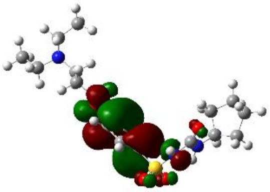
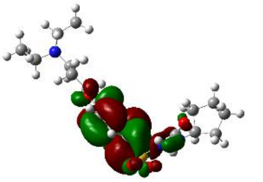
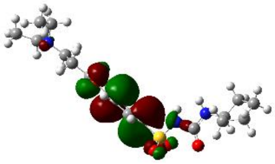
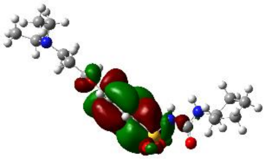
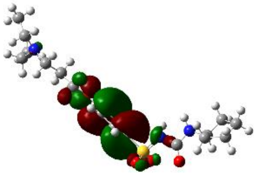
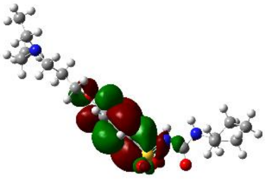
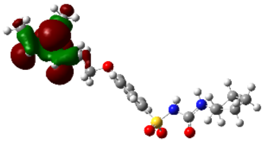
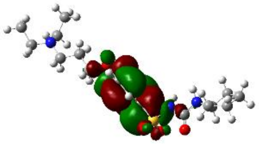
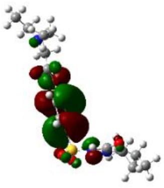
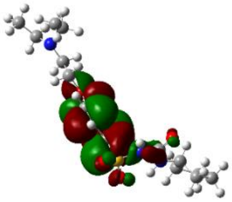
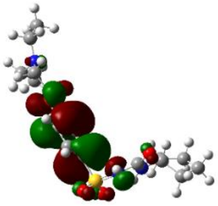
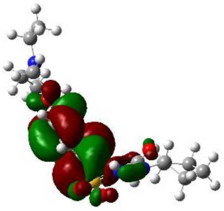
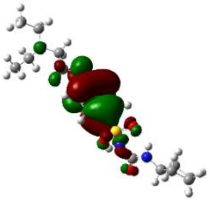
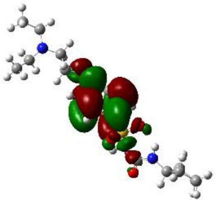
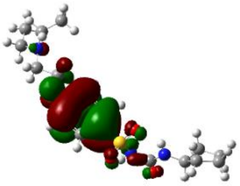
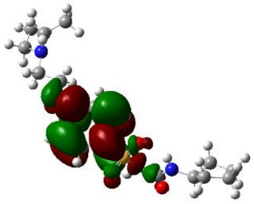
ALP-k-r-u3 HOMO	ALP-k-r-u3 LUMO	ALP-m-r-u2 HOMO	ALP-m-r-u2 LUMO
			
ALP-m-s-u2 HOMO	ALP-m-s-u2 LUMO	ALP-m-q-u2 HOMO	ALP-m-q-u2 LUMO
			
ALP-j-q-u3 HOMO	ALP-j-q-u3 LUMO	ALP-j-r-u3 HOMO	ALP-j-r-u3 LUMO
			
ALP-j-s-u3 HOMO	ALP-j-s-u3 LUMO		

Figure 6.42: Shapes of HOMO and LUMO for the calculated conformers of compound ALQ.

			
ALQ-m-r-u1 HOMO	ALQ-m-r-u1 LUMO	ALQ-m-q-u1 HOMO	ALQ-m-q-u1 LUMO
			

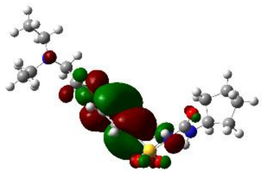
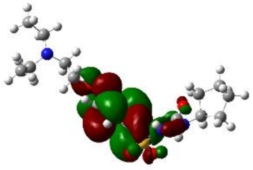
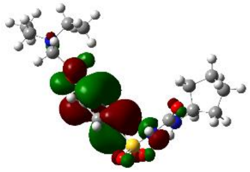
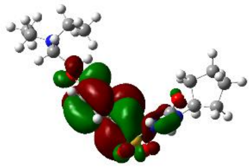
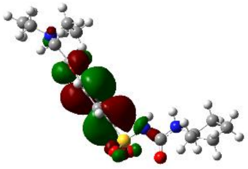
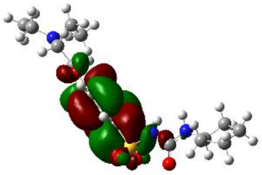
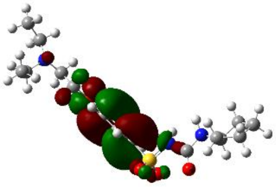
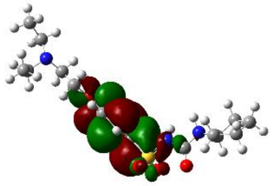
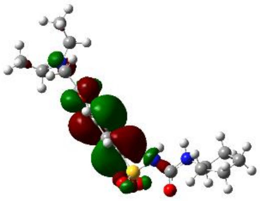
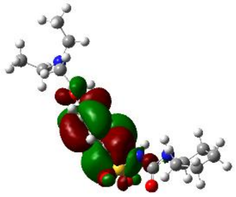
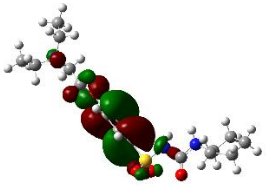
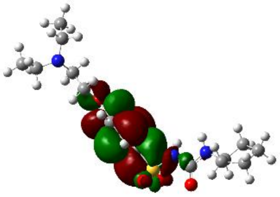
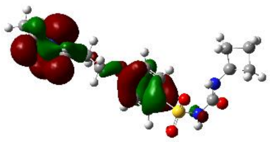
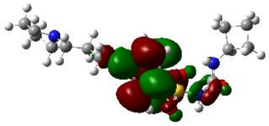
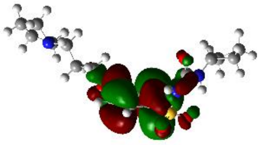
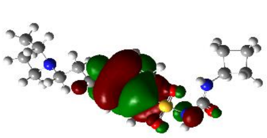
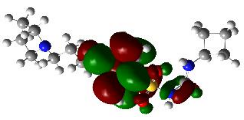
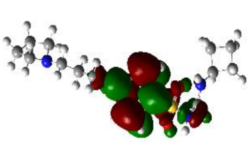
ALQ-k-q-u1 HOMO	ALQ-k-q-u1 LUMO	ALQ-k-r-u1 HOMO	ALQ-k-r-u1 LUMO
			
ALQ-m-r-u2 HOMO	ALQ-m-r-u2 LUMO	ALQ-m-q-u2 HOMO	ALQ-m-q-u2 LUMO
			
ALQ-j-q-u3 HOMO	ALQ-j-q-u3 LUMO	ALQ-j-r-u3 HOMO	ALQ-j-r-u3 LUMO
			
ALQ-j-q-u3 HOMO	ALQ-j-q-u3 LUMO	ALQ-j-r-u3 HOMO	ALQ-j-r-u3 LUMO

Figure 6.43: Shapes of HOMO and LUMO for the calculated conformers of compound BGP.

			
BGP-p-s-v3 HOMO	BGP-p-s-v3 LUMO	BGP-p-t-v3 HOMO	BGP-p-t-v3 LUMO
			
BGP-m-r-v1 HOMO	BGP-m-r-v1 LUMO	BGP-m-s-v1 HOMO	BGP-m-s-v1 LUMO

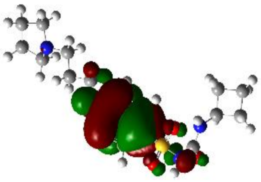
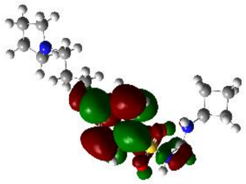
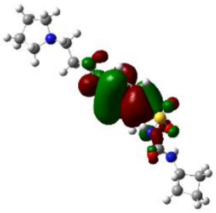
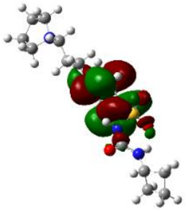
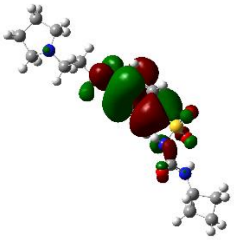
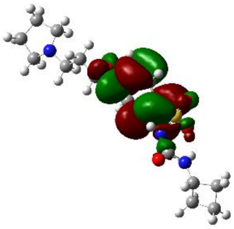
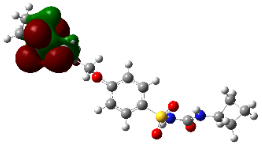
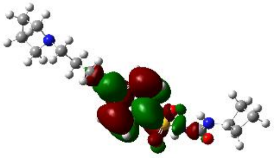
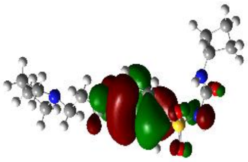
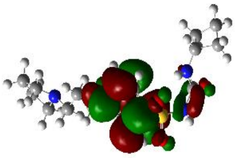
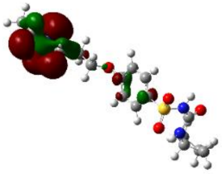
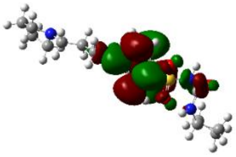
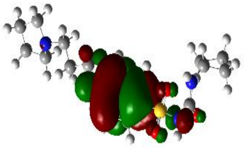
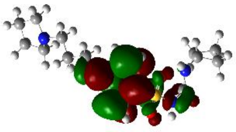
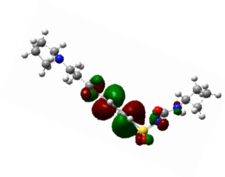
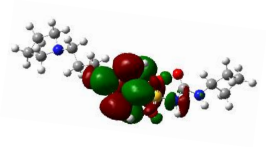
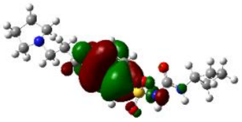
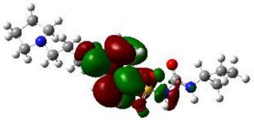
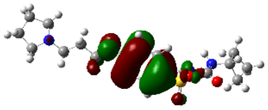
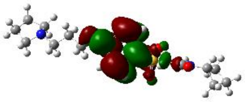
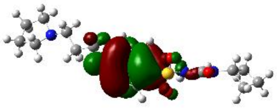
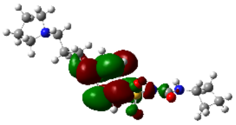
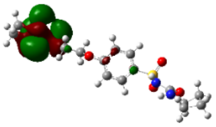
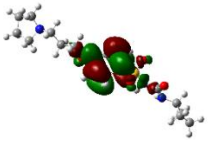
			
BGP-m-q-v1 HOMO	BGP-m-q-v1 LUMO	BGP-k-q-v3 LUMO	BGP-k-q-v3 HOMO
			
BGP-k-r-v3 HOMO	BGP-k-r-v3 LUMO	BGP-k-s-v3 HOMO	BGP-k-s-v3 LUMO
			
BGP-m-r-v2 HOMO	BGP-m-r-v2 LUMO	BGP-m-s-v2 HOMO	BGP-m-s-v2 LUMO
			
BGP-m-q-v2 HOMO	BGP-m-q-v2 LUMO	BGP-g-r-v1 HOMO	BGP-g-r-v1 LUMO
			
BGP-g-q-v1 HOMO	BGP-g-q-v1 LUMO	BGP-j-q-v5 HOMO	BGP-j-q-v5 LUMO
			
BGP-j-r-v5 HOMO	BGP-j-r-v5 LUMO	BGP-j-s-v5 HOMO	BGP-j-s-v5 LUMO

Figure 6.44: Shapes of HOMO and LUMO for the calculated conformers of compound BGQ.

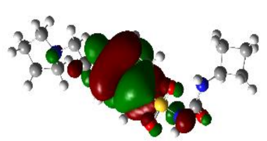
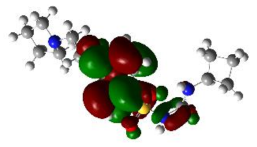
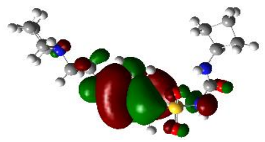
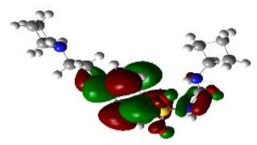
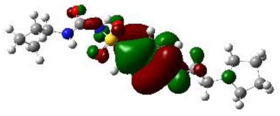
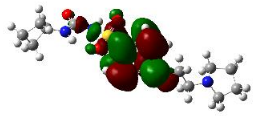
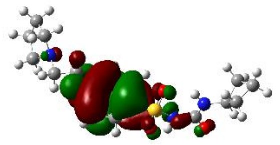
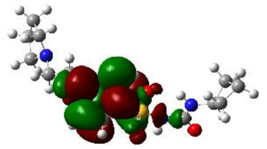
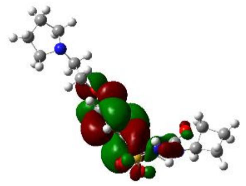
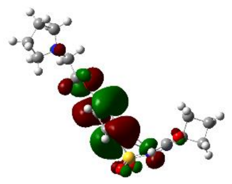
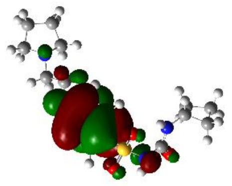
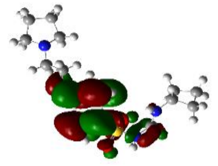
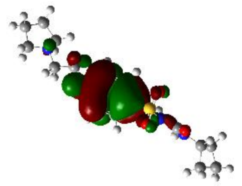
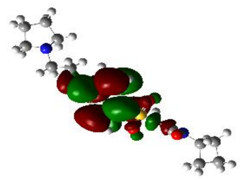
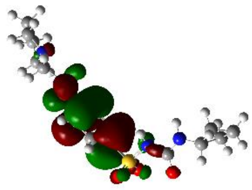
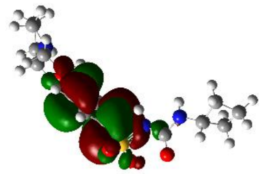
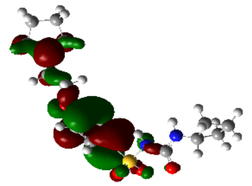
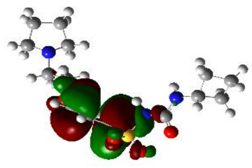
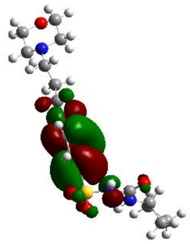
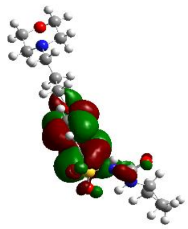
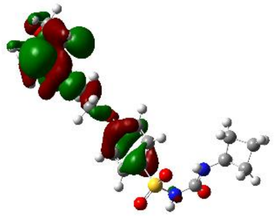
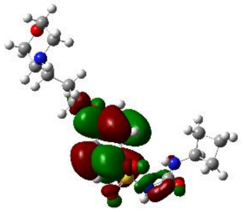
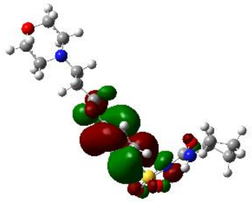
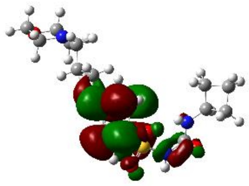
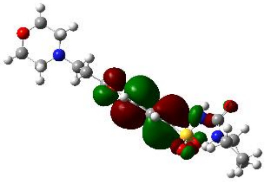
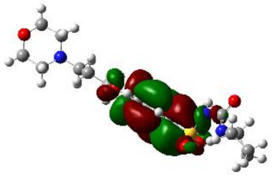
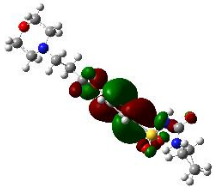
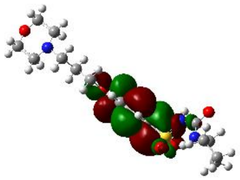
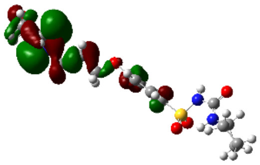
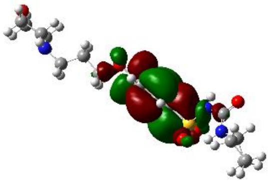
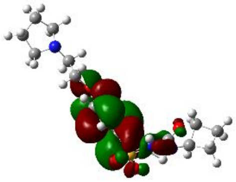
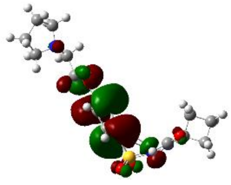
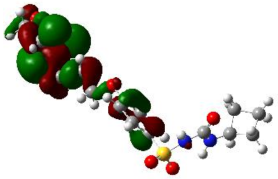
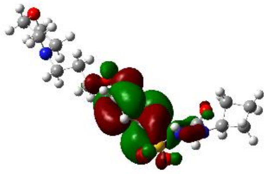
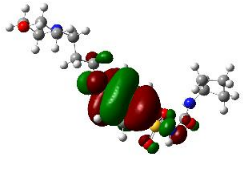
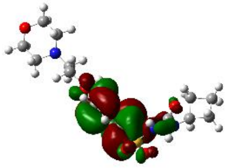
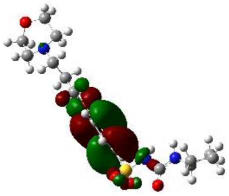
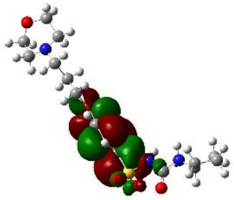
			
BGQ-m-r-v1 HOMO	BGQ-m-r-v1 LUMO	BGQ-m-q-v1 HOMO	BGQ-m-q-v1 LUMO
			
BGQ-k-q-v1 HOMO	BGQ-k-q-v1 LUMO	BGQ-k-r-v1 HOMO	BGQ-k-r-v1 LUMO
			
BGQ-m-r-v2 HOMO	BGQ-m-r-v2 LUMO	BGQ-m-q-v2 HOMO	BGQ-m-q-v2 LUMO
			
BGQ-j-q-v3 HOMO	BGQ-j-q-v3 LUMO	BGQ-j-r-v3 HOMO	BGQ-j-r-v3 LUMO
			
BGQ-j-t-v3 HOMO	BGQ-j-t-v3 LUMO		

Figure 6.45: Shapes of HOMO and LUMO for the calculated conformers of compound BJP.

			
BJP-p-q-v3 HOMO	BJP-p-q-v3 LUMO	BJP-p-s-v3 HOMO	BJP-p-s-v3 LUMO
			
BJP-p-r-v3 HOMO	BJP-p-r-v3 LUMO	BJP-k-q-v1 HOMO	BJP-k-q-v1 LUMO
			
BJP-k-r-v1 HOMO	BJP-k-r-v1 LUMO	BJP-k-s-v1 HOMO	BJP-k-s-v1 LUMO
			
BJP-m-r-v2 HOMO	BJP-m-r-v2 LUMO	BJP-m-s-v2 HOMO	BJP-m-s-v2 LUMO
			
BJP-m-q-v2 HOMO	BJP-m-q-v2 LUMO	BJP-j-r-v3 HOMO	BJP-j-r-v3 LUMO

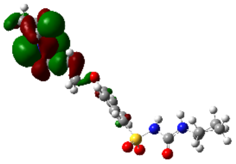
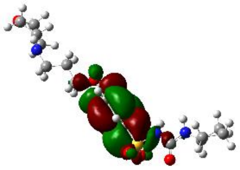
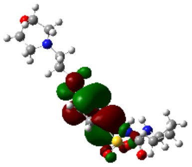
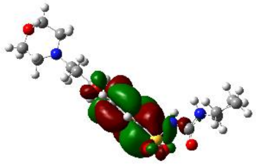
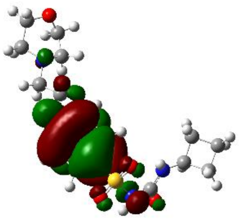
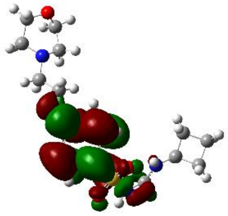
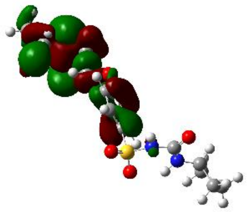
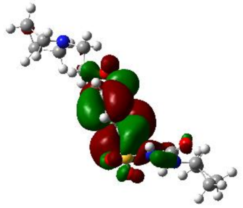
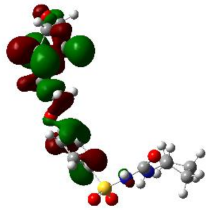
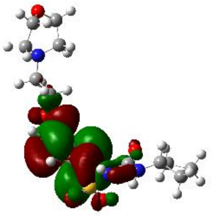
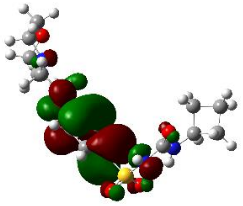
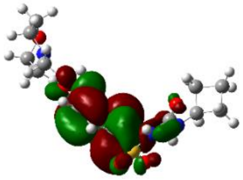
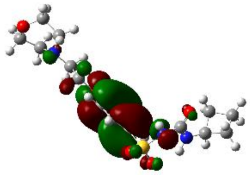
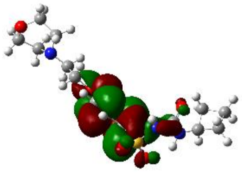
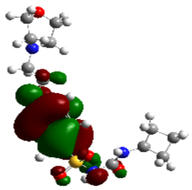
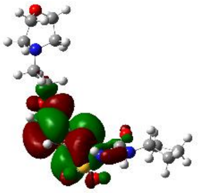
			
BJP-j-s-v3 HOMO	BJP-j-s-v3 LUMO	BJP-j-q-v3 HOMO	BJP-j-q-v3 LUMO

Figure 6.46: Shapes of HOMO and LUMO for the calculated conformers of compound BJQ.

			
BJQ-p-r-v3 HOMO	BJQ-p-r-v3 LUMO	BJQ-m-s-v1 HOMO	BJQ-m-s-v1 LUMO
			
BJQ-m-t-v1 HOMO	BJQ-m-t-v1 LUMO	BJQ-m-q-v2 HOMO	BJQ-m-q-v2 LUMO
			
BJQ-m-r-v2 HOMO	BJQ-m-r-v2 LUMO	BJQ-m-q-v1 HOMO	BJQ-m-q-v1 LUMO

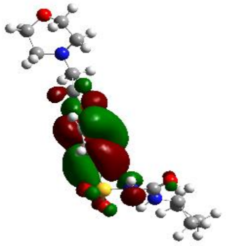
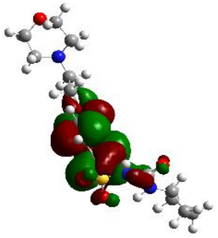
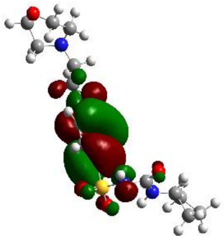
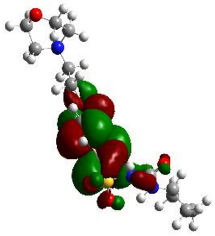
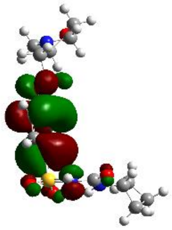
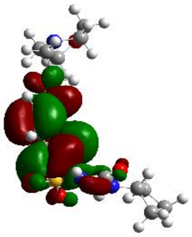
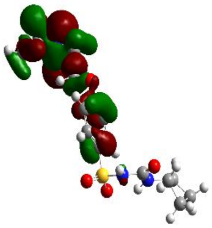
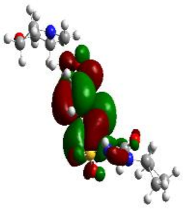
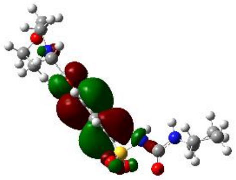
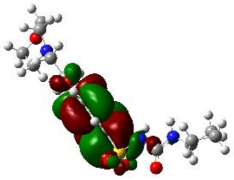
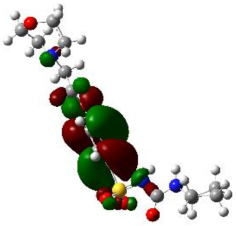
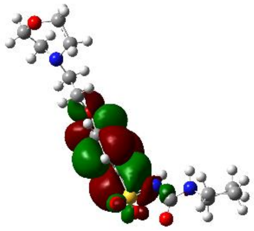
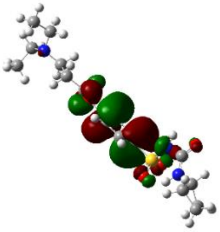
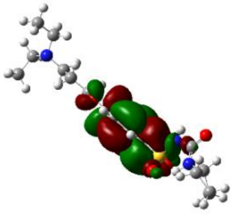
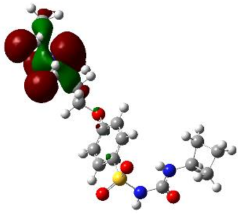
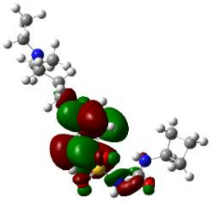
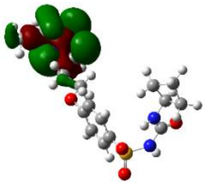
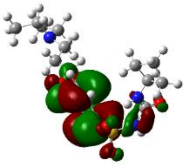
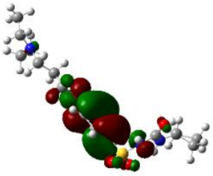
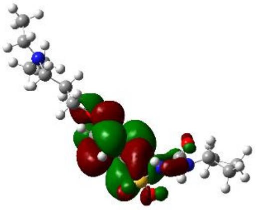
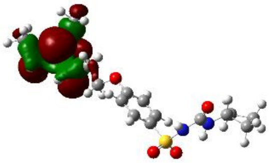
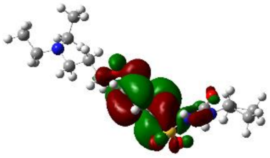
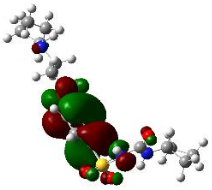
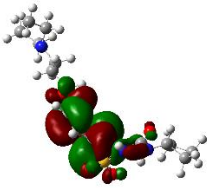
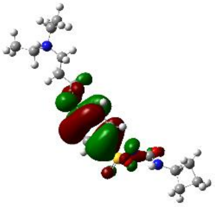
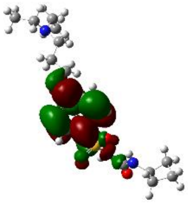
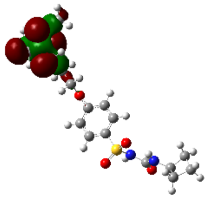
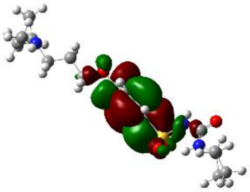
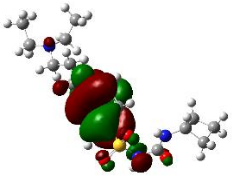
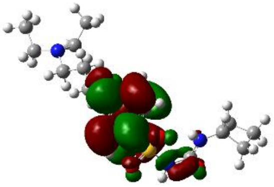
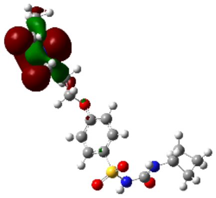
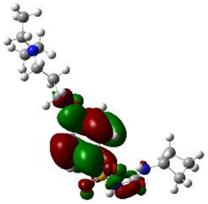
			
BJQ-p-q-v3 HOMO	BJQ-p-q-v3 LUMO	BJQ-p-q-v3′ HOMO	BJQ-p-q-v3′ LUMO
			
BJQ-p-r-v3 HOMO	BJQ-p-r-v3 LUMO	BJQ-p-s-v3 HOMO	BJQ-p-s-v3 LUMO
			
BJQ-j-q-v3 HOMO	BJQ-j-q-v3 LUMO	BJQ-j-r-v3 HOMO	BJQ-j-r-v3 LUMO

Figure 6.47: Shapes of HOMO and LUMO for the calculated conformers of compound BLP.

			
BLP-k-q-v1 HOMO	BLP-k-q-v1 LUMO	BLP-p-s-v3 HOMO	BLP-p-s-v3 LUMO
			
BLP-p-t-v3 HOMO	BLP-p-t-v3 LUMO	BLP-m-r-v1 HOMO	BLP-m-r-v1 LUMO
			
BLP-m-s-v1 HOMO	BLP-m-s-v1 LUMO	BLP-m-r-v1′ HOMO	BLP-m-r-v1′ LUMO
			
BLP-k-r-v1 HOMO	BLP-k-r-v1 LUMO	BLP-k-s-v1 HOMO	BLP-k-s-v1 LUMO
			
BLP-p-q-v4 HOMO	BLP-p-q-v4 LUMO	BLP-p-s-v4 HOMO	BLP-p-s-v4 LUMO

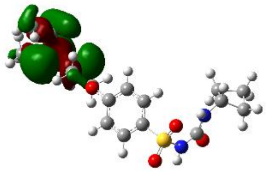
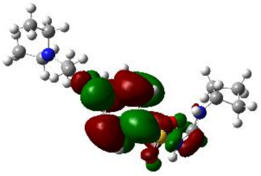
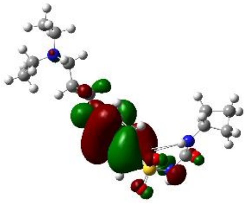
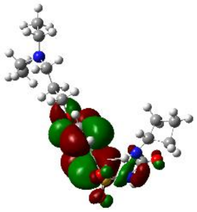
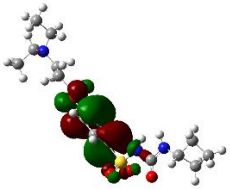
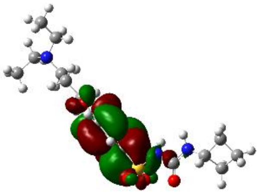
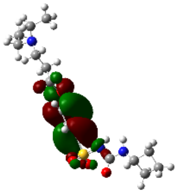
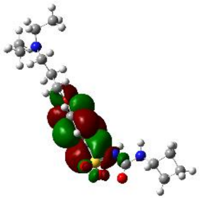
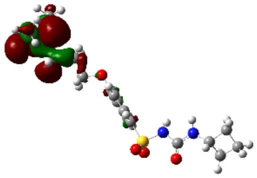
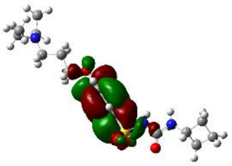
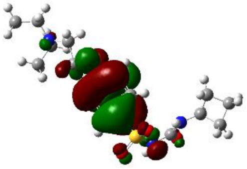
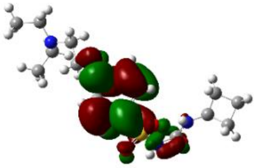
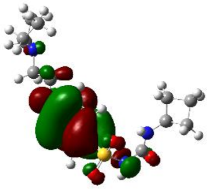
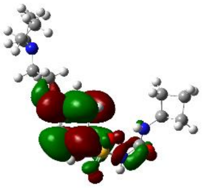
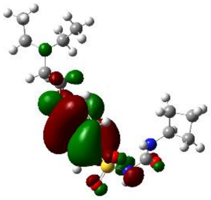
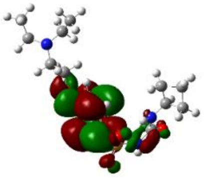
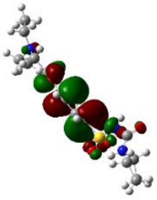
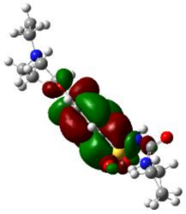
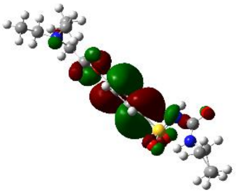
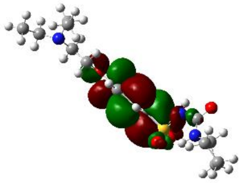
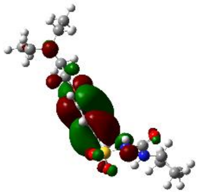
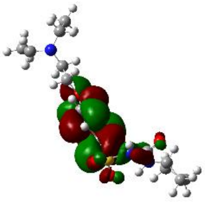
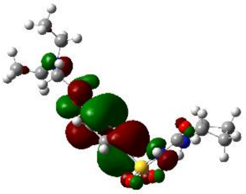
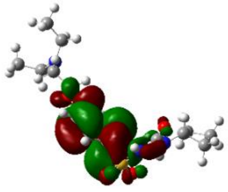
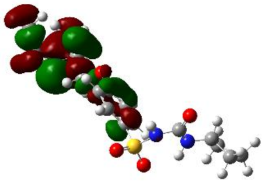
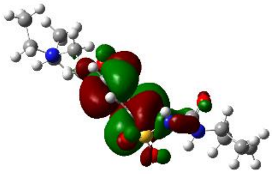
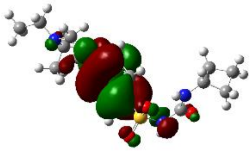
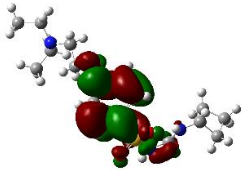
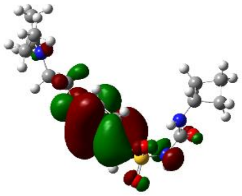
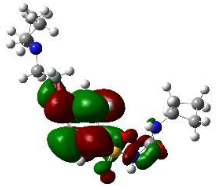
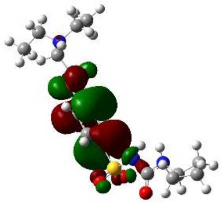
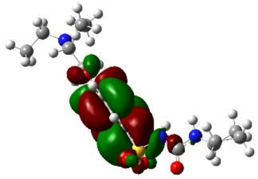
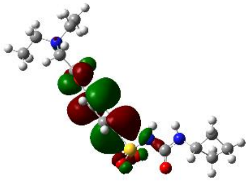
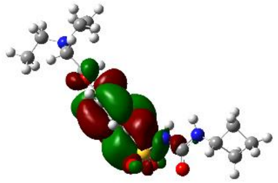
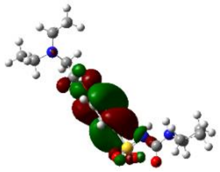
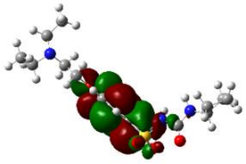
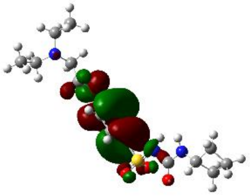
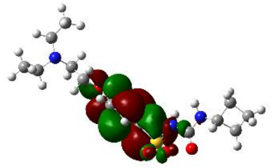
			
BLP-p-t-v4 HOMO	BLP-p-t-v4 LUMO	BLP-p-r-v4 HOMO	BLP-p-r-v4 LUMO
			
BLP-j-q-v5 HOMO	BLP-j-q-v5 LUMO	BLP-j-r-v5 HOMO	BLP-j-r-v5 LUMO
			
BLP-j-s-v5 HOMO	BLP-j-s-v5 LUMO		

Figure 6.48: Shapes of HOMO and LUMO for the calculated conformers of compound BLQ.

			
BLQ-p-q-v3 HOMO	BLQ-p-q-v3 LUMO	BLQ-p-r-v3 HOMO	BLQ-p-r-v3 LUMO
			
BLQ-p-r-v3 HOMO	BLQ-p-r-v3 LUMO	BLQ-k-q-v1 HOMO	BLQ-k-q-v1 LUMO

			
BLQ-k-r-v1 HOMO	BLQ-k-r-v1 LUMO	BLQ-m-r-v1 HOMO	BLQ-m-r-v1 LUMO
			
BLQ-m-q-v1 HOMO	BLQ-m-q-v1 LUMO	BLQ-m-s-v1 HOMO	BLQ-m-s-v1 LUMO
			
BLQ-p-q-v4 HOMO	BLQ-p-q-v4 LUMO	BLQ-p-r-v4 HOMO	BLQ-p-r-v4 LUMO
			
BLQ-j-q-v3 HOMO	BLQ-j-q-v3 LUMO	BLQ-j-q-v5 HOMO	BLQ-j-q-v5 LUMO
			
BLQ-j-r-v3 HOMO	BLQ-j-r-v3 LUMO	BLQ-j-r-v5 HOMO	BLQ-j-r-v5 LUMO

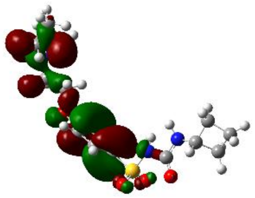
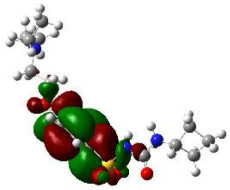
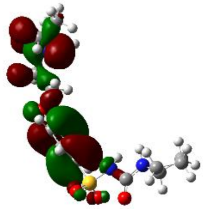
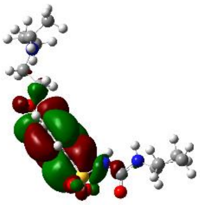
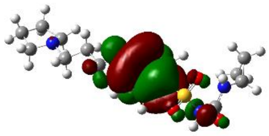
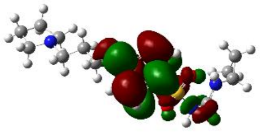
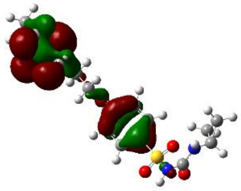
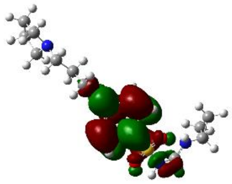
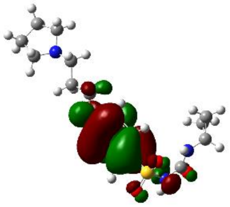
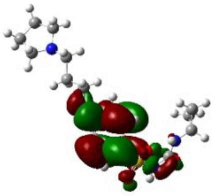
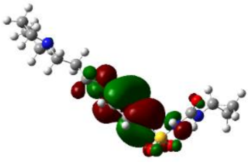
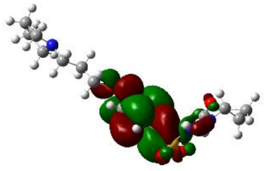
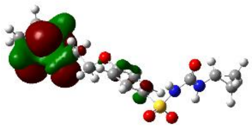
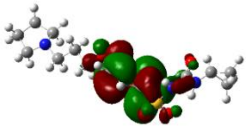
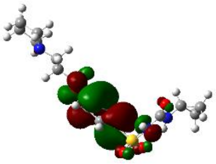
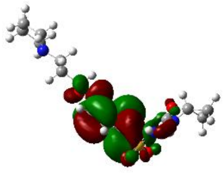
			
BLQ-j-t-v3 HOMO	BLQ-j-t-v3 LUMO	BLQ-j-t-v5 HOMO	BLQ-j-t-v5 LUMO

Figure 6.49: Shapes of HOMO and LUMO for the calculated conformers of compound CGP.

			
CGP-p-q-w5 HOMO	CGP-p-q-w5 LUMO	CGP-p-s-w5 HOMO	CGP-p-s-w5 LUMO
			
CGP-p-r-w5 HOMO	CGP-p-r-w5 LUMO	CGP-m-r-w1 HOMO	CGP-m-r-w1 LUMO
			
CGP-m-s-w1 HOMO	CGP-m-s-w1 LUMO	CGP-m-q-w1 HOMO	CGP-m-q-w1 LUMO

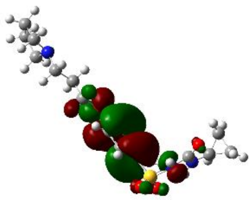
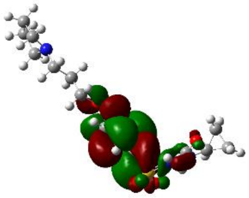
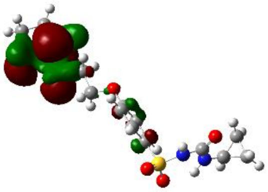
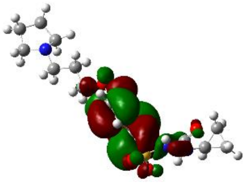
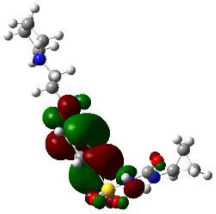
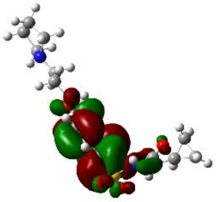
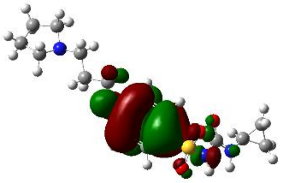
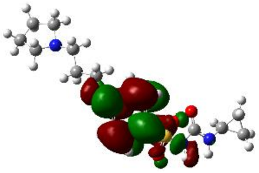
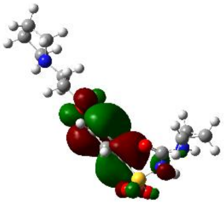
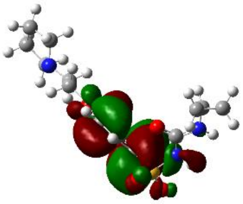
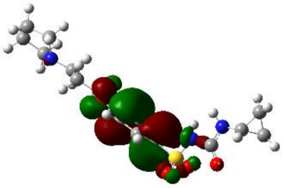
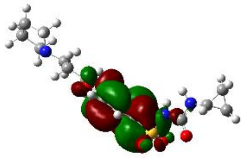
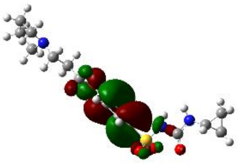
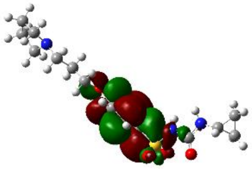
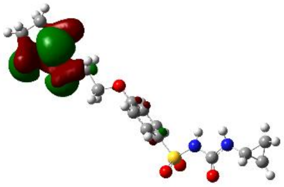
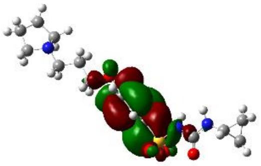
			
CGP-m-r-w2 HOMO	CGP-m-r-w2 LUMO	CGP-m-s-w2 HOMO	CGP-m-s-w2 LUMO
			
CGP-m-q-w2 HOMO	CGP-m-q-w2 LUMO	CGP-g-r-w5 HOMO	CGP-g-r-w5 LUMO
			
CGP-g-q-w5 HOMO	CGP-g-q-w5 LUMO	CGP-j-q-w5 HOMO	CGP-j-q-w5 LUMO
			
CGP-j-r-w5 HOMO	CGP-j-r-w5 LUMO	CGP-j-s-w5 HOMO	CGP-j-s-w5 LUMO

Figure 6.50: Shapes of HOMO and LUMO for the calculated conformers of compound CGQ.

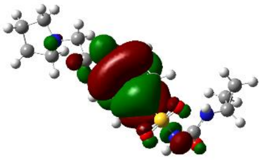
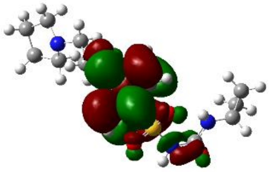
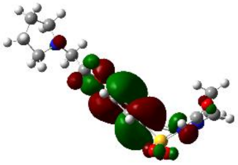
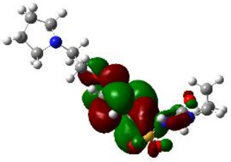
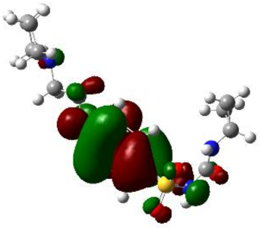
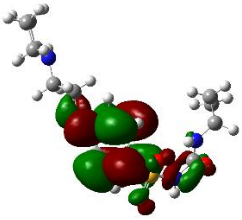
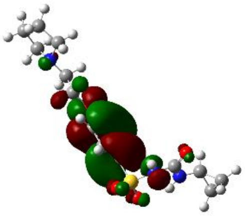
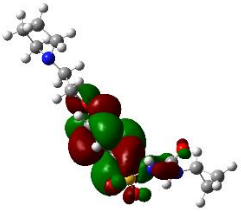
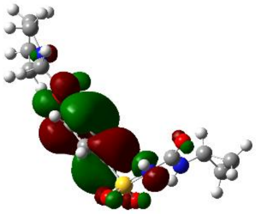
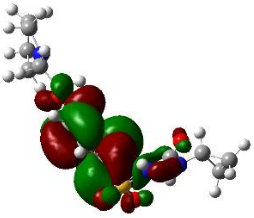
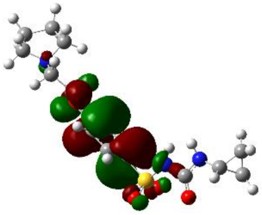
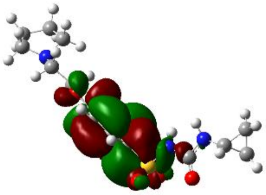
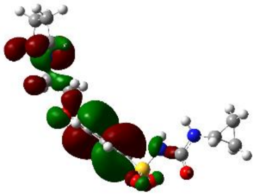
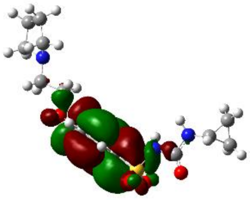
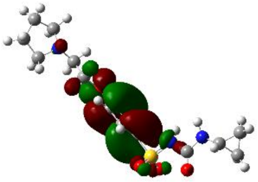
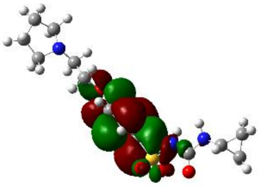
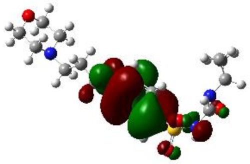
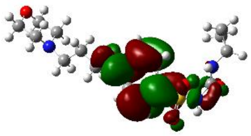
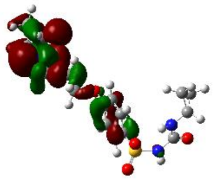
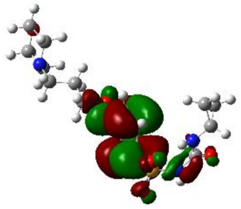
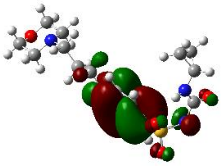
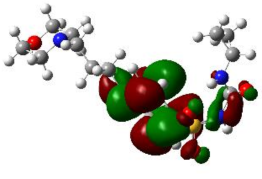
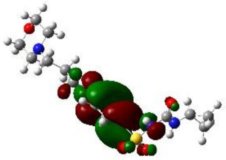
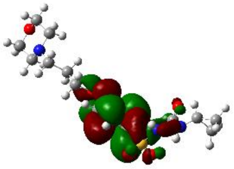
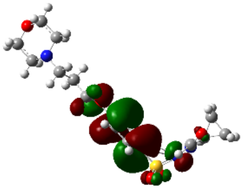
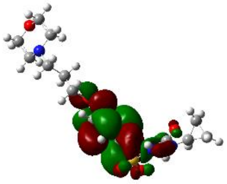
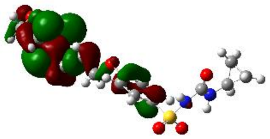
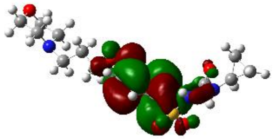
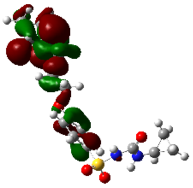
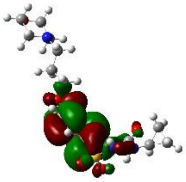
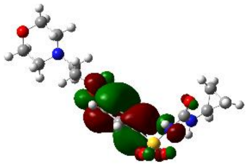
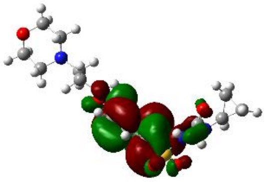
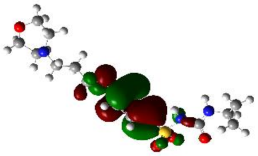
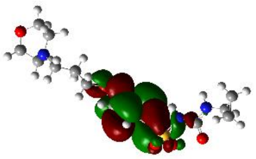
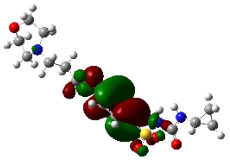
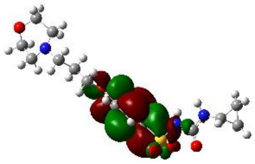
			
CGQ-p-q-w5 HOMO	CGQ-p-q-w5 LUMO	CGQ-m-q-w3 HOMO	CGQ-m-q-w3 LUMO
			
CGQ-p-r-w5 HOMO	CGQ-p-r-w5 LUMO	CGQ-m-r-w1 HOMO	CGQ-m-r-w1 LUMO
			
CGQ-m-q-w1 HOMO	CGQ-m-q-w1 LUMO	CGQ-j-q-w5 HOMO	CGQ-j-q-w5 LUMO
			
CGQ-j-r-w5 HOMO	CGQ-j-r-w5 LUMO	CGQ-j-t-w5 HOMO	CGQ-j-t-w5 LUMO

Figure 6.51: Shapes of HOMO and LUMO for the calculated conformers of compound CJP.

			
CJP-p-q-w3 HOMO	CJP-p-q-w3 LUMO	CJP-p-s-w3 HOMO	CJP-p-s-w3 LUMO
			
CJP-p- r-w3 HOMO	CJP-p- r-w3 LUMO	CJP-m-r-w1 HOMO	CJP-m-r-w1 LUMO
			
CJP-m-r-w2 HOMO	CJP-m-r-w2 LUMO	CJP-m-s-w2 HOMO	CJP-m-s-w2 LUMO
			
CJP-m-t-w2 HOMO	CJP-m-t-w2 LUMO	CJP-m-q-w2 HOMO	CJP-m-q-w2 LUMO
			
CJP-j-q-w1 HOMO	CJP-j-q-w1 LUMO	CJP-j-r-w1 HOMO	CJP-j-r-w1 LUMO

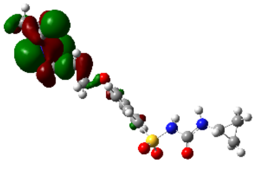
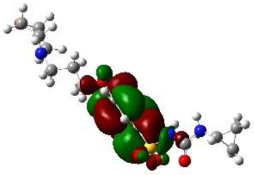
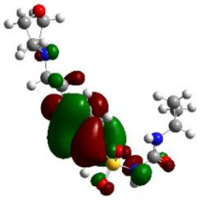
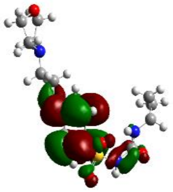
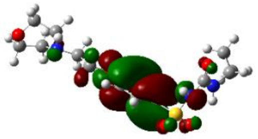
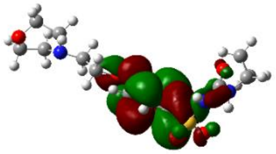
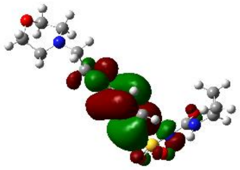
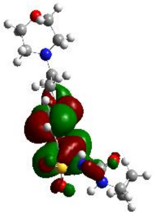
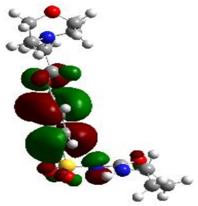
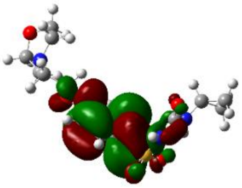
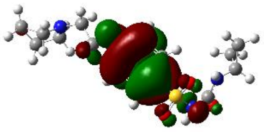
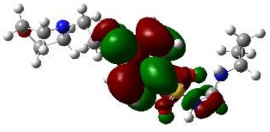
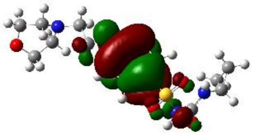
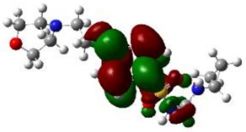
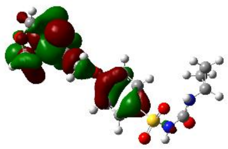
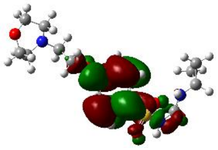
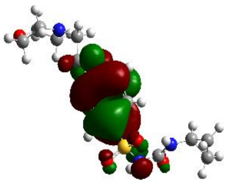
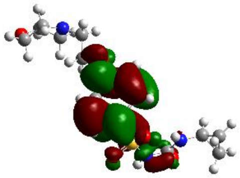
			
CJP-j-s-w1 HOMO	CJP-j-s-w1 LUMO		

Figure 6.52: Shapes of HOMO and LUMO for the calculated conformers of compound CJQ.

			
CJQ-m-q-w6 HOMO	CJQ-m-q-w6 LUMO	CJQ-m-r-w6 HOMO	CJQ-m-r-w6 LUMO
			
CJQ-p-q-w5 HOMO	CJQ-p-q-w5 LUMO	CJQ-m-q-w HOMO	CJQ-m-q-w1 LUMO
			
CJQ-p-q-w5 HOMO	CJQ-p-q-w5 LUMO	CJQ-p-q-w5′ HOMO	CJQ-p-q-w5′ LUMO
			
CJQ-p-s-w5 HOMO	CJQ-p-s-w5 LUMO	CJQ-m-r-w1 HOMO	CJQ-m-r-w1 LUMO

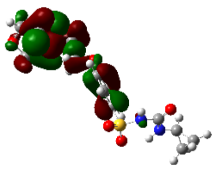
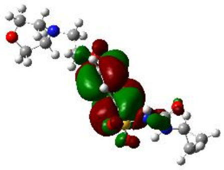
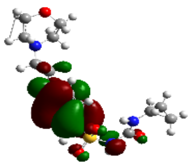
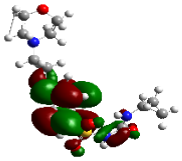
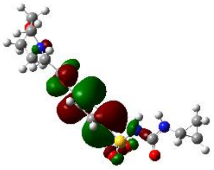
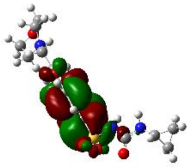
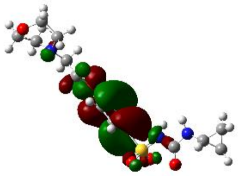
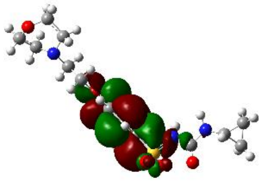
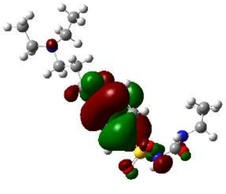
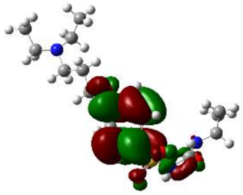
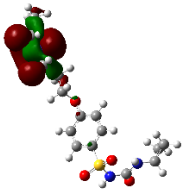
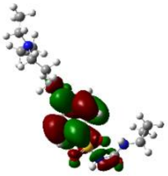
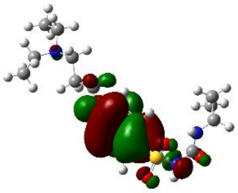
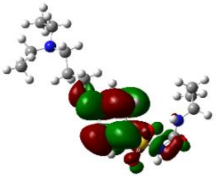
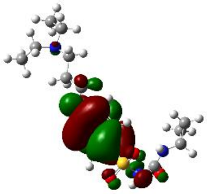
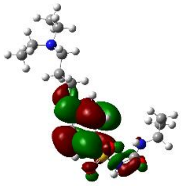
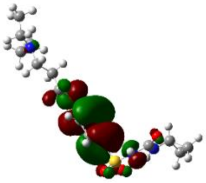
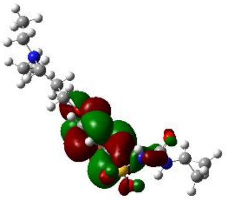
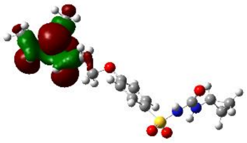
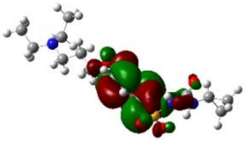
			
CJQ-m-s-w1 HOMO	CJQ-m-s-w1 LUMO	CJQ-m-q-w1′ HOMO	CJQ-m-q-w1′ LUMO
			
CJQ-j-q-w5 HOMO	CJQ-j-q-w5 LUMO	CJQ-j-r-w5 HOMO	CJQ-j-r-w5 LUMO

Figure 6.53: Shapes of HOMO and LUMO for the calculated conformers of compound CLP.

			
CLP-p-q-w5 HOMO	CLP-p-q-w5 LUMO	CLP-p-s-w5 HOMO	CLP-p-s-w5 LUMO
			
CLP-p-r-w5 HOMO	CLP-p-r-w5 LUMO	CLP-p-r-w5′ HOMO	CLP-p-r-w5′ LUMO
			
CLP-m-r-w1 HOMO	CLP-m-r-w1 LUMO	CLP-m-s-w1 HOMO	CLP-m-s-w1 LUMO

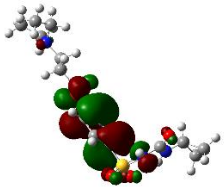
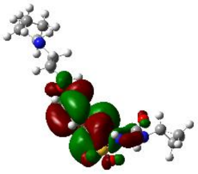
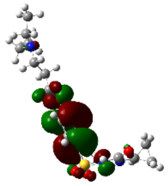
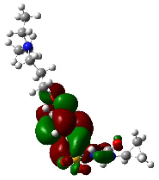
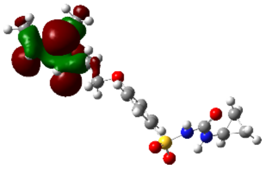
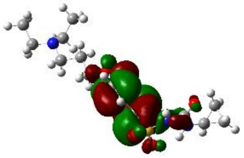
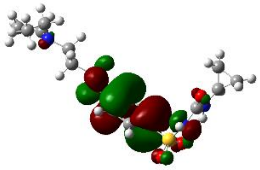
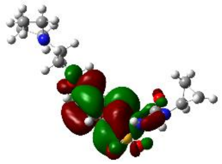
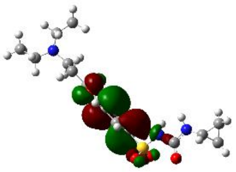
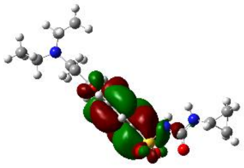
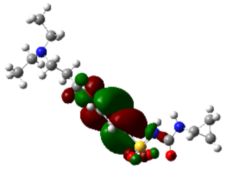
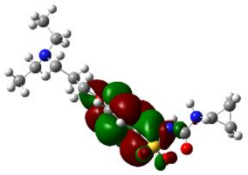
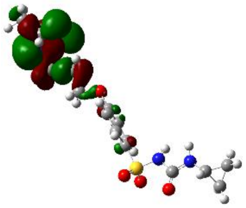
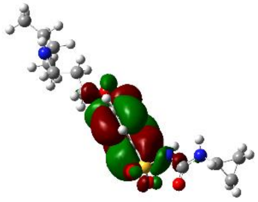
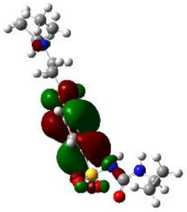
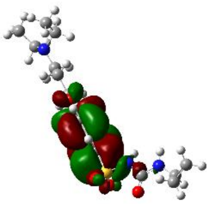
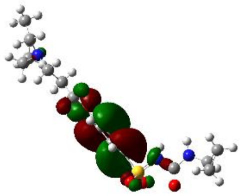
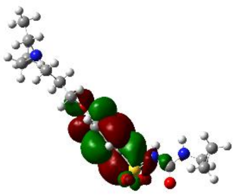
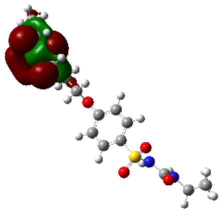
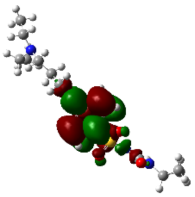
			
CLP-m-q-w1 HOMO	CLP-m-q-w1 LUMO	CLP-m-q-w2 HOMO	CLP-m-q-w2 LUMO
			
CLP-m-s-w2 HOMO	CLP-m-s-w2 LUMO	CLP-m-q-w2 HOMO	CLP-m-q-w2 LUMO
			
CLP-j-q-w5 HOMO	CLP-j-q-w5 LUMO	CLP-j-r-w5 HOMO	CLP-j-r-w5 LUMO
			
CLP-j-s-w5 HOMO	CLP-j-s-w5 LUMO	CLP-j-q-w6 HOMO	CLP-j-q-w6 LUMO
			
CLP-j-r-w6 HOMO	CLP-j-r-w6 LUMO	CLP-j-s-w6 HOMO	CLP-j-s-w6 LUMO

Figure 6.54: Shapes of HOMO and LUMO for the calculated conformers of compound CLQ.

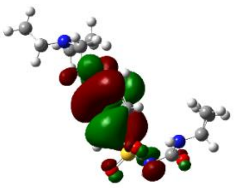
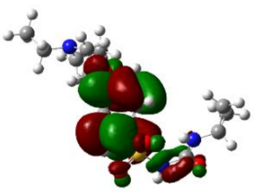
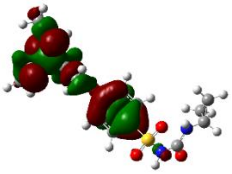
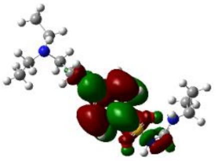
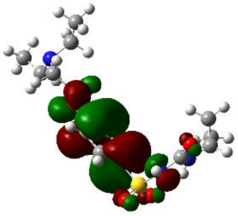
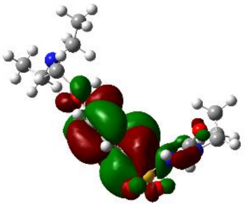
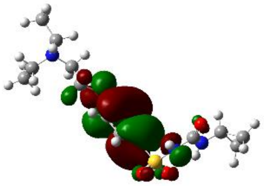
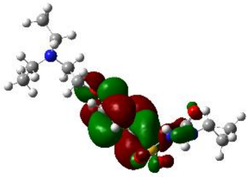
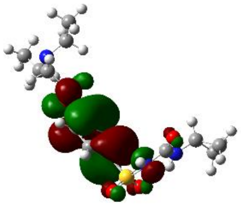
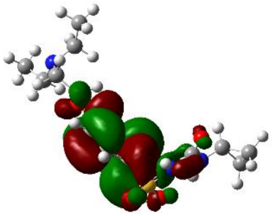
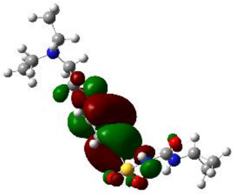
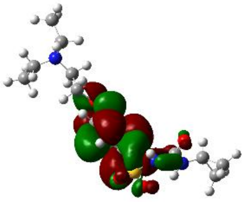
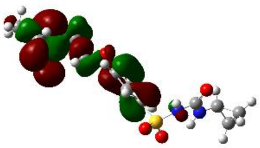
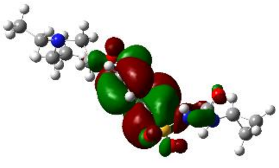
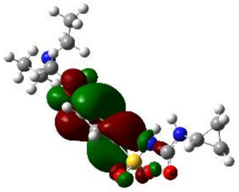
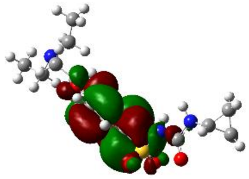
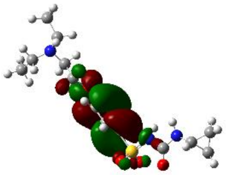
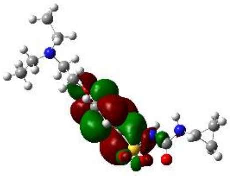
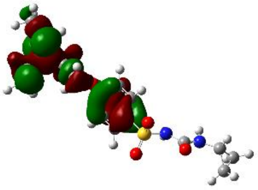
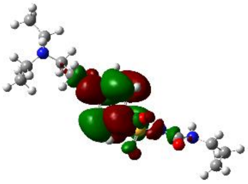
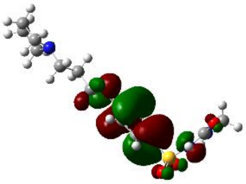
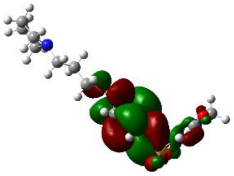
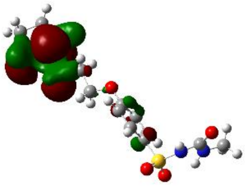
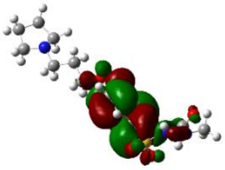
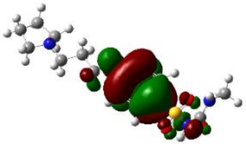
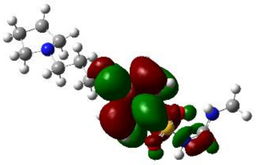
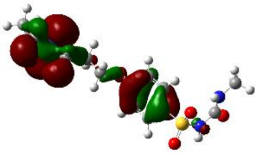
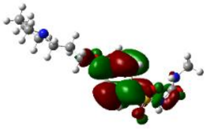
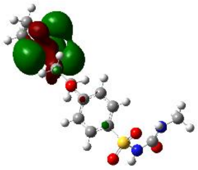
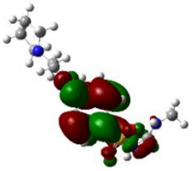
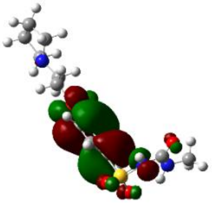
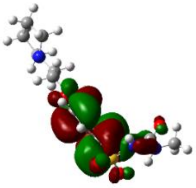
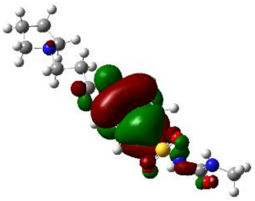
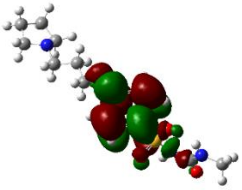
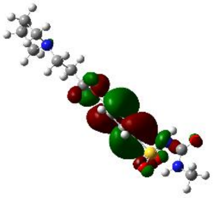
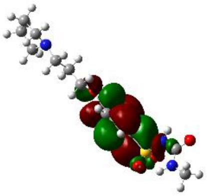
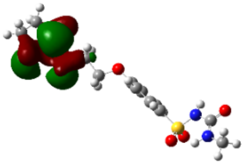
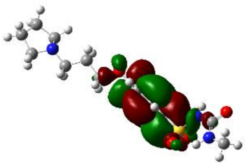
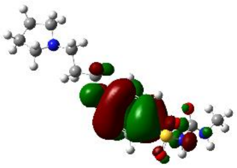
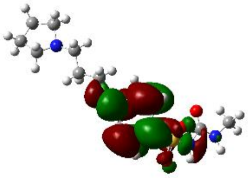
			
CLQ-p-q-w5 HOMO	CLQ-p-q-w5 LUMO	CLQ-p-s-w5 HOMO	CLQ-p-s-w5 LUMO
			
CLQ-m-q-w1 HOMO	CLQ-m-q-w1 LUMO	CLQ-m-q-w1′ HOMO	CLQ-m-q-w1′ LUMO
			
CLQ-m-r-w1′ HOMO	CLQ-m-r-w1′ LUMO	CLQ-m-r-w1 HOMO	CLQ-m-r-w1 LUMO
			
CLQ-m-s-w1 HOMO	CLQ-m-s-w1 LUMO	CLQ-j-q-w5 HOMO	CLQ-j-q-w5 LUMO
			
CLQ-j-r-w5 HOMO	CLQ-j-r-w5 LUMO	CLQ-j-s-w6 HOMO	CLQ-j-s-w6 LUMO

Figure 6.55: Shapes of HOMO and LUMO for the calculated conformers of compound DGP.

			
DGP-m-r HOMO	DGP-m-r LUMO	DGP-m-s HOMO	DGP-m-s LUMO
			
DGP-p-q HOMO	DGP-p-q LUMO	DGP-p-s HOMO	DGP-p-s LUMO
			
DGP-p-t HOMO	DGP-p-t LUMO	DGP-m-q HOMO	DGP-m-q LUMO
			
DGP-k-q HOMO	DGP-k-q LUMO	DGP-k-r HOMO	DGP-k-r LUMO
			
DGP-k-s HOMO	DGP-k-s LUMO	DGP-g-r HOMO	DGP-g-r LUMO

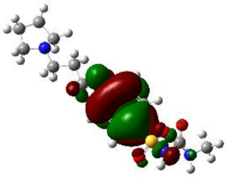
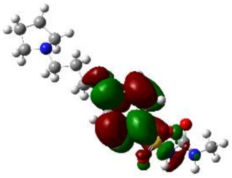
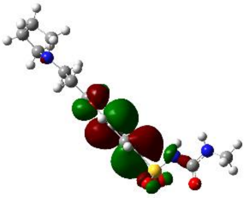
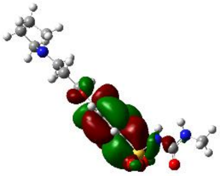
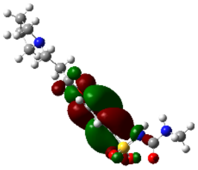
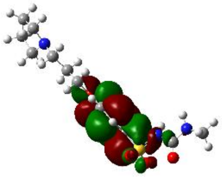
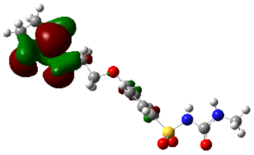
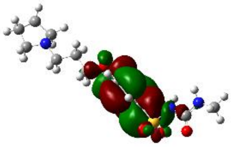
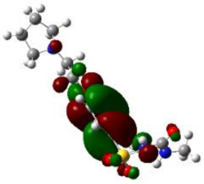
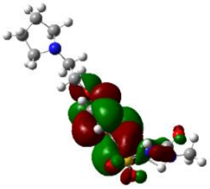
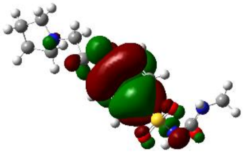
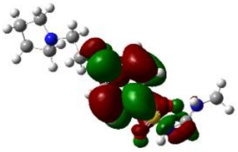
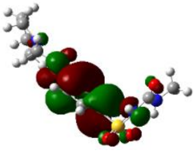
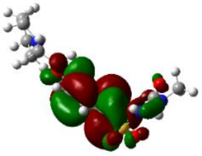
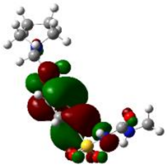
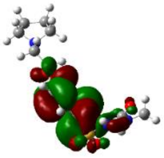
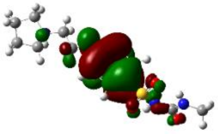
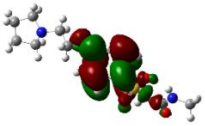
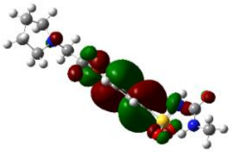
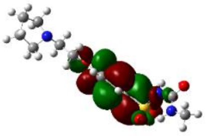
			
DGP-g-q HOMO	DGP-g-q LUMO	DGP-j-q HOMO	DGP-j-q LUMO
			
DGP-j-r HOMO	DGP-j-r LUMO	DGP-j-s HOMO	DGP-j-s LUMO

Figure 6.56: Shapes of HOMO and LUMO for the calculated conformers of compound DGQ.

			
DGQ-m-r HOMO	DGQ-m-r LUMO	DGQ-p-q HOMO	DGQ-p-q LUMO
			
DGQ-m-q HOMO	DGQ-m-q LUMO	DGQ-m-q′ HOMO	DGQ-m-q′ LUMO
			
DGQ-k-q HOMO	DGQ-k-q LUMO	DGQ-k-r HOMO	DGQ-k-r LUMO

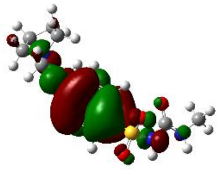
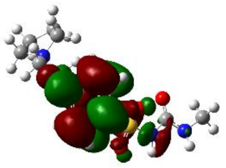
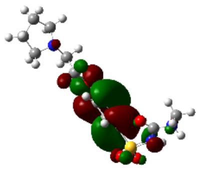
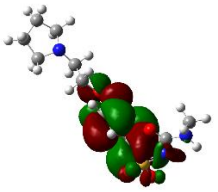
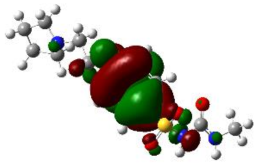
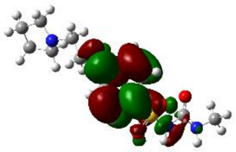
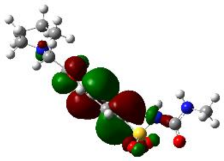
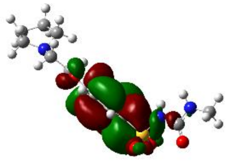
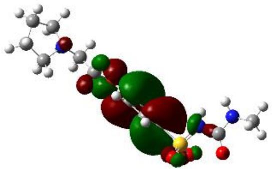
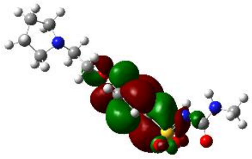
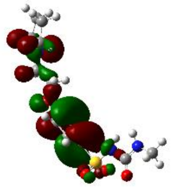
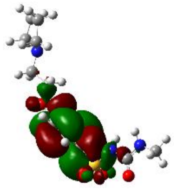
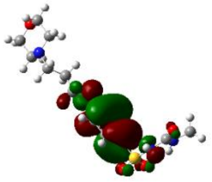
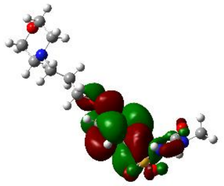
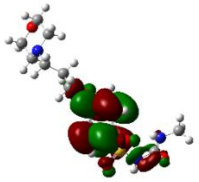
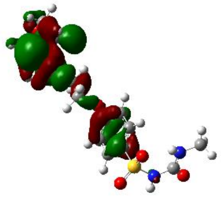
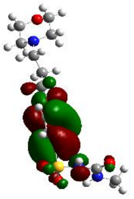
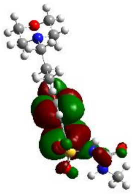
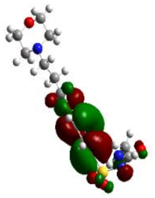
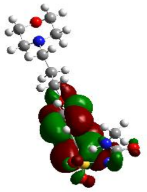
			
DGQ-g-r HOMO	DGQ-g-r LUMO	DGQ-g-t HOMO	DGQ-g-t LUMO
			
DGQ-g-q HOMO	DGQ-g-q LUMO	DGQ-j-q HOMO	DGQ-j-q LUMO
			
DGQ-j-r HOMO	DGQ-j-r LUMO	DGQ-j-t HOMO	DGQ-j-t LUMO

Figure 6.57: Shapes of HOMO and LUMO for the calculated conformers of compound DJP.

			
DJP-m-r HOMO	DJP-m-r LUMO	DJP-p-s HOMO	DJP-p-s LUMO
			
DJP-p-q HOMO	DJP-p-q LUMO	DJP-m-q HOMO	DJP-m-q LUMO

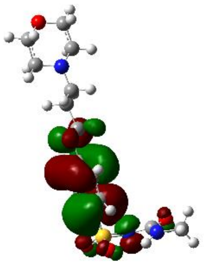
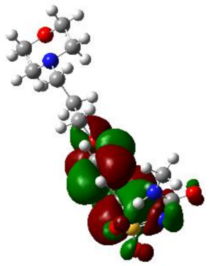
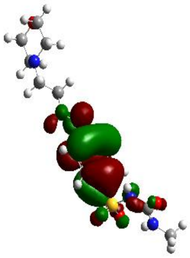
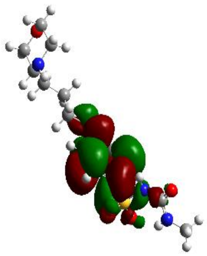
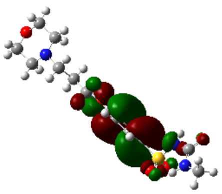
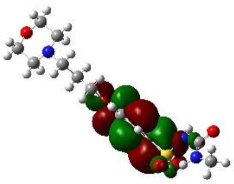
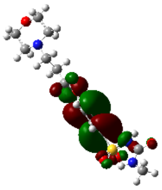
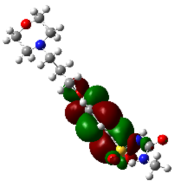
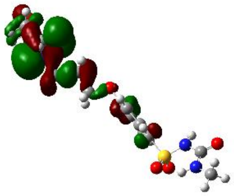
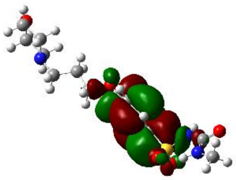
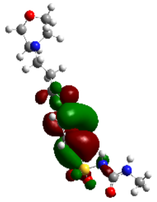
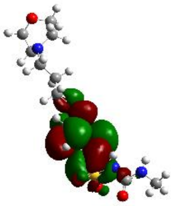
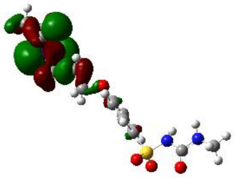
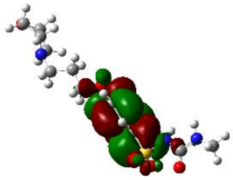
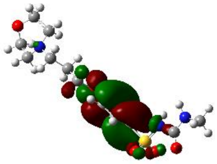
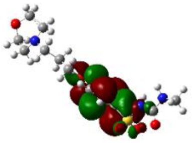
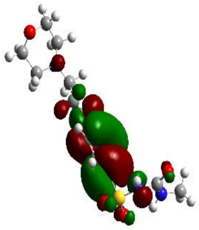
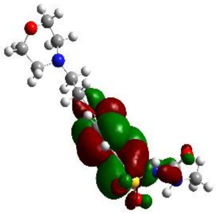
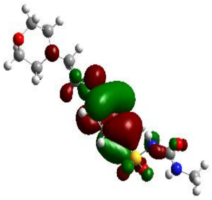
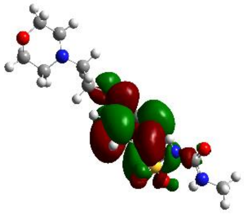
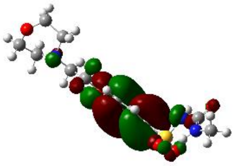
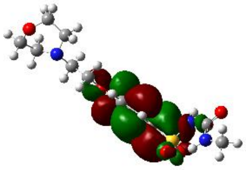
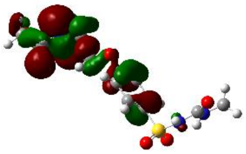
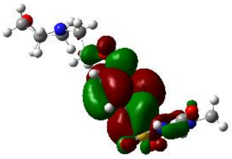
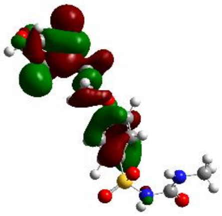
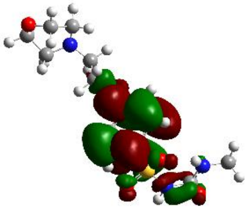
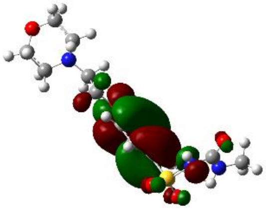
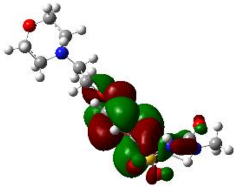
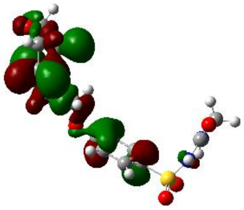
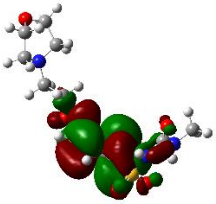
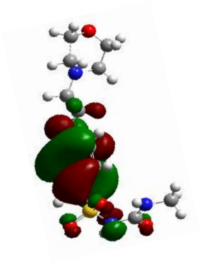
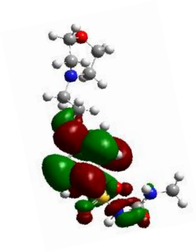
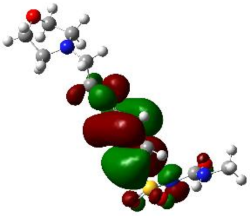
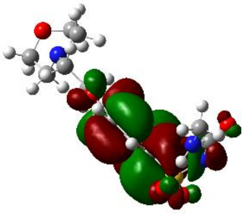
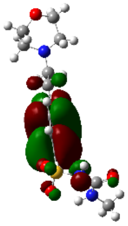
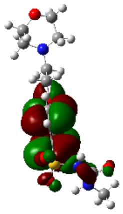
			
DJP-p-r HOMO	DJP-p-r LUMO	DJP-k-q HOMO	DJP-k-q LUMO
			
DJP-k-r HOMO	DJP-k-r LUMO	DJP-k-r′ HOMO	DJP-k-r′ LUMO
			
DJP-k-s HOMO	DJP-k-s LUMO	DJP-j-q HOMO	DJP-j-q LUMO
			
DJP-j-s HOMO	DJP-j-s LUMO	DJP-j-r HOMO	DJP-j-r LUMO

Figure 6.58: Shapes of HOMO and LUMO for the calculated conformers of compound DJQ.

			
DJQ-m-q HOMO	DJQ-m-q LUMO	DJQ-k-q HOMO	DJQ-k-q LUMO
			
DJQ-k-r HOMO	DJQ-k-r LUMO	DJQ-m-r HOMO	DJQ-m-r LUMO
			
DJQ-m-s HOMO	DJQ-m-s LUMO	DJQ-m-t HOMO	DJQ-m-t LUMO
			
DJQ-m-s′ HOMO	DJQ-m-s′ LUMO	DJQ-m-q HOMO	DJQ-m-q LUMO
			
DJQ-p-q HOMO	DJQ-p-q LUMO	DJQ-m-r′ HOMO	DJQ-m-r′ LUMO

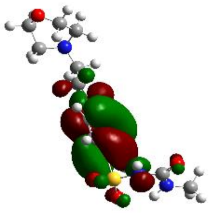
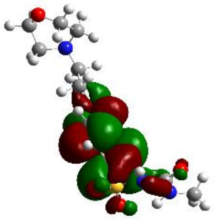
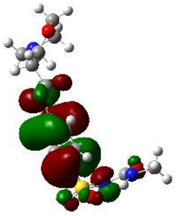
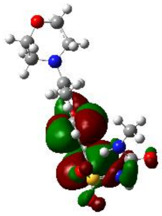
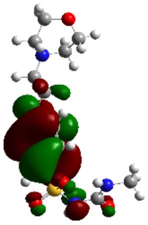
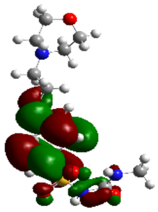
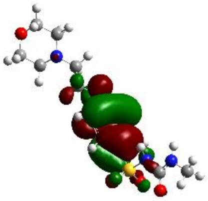
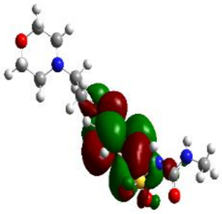
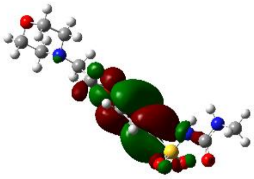
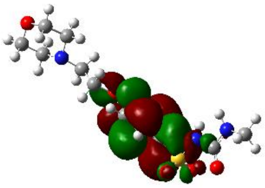
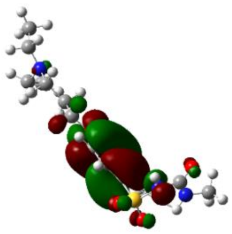
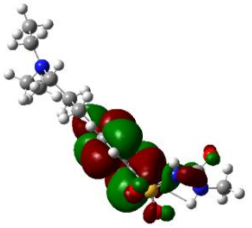
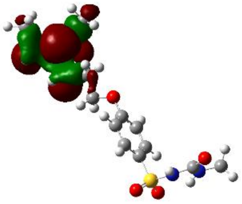
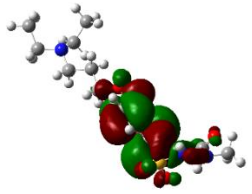
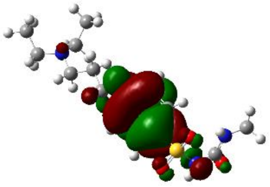
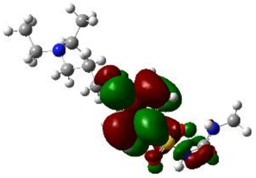
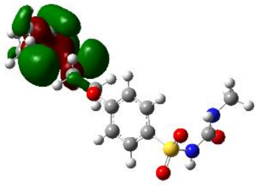
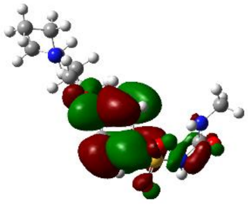
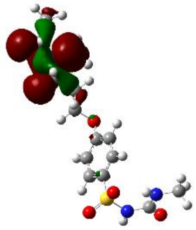
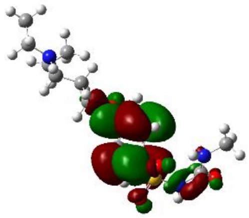
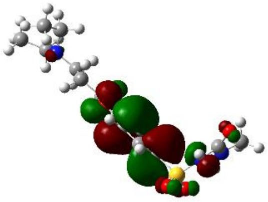
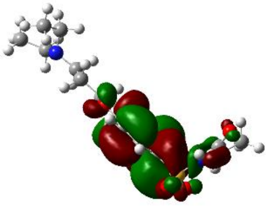
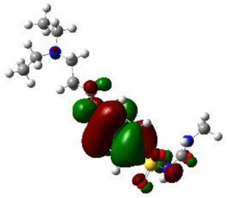
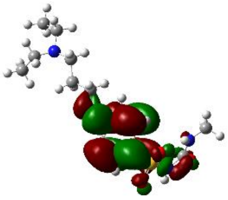
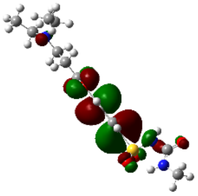
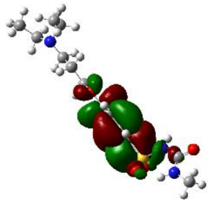
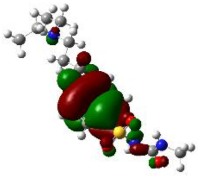
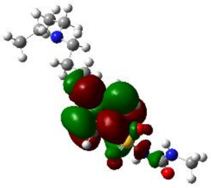
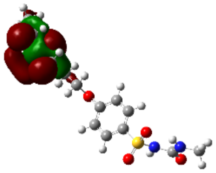
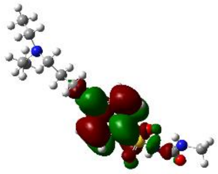
			
DJQ-p-q′ HOMO	DJQ-p-q′ LUMO	DJQ-p-r HOMO	DJQ-p-r LUMO
			
DJQ-m-q HOMO	DJQ-m-q LUMO	DJQ-j-q HOMO	DJQ-j-q LUMO
			
DJQ-j-r HOMO	DJQ-j-r LUMO		

Figure 6.59: Shapes of HOMO and LUMO for the calculated conformers of compound DLP.

			
DLP-m-r HOMO	DLP-m-r LUMO	DLP-m-s HOMO	DLP-m-s LUMO
			
DLP-p-q HOMO	DLP-p-q LUMO	DLP-p-s HOMO	DLP-p-s LUMO
			
CLP-p-t HOMO	CLP-p-t LUMO	DLP-m-q HOMO	DLP-m-q LUMO
			
DLP-p-r HOMO	DLP-p-r LUMO	DLP-k-q HOMO	DLP-k-q LUMO
			
DLP-k-r HOMO	DLP-k-r LUMO	DLP-k-s HOMO	DLP-k-s LUMO

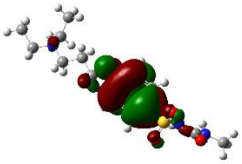
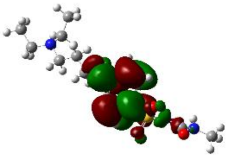
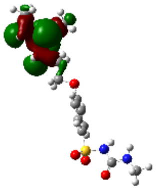
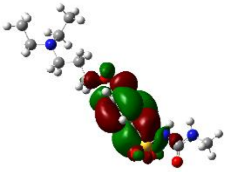
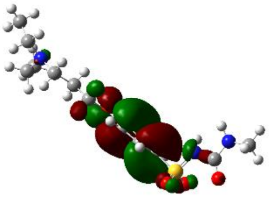
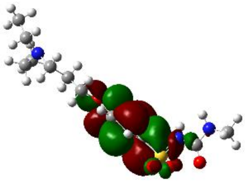
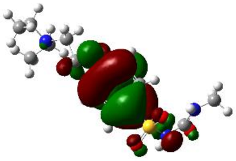
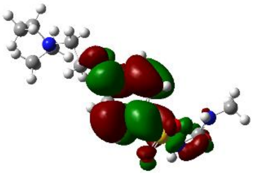
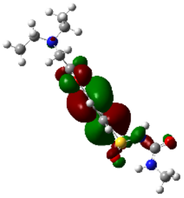
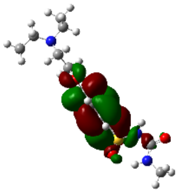
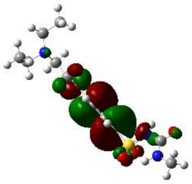
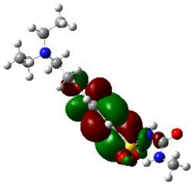
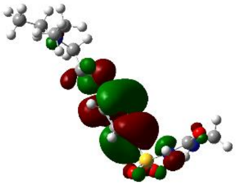
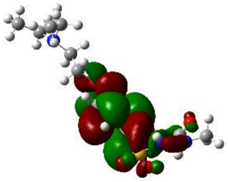
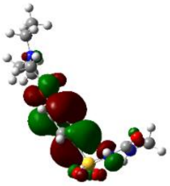
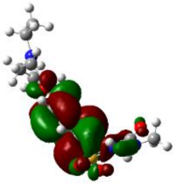
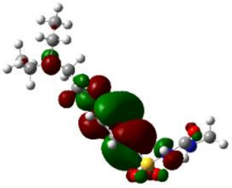
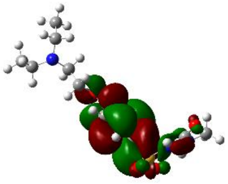
			
DLP-j-q HOMO	DLP-j-q LUMO	DLP-j-s HOMO	DLP-j-s LUMO
			
DLP-j-r HOMO	DLP-j-r LUMO		

Figure 6.60: Shapes of HOMO and LUMO for the calculated conformers of compound DLQ.

			
DLQ-p-q HOMO	DLQ-p-q LUMO	DLQ-k-q HOMO	DLQ-k-q LUMO
			
DLQ-k-r HOMO	DLQ-k-r LUMO	DLQ-m-r HOMO	DLQ-m-r LUMO
			
DLQ-m-q HOMO	DLQ-m-q LUMO	DLQ-m-r′ HOMO	DLQ-m-r′ UMO

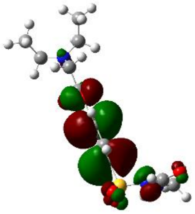
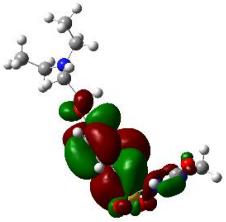
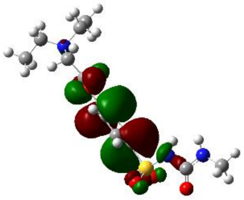
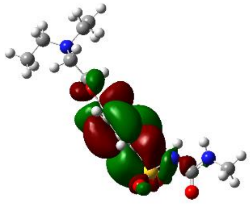
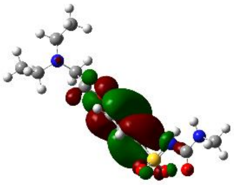
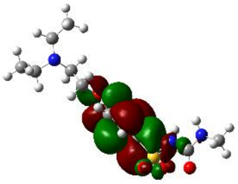
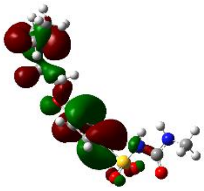
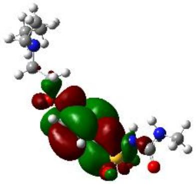
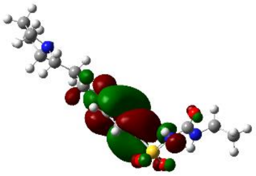
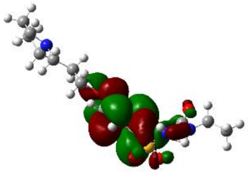
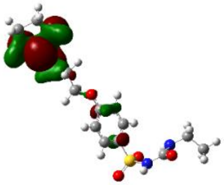
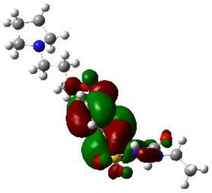
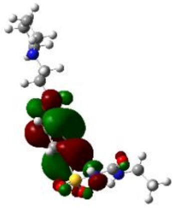
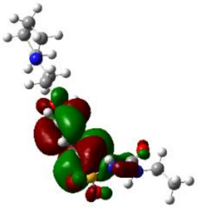
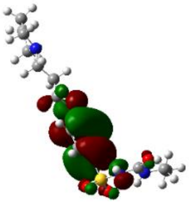
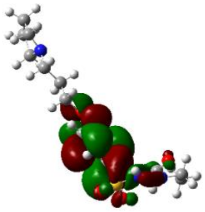
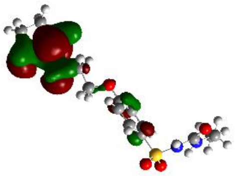
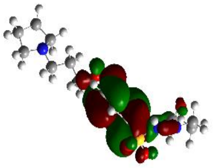
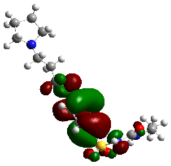
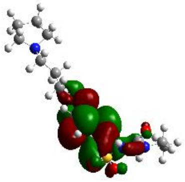
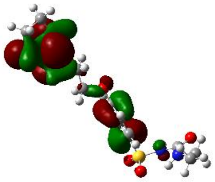
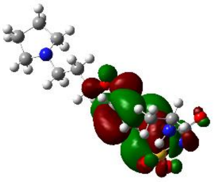
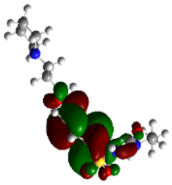
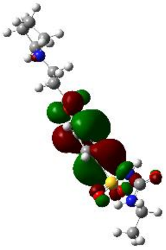
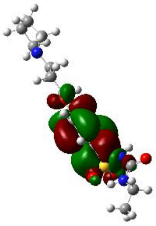
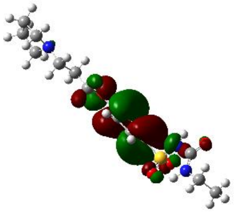
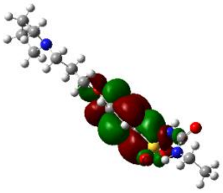
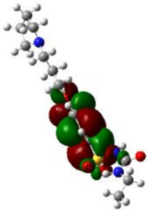
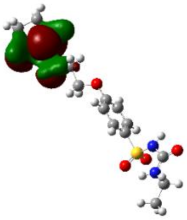
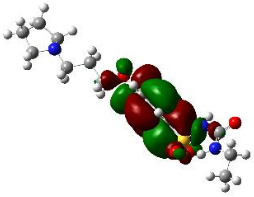
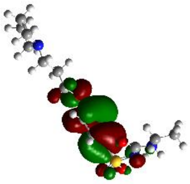
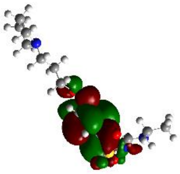
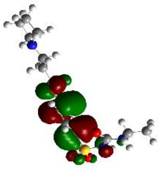
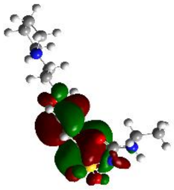
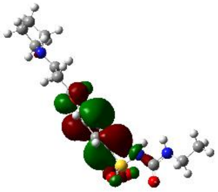
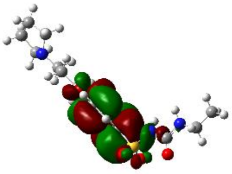
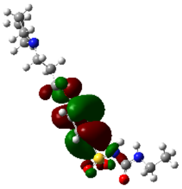
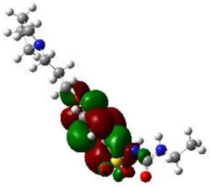
			
DLQ-m-q′ HOMO	DLQ-m-q′ LUMO	DLQ-j-q HOMO	DLQ-j-q LUMO
			
DLQ-j-r HOMO	DLQ-j-r LUMO	DLQ-j-t HOMO	DLQ-j-t LUMO

Figure 6.61: Shapes of HOMO and LUMO for the calculated conformers of compound EGP.

			
EGP-m-r-x4 HOMO	EGP-m-r-x4 LUMO	EGP-m-s-x4 HOMO	EGP-m-s-x4 LUMO
			
EGP-m-q-x4 HOMO	EGP-m-q-x4 LUMO	EGP-m-r-x1 HOMO	EGP-m-r-x1 LUMO
			
EGP-m-s-x1 HOMO	EGP-m-s-x1 LUMO	EGP-p-q-x3 HOMO	EGP-p-q-x3 LUMO

			
EGP-p-s-x3 HOMO	EGP-p-s-x3 LUMO	EGP-m-q-x1 HOMO	EGP-m-q-x1 LUMO
			
EGP-k-q-x1 HOMO	EGP-k-q-x1 LUMO	EGP-k-r-x2 HOMO	EGP-k-r-x2 LUMO
			
EGP-k-q-x1′ HOMO	EGP-k-q-x1′ LUMO	EGP-k-s-x1 HOMO	EGP-k-s-x1 LUMO
			
EGP-g-r-x1 HOMO	EGP-g-r-x1 LUMO	EGP-g-q-x1 HOMO	EGP-g-q-x1 LUMO
			
EGP-j-q-x3 HOMO	EGP-j-q-x3 LUMO	EGP-j-r-x3 HOMO	EGP-j-r-x3 LUMO

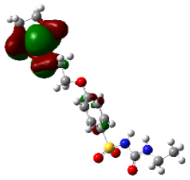
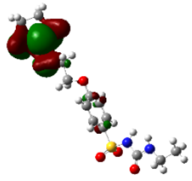
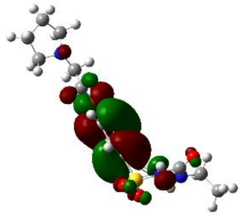
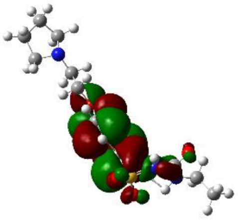
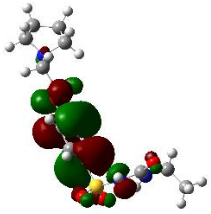
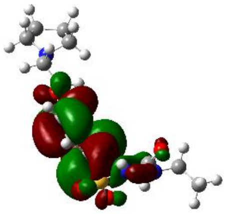
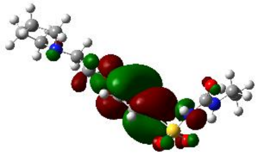
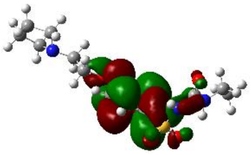
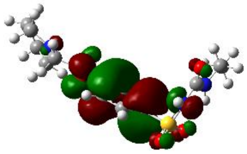
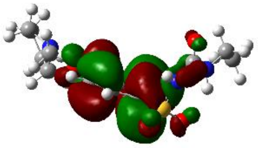
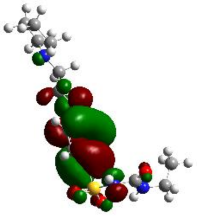
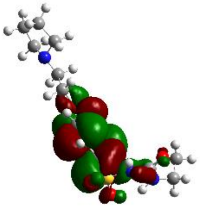
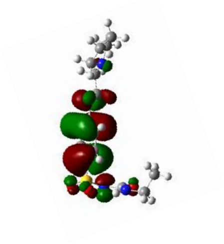
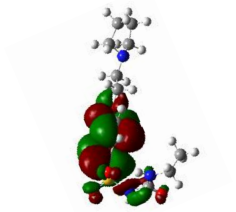
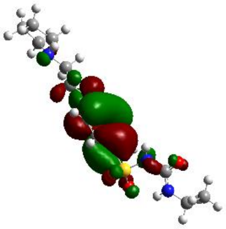
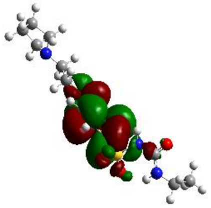
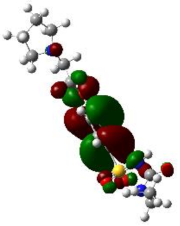
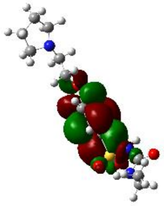
			
EGP-j-s-x3 HOMO	EGP-j-s-x3 LUMO		

Figure 6.62: Shapes of HOMO and LUMO for the calculated conformers of compound EGQ.

			
EGQ-m-r-x4 HOMO	EGQ-m-r-x4 LUMO	EGQ-m-q-x4 HOMO	EGQ-m-q-x4 LUMO
			
EGQ-m-r-x1 HOMO	EGQ-m-r-x1 LUMO	EGQ-m-q-x1 HOMO	EGQ-m-q-x1 LUMO
			
EGQ-p-q-x3 HOMO	EGQ-p-q-x3 LUMO	EGQ-p-r-x3 HOMO	EGQ-p-r-x3 LUMO
			
EGQ-k-q-x4 HOMO	EGQ-k-q-x4 LUMO	EGQ-k-r-x4 HOMO	EGQ-k-r-x4 LUMO

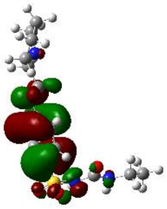
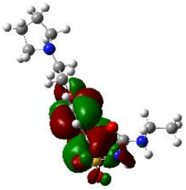
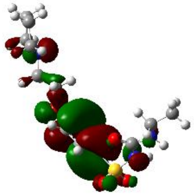
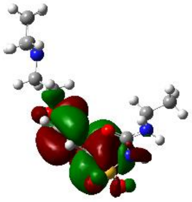
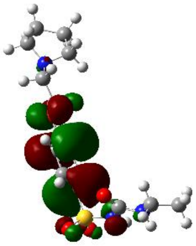
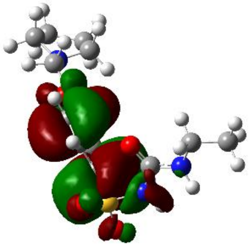
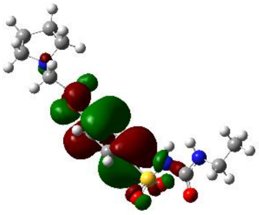
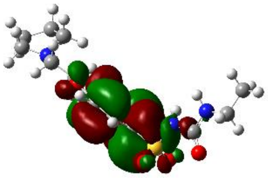
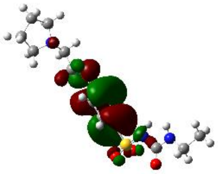
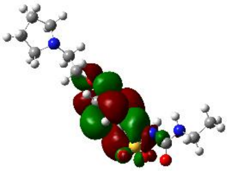
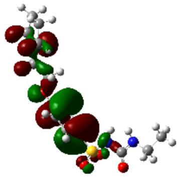
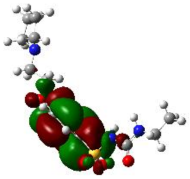
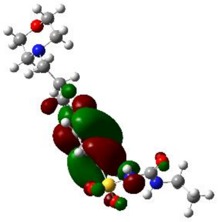
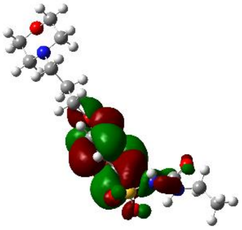
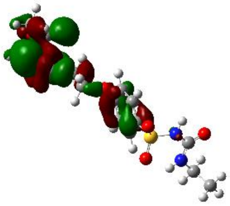
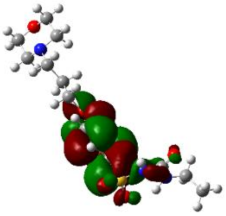
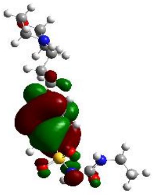
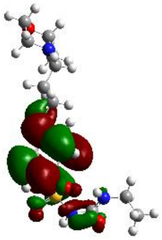
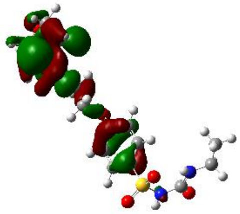
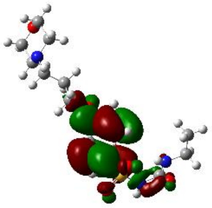
			
EGQ-g-r-x1 HOMO	EGQ-g-r-x1 LUMO	EGQ-g-t-x1 HOMO	EGQ-g-t-x1 LUMO
			
EGQ-g-q-x1 HOMO	EGQ-g-q-x1 LUMO	EGQ-j-q-x3 HOMO	EGQ-j-q-x3 LUMO
			
EGQ-j-r-x3 HOMO	EGQ-j-r-x3 LUMO	EGQ-j-t-x3 HOMO	EGQ-j-t-x3 LUMO

Figure 6.63: Shapes of HOMO and LUMO for the calculated conformers of compound EJP.

			
EJP-m-s-x4 HOMO	EJP-m-s-x4 LUMO	EJP-m-r-x4 HOMO	EJP-m-r-x4 LUMO
			
EJP-m-q-x4 HOMO	EJP-m-q-x4 LUMO	EJP-p-s-x4 HOMO	EJP-p-s-x4 LUMO

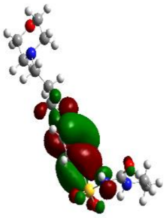
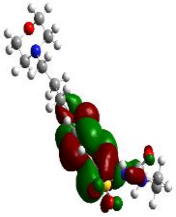
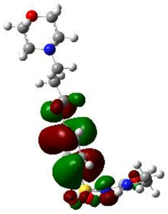
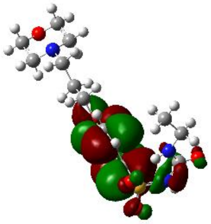
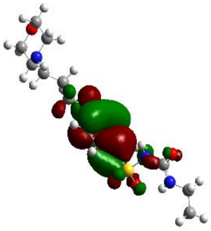
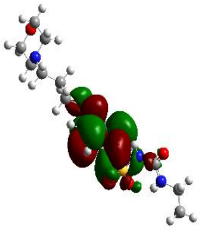
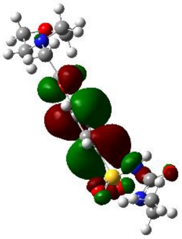
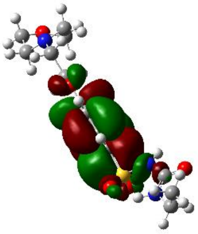
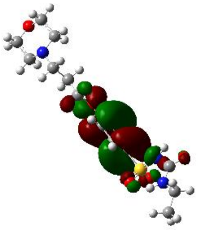
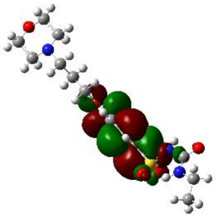
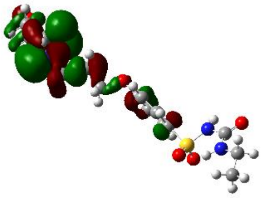
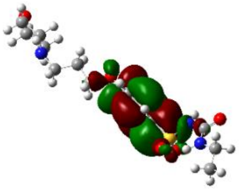
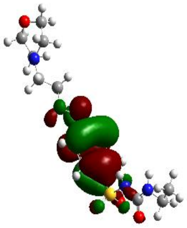
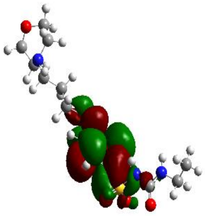
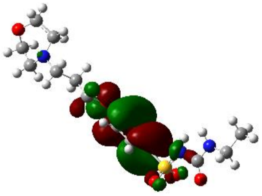
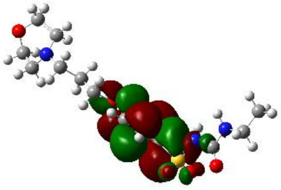
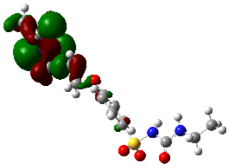
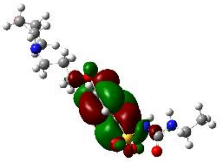
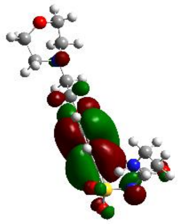
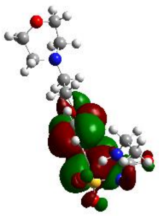
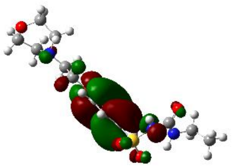
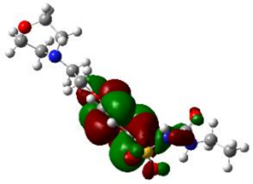
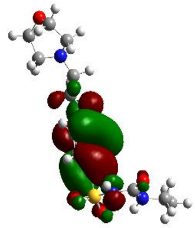
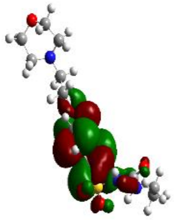
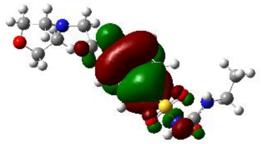
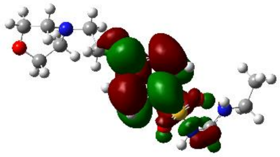
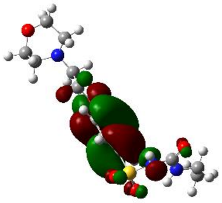
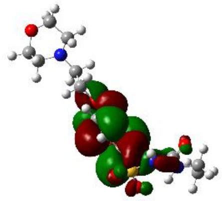
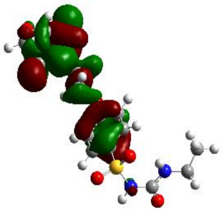
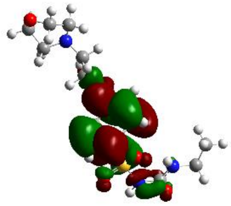
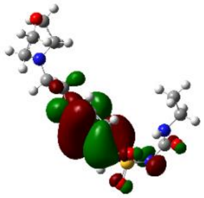
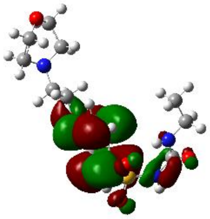
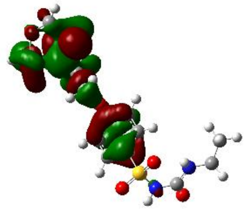
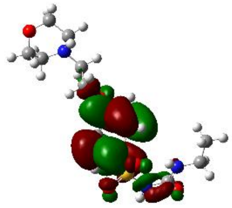
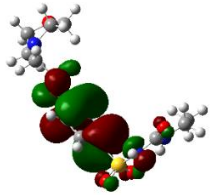
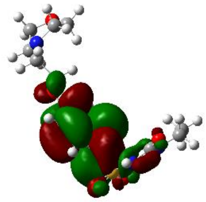
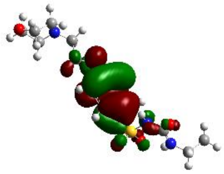
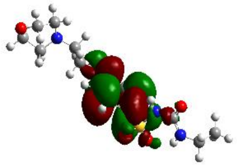
			
EJP-p-q-x4 HOMO	EJP-p-q-x4 LUMO	EJP-p-r-x4 HOMO	EJP-p-r-x4 LUMO
			
EJP-k-q-x1 HOMO	EJP-k-q-x1 LUMO	EJP-k-r-x1 HOMO	EJP-k-r-x1 LUMO
			
EJP-k-r-x1′ HOMO	EJP-k-r-x1′ LUMO	EJP-k-s-x1 HOMO	EJP-k-s-x1 LUMO
			
EJP-j-q-x3 HOMO	EJP-j-q-x3 LUMO	EJP-j-r-x3 HOMO	EJP-j-r-x3 LUMO
			
EJP-j-s-x3 HOMO	EJP-j-s-x3 LUMO		

Figure 6.64: Shapes of HOMO and LUMO for the calculated conformers of compound EJQ.

			
EJQ-m-q-x4 HOMO	EJQ-m-q-x4 LUMO	EJQ-m-r-x4 HOMO	EJQ-m-r-x4 LUMO
			
EJQ-p-q-x4 HOMO	EJQ-p-q-x4 LUMO	EJQ-p-q-x4′ HOMO	EJQ-p-q-x4′ LUMO
			
EJQ-m-r-x1 HOMO	EJQ-m-r-x1 LUMO	EJQ-m-s-x1 HOMO	EJQ-m-s-x1 LUMO
			
EJQ-p-r-x4 HOMO	EJQ-p-r-x4 LUMO	EJQ-p-s-x4 HOMO	EJQ-p-s-x4 LUMO
			
EJQ-m-q-x1 HOMO	EJQ-m-q-x1 LUMO	EJQ-k-q-x4 HOMO	EJQ-k-q-x4 LUMO

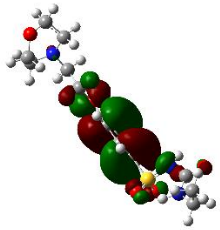
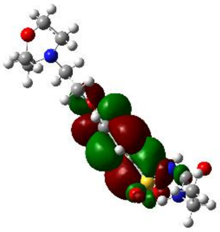
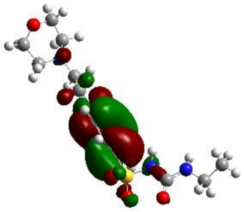
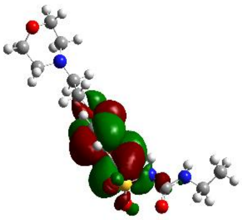
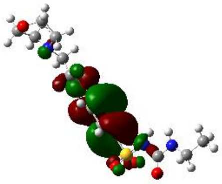
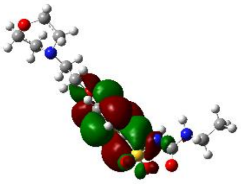
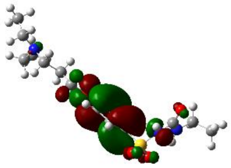
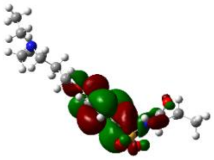
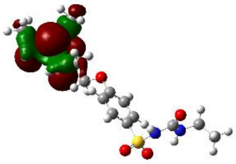
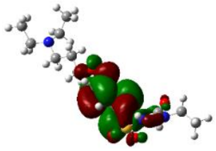
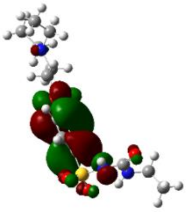
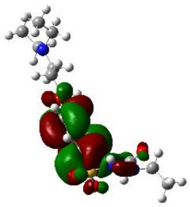
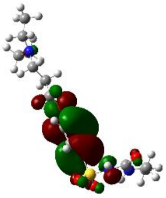
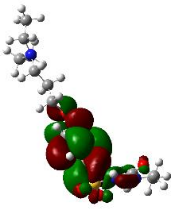
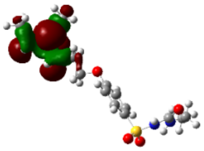
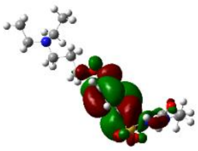
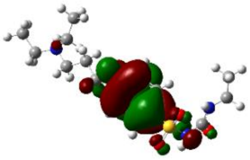
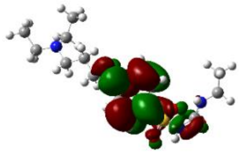
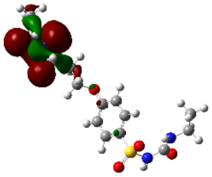
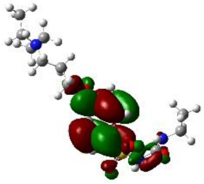
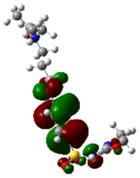
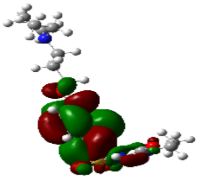
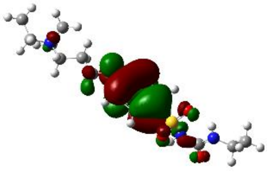
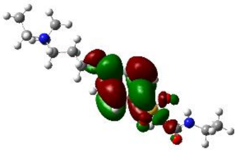
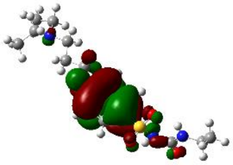
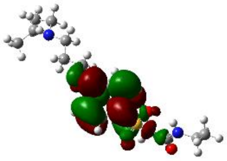
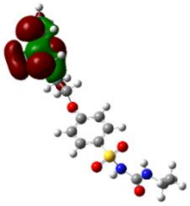
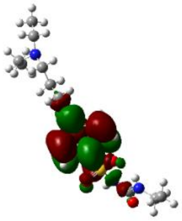
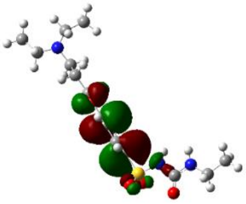
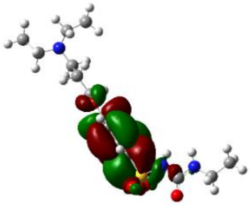
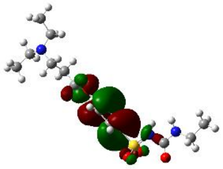
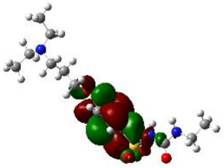
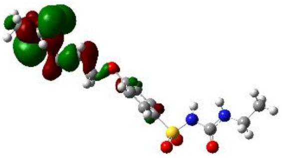
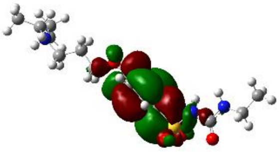
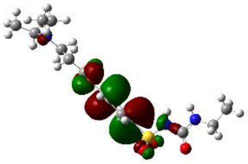
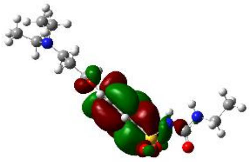
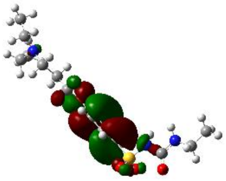
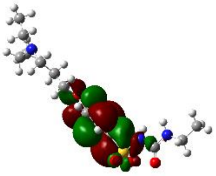
			
EJQ-k-r-x4 HOMO	EJQ-k-r-x4 LUMO	EJQ-j-q-x3 HOMO	EJQ-j-q-x3 LUMO
			
EJQ-j-r-x3 HOMO	EJQ-j-r-x3 LUMO		

Figure 6.65: Shapes of HOMO and LUMO for the calculated conformers of compound ELP.

			
ELP-m-s-x4 HOMO	ELP-m-s-x4 LUMO	ELP-m-q-x4 HOMO	ELP-m-q-x4 LUMO
			
ELP-m-q-x4 HOMO	ELP-m-q-x4 LUMO	ELP-m-r-x1 HOMO	ELP-m-r-x1 LUMO
			

ELP-m-s-x1 HOMO	ELP-m-s-x1 LUMO	ELP-p-s-x4 HOMO	ELP-p-s-x4 LUMO
			
ELP-p-s-x4′ HOMO	ELP-p-s-x4′ LUMO	ELP-m-q-x1 HOMO	ELP-m-q-x1 LUMO
			
ELP-k-q-x1 HOMO	ELP-k-q-x1 LUMO	ELP-k-r-x1 HOMO	ELP-k-r-x1 LUMO
			
ELP-k-s-x1 HOMO	ELP-k-s-x1 LUMO	ELP-j-q-x3 HOMO	ELP-j-q-x3 LUMO
			
ELP-j-r-x3 HOMO	ELP-j-r-x3 LUMO	ELP-j-s-x3 HOMO	ELP-j-s-x3 LUMO
			
ELP-j-q-x3′ HOMO	ELP-j-q-x3′ LUMO	ELP-j-r-x3′ HOMO	ELP-j-r-x3′ LUMO

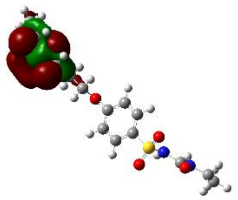
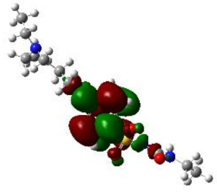
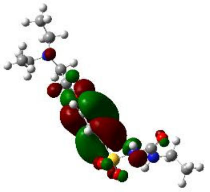
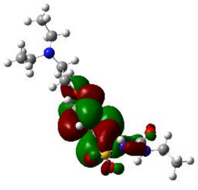
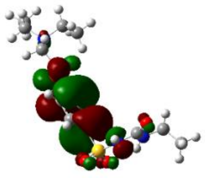
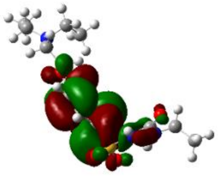
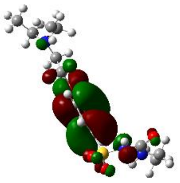
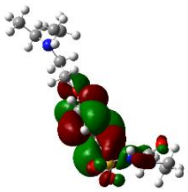
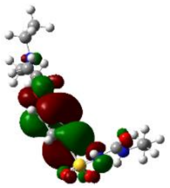
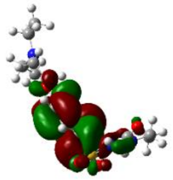
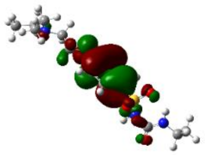
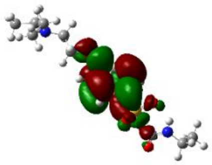
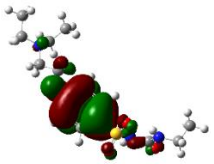
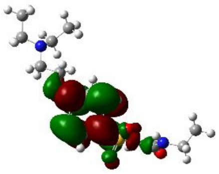
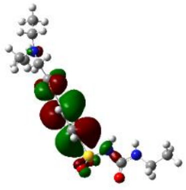
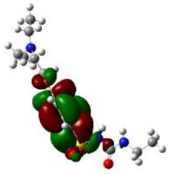
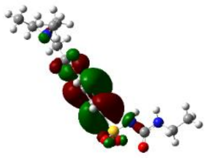
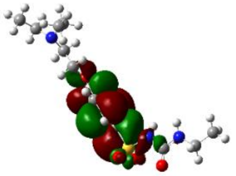
			
ELP-j-s-x3′ HOMO	ELP-j-s-x3′ LUMO		

Figure 6.66: Shapes of HOMO and LUMO for the calculated conformers of compound ELQ.

			
ELQ-m-r-x4 HOMO	ELQ-m-r-x4 LUMO	ELQ-m-q-x4 HOMO	ELQ-m-q-x4 LUMO
			
ELQ-m-r-x1 HOMO	ELQ-m-r-x1 LUMO	ELQ-m-q-x1 HOMO	ELQ-m-q-x1 LUMO
			
ELQ-k-q-x4 HOMO	ELQ-k-q-x4 LUMO	ELQ-k-r-x4 HOMO	ELQ-k-r-x4 LUMO
			
ELQ-j-q-x3 HOMO	ELQ-j-q-x3 LUMO	ELQ-j-r-x3 HOMO	ELQ-j-r-x3 LUMO

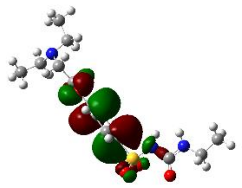
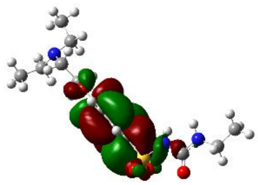
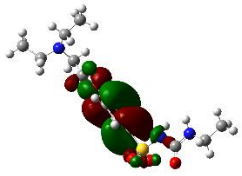
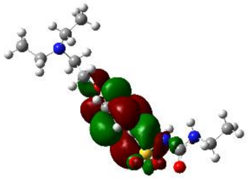
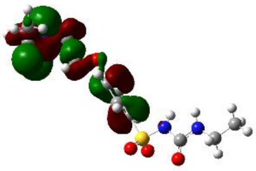
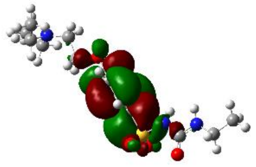
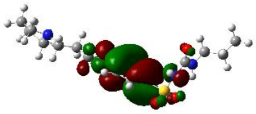
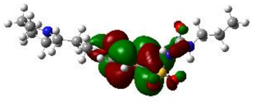
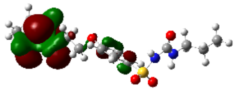
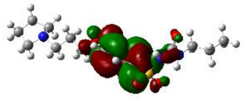
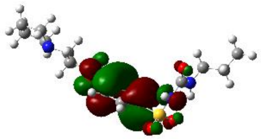
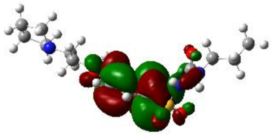
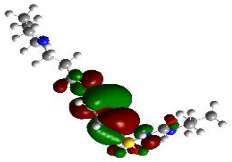
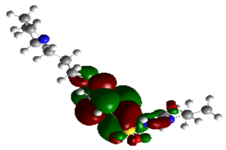
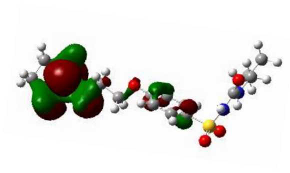
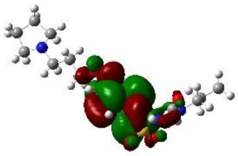
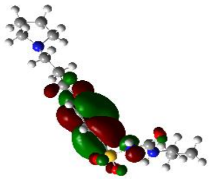
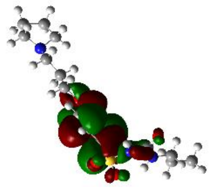
			
ELQ-j-q-x3′ HOMO	ELQ-j-q-x3′ LUMO	ELQ-j-r-x3′ HOMO	ELQ-j-r-x3′ LUMO
			
ELQ-j-s-x3 HOMO	ELQ-j-s-x3 LUMO		

Figure 6.67: Shapes of HOMO and LUMO for the calculated conformers of compound FGP.

			
FGP-m-r-x4 HOMO	FGP-m-r-x4 LUMO	FGP-m-s-x4 HOMO	FGP-m-s-x4 LUMO
			
FGP-m-q-x4 HOMO	FGP-m-q-x4 LUMO	FGP-m-r-x1 HOMO	FGP-m-r-x1 LUMO
			
FGP-m-s-x1 HOMO	FGP-m-s-x1 LUMO	FGP-p-q-x4 HOMO	FGP-p-q-x4 LUMO

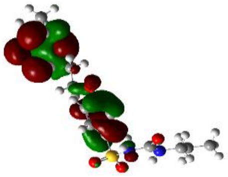
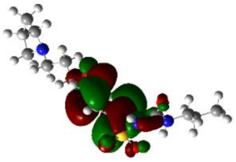
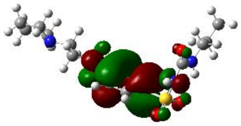
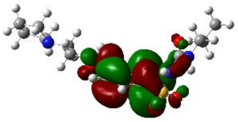
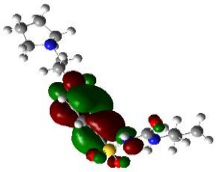
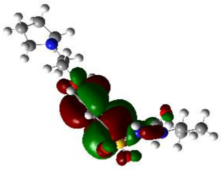
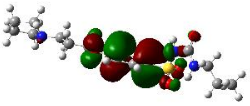
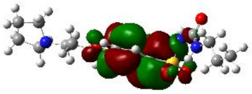
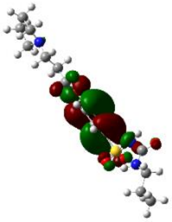
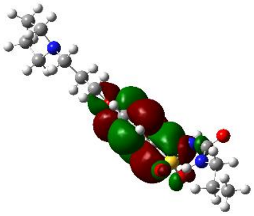
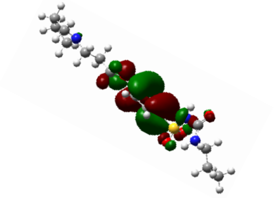
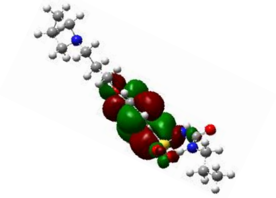
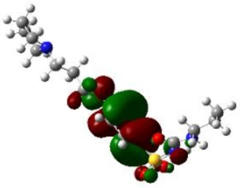
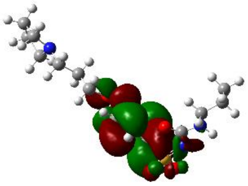
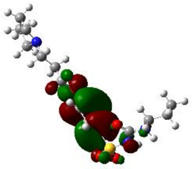
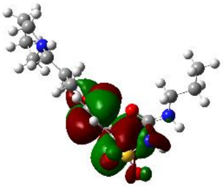
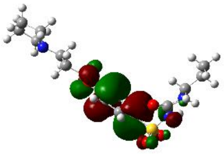
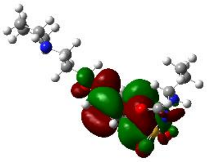
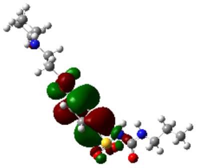
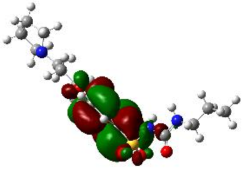
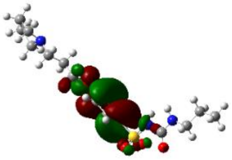
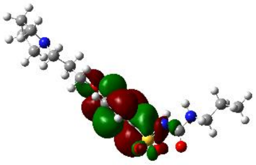
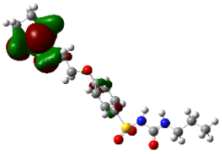
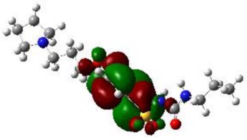
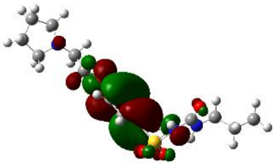
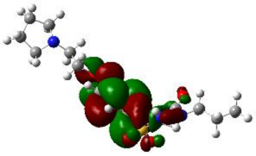
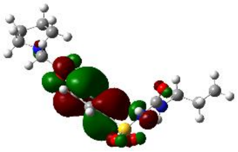
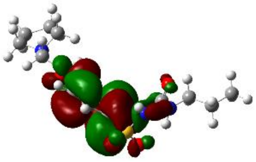
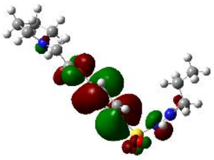
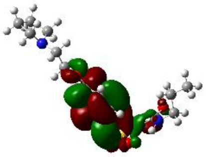
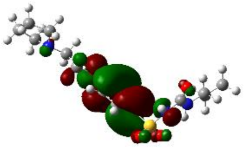
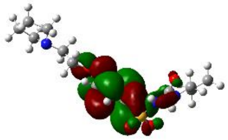
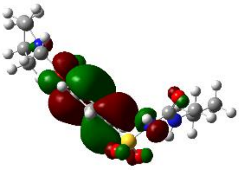
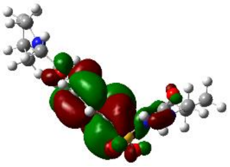
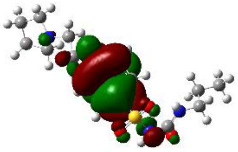
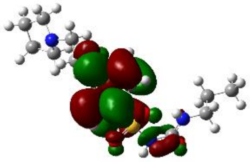
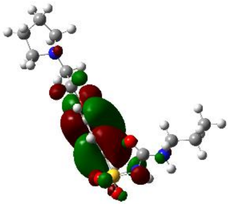
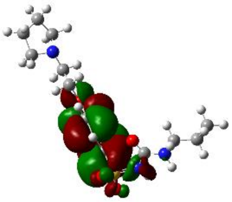
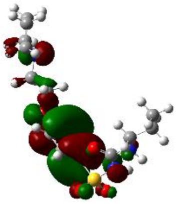
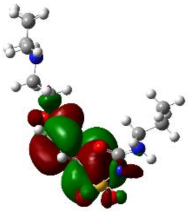
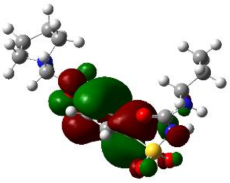
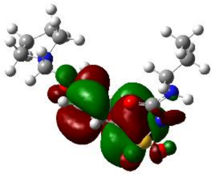
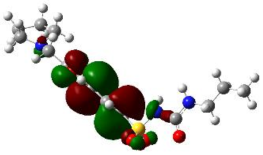
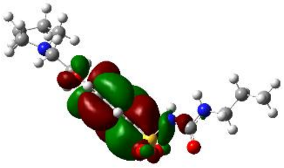
			
FGP-p-s-x4 HOMO	FGP-p-s-x4 LUMO	FGP-m-q-x1 HOMO	FGP-m-q-x1 LUMO
			
FGP-p-r-x4 HOMO	FGP-p-r-x4 LUMO	FGP-k-q-x1 HOMO	FGP-k-q-x1 LUMO
			
FGP-k-r-x1 HOMO	FGP-k-r-x1 LUMO	FGP-k-r-x1 HOMO	FGP-k-r-x1 LUMO
			
FGP-g-r-x1 HOMO	FGP-g-r-x1 LUMO	FGP-g-r-x1′ HOMO	FGP-g-r-x1′ LUMO
			
FGP-g-q-x1 HOMO	FGP-g-q-x1 LUMO	FGP-j-q-x3 HOMO	FGP-j-q-x3 LUMO
			
FGP-j-r-x3 HOMO	FGP-j-r-x3 LUMO	FGP-j-s-x3 HOMO	FGP-j-s-x3 LUMO

Figure 6.68: Shapes of HOMO and LUMO for the calculated conformers of compound FGQ.

			
FGQ-m-r-x4 HOMO	FGQ-m-r-x4 LUMO	FGQ-m-q-x4 HOMO	FGQ-m-q-x4 LUMO
			
FGQ-p-q-x4 HOMO	FGQ-p-q-x4 LUMO	FGQ-m-r-x1 HOMO	FGQ-m-r-x1 LUMO
			
FGQ-m-q-x1 HOMO	FGQ-m-q-x1 LUMO	FGQ-k-r-x4 HOMO	FGQ-k-r-x4 LUMO
			
FGQ-g-r-x1 HOMO	FGQ-g-r-x1 LUMO	FGQ-g-t-x1 HOMO	FGQ-g-t-x1 LUMO
			
FGQ-g-q-x1 HOMO	FGQ-g-q-x1 LUMO	FGQ-j-q-x3 HOMO	FGQ-j-q-x3 LUMO

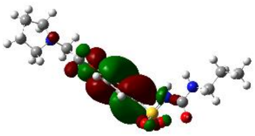
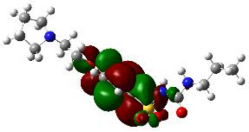
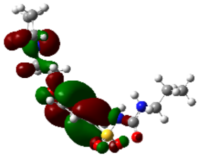
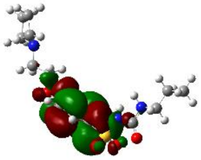
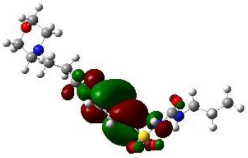
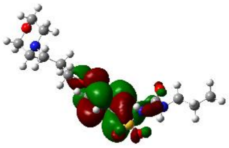
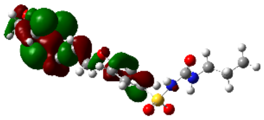
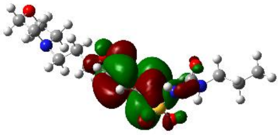
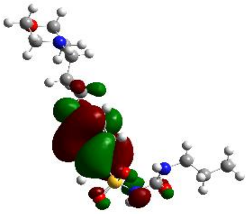
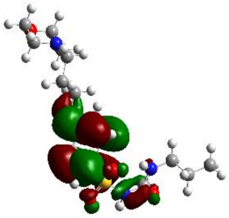
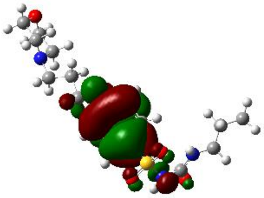
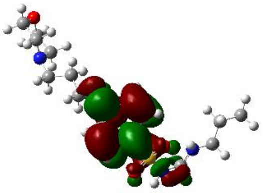
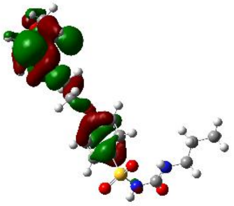
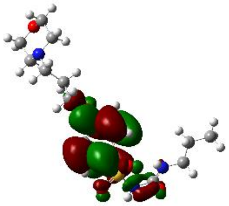
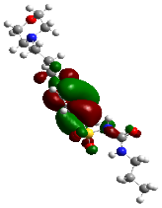
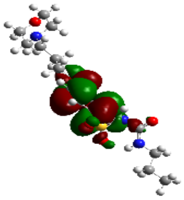
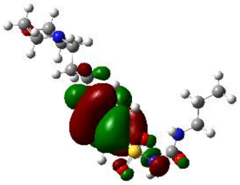
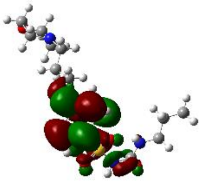
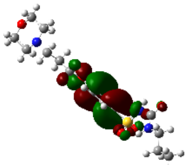
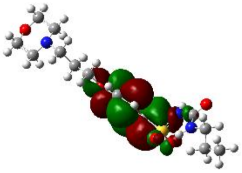
			
FGQ-j-r-x3 HOMO	FGQ-j-r-x3 LUMO	FGQ-j-t-x3 HOMO	FGQ-j-t-x3 LUMO

Figure 6.69: Shapes of HOMO and LUMO for the calculated conformers of compound FJP.

			
FJP-m-r-x4 HOMO	FJP-m-r-x4 LUMO	FJP-m-s-x4 HOMO	FJP-m-s-x4 LUMO
			
FJP-m-q-x4 HOMO	FJP-m-q-x4 LUMO	FJP-p-q-x4 HOMO	FJP-p-q-x4 LUMO
			
FJP-p-s-x4 HOMO	FJP-p-s-x4 LUMO	FJP-k-q-x1 HOMO	FJP-k-q-x1 LUMO
			
FJP-p-r-x1 HOMO	FJP-p-r-x1 LUMO	FJP-k-r-x1 HOMO	FJP-k-r-x1 LUMO

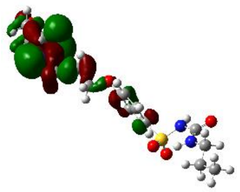
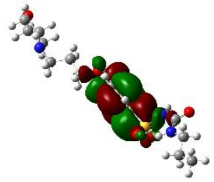
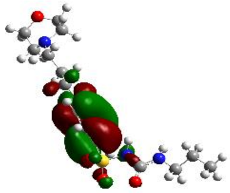
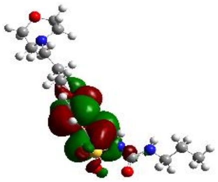
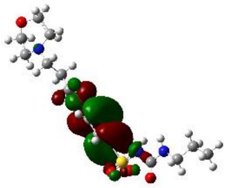
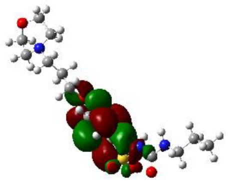
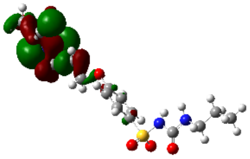
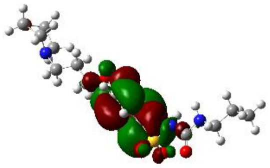
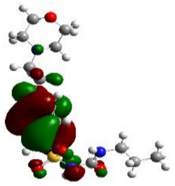
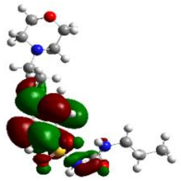
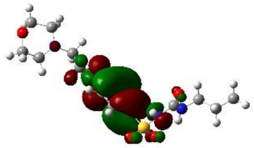
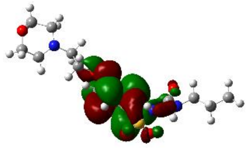
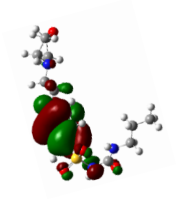
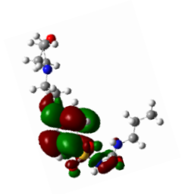
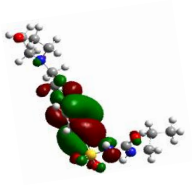
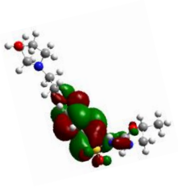
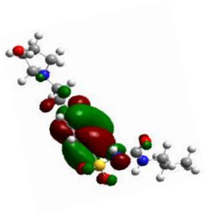
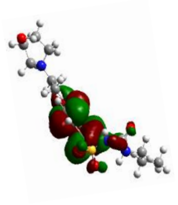
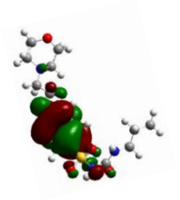
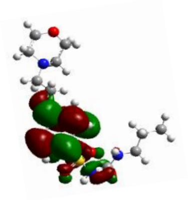
			
FJP-k-s-x1 HOMO	FJP-k-s-x1 LUMO	FJP-j-q-x3 HOMO	FJP-j-q-x3 LUMO
			
FJP-j-r-x3 HOMO	FJP-j-r-x3 LUMO	FJP-j-s-x3 HOMO	FJP-j-s-x3 LUMO

Figure 6.70: Shapes of HOMO and LUMO for the calculated conformers of compound FJQ.

			
FJQ-m-q-x4 HOMO	FJQ-m-q-x4 LUMO	FJQ-m-r-x4 HOMO	FJQ-m-r-x4 LUMO
			
FJQ-p-r-x4 HOMO	FJQ-p-r-x4 LUMO	FJQ-p-q-x4 HOMO	FJQ-p-q-x4 LUMO
			
FJQ-p-q-x4′ HOMO	FJQ-p-q-x4′ LUMO	FJQ-m-q-x1 HOMO	FJQ-m-q-x1 LUMO

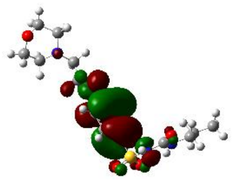
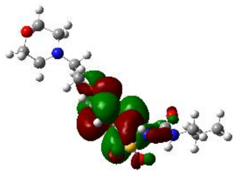
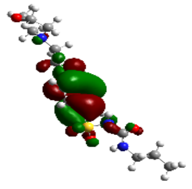
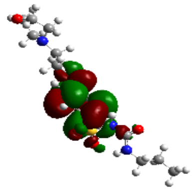
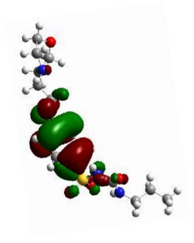
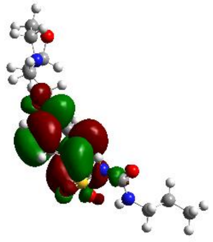
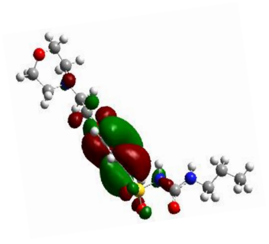
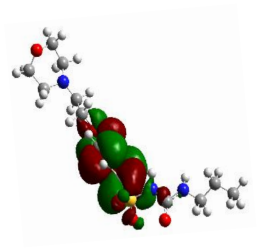
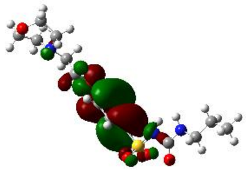
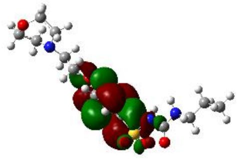
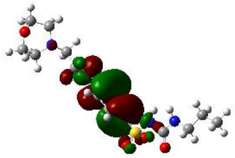
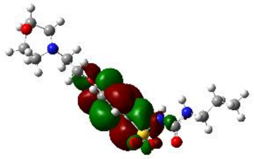
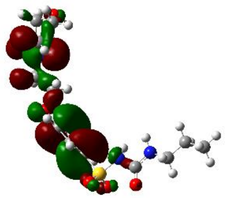
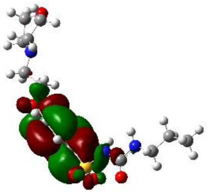
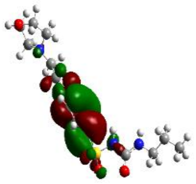
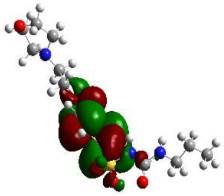
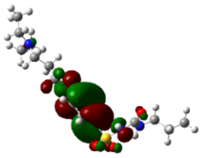
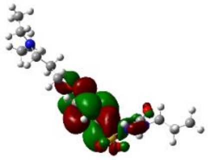
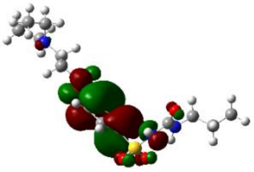
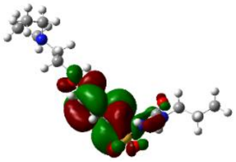
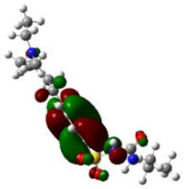
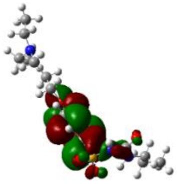
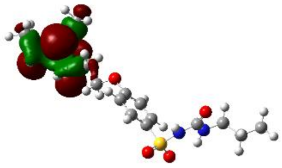
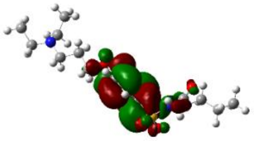
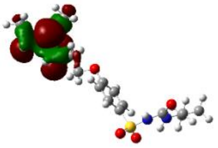
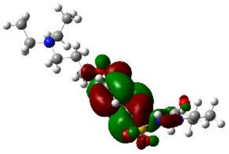
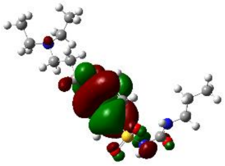
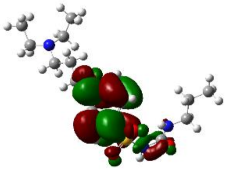
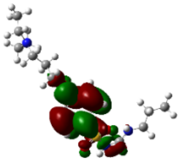
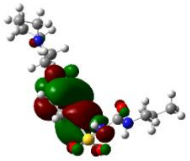
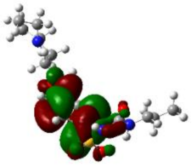
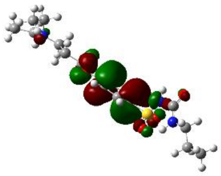
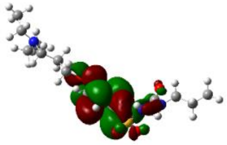
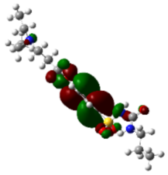
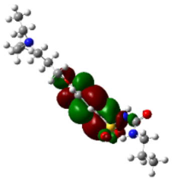
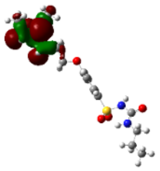
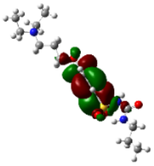
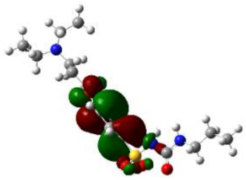
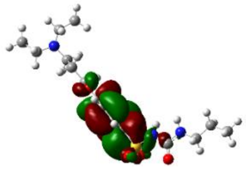
			
FJQ-m-r-x1 HOMO	FJQ-m-r-x1 LUMO	FJQ-k-q-x4 HOMO	FJQ-k-q-x4 LUMO
			
FJQ-k-r-x4 HOMO	FJQ-k-r-x4 LUMO	FJQ-j-q-x3 HOMO	FJQ-j-q-x3 LUMO
			
FJQ-j-r-x3 HOMO	FJQ-j-r-x3 LUMO	FJQ-j-r-x3′ HOMO	FJQ-j-r-x3′ LUMO
			
FJQ-j-t-x3 HOMO	FJQ-j-t-x3 LUMO	FJQ-j-q-x3′ HOMO	FJQ-j-q-x3′ LUMO

Figure 6.71: Shapes of HOMO and LUMO for the calculated conformers of compound FLP.

			
FLP-m-r-x4 HOMO	FLP-m-r-x4 LUMO	FLP-m-q-x4 HOMO	FLP-m-q-x4 LUMO
			
FLP-m-r-x1 HOMO	FLP-m-r-x1 LUMO	FLP-m-s-x4 HOMO	FLP-m-s-x4 LUMO
			
FLP-m-s-x1 HOMO	FLP-m-s-x1 LUMO	FLP-p-q-x4 HOMO	FLP-p-q-x4 LUMO
			
FLP-p-s-x4 HOMO	FLP-p-s-x4 LUMO	FLP-m-q-x1 HOMO	FLP-m-q-x1 LUMO
			
FLP-k-q-x1 HOMO	FLP-k-q-x1 LUMO	FLP-k-r-x1 HOMO	FLP-k-r-x1 LUMO
			
FLP-k-s-x1 HOMO	FLP-k-s-x1 LUMO	FLP-j-q-x3 HOMO	FLP-j-q-x3 LUMO

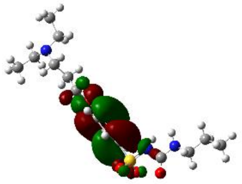
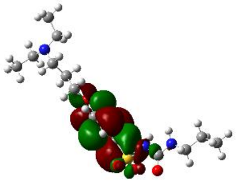
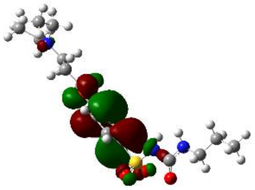
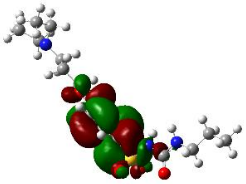
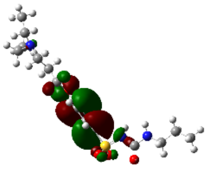
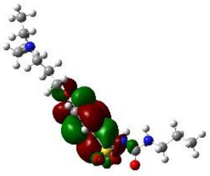
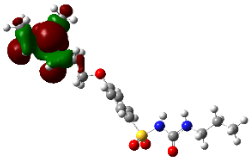
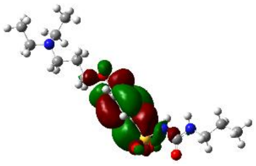
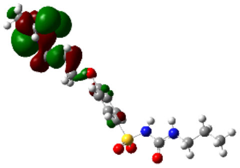
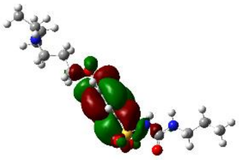
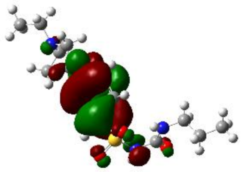
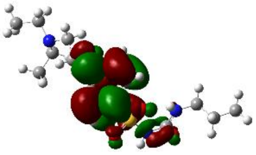
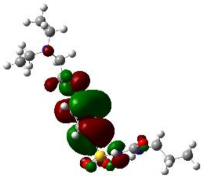
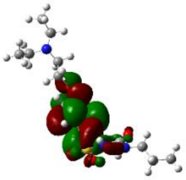
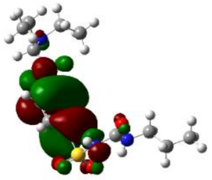
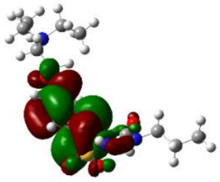
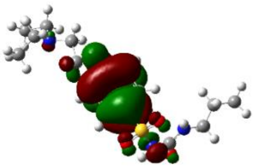
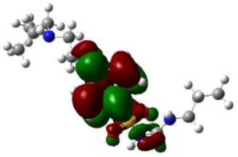
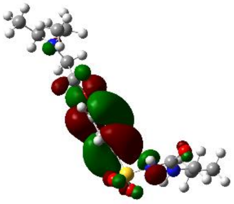
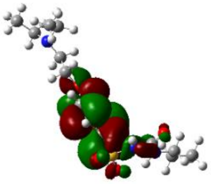
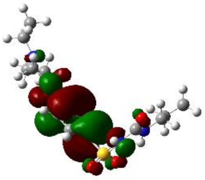
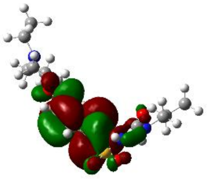
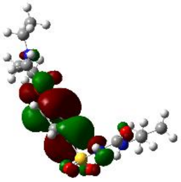
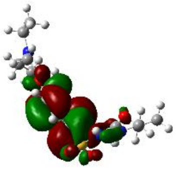
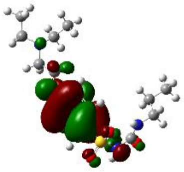
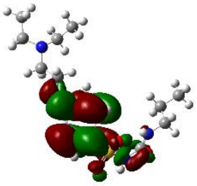
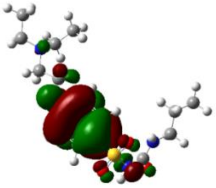
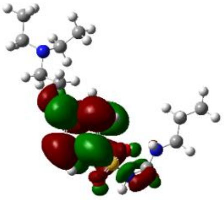
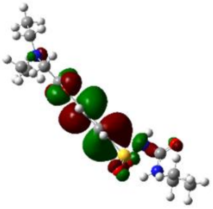
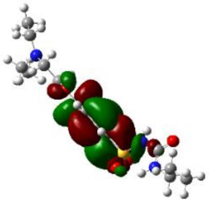
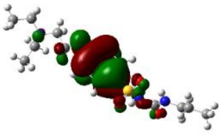
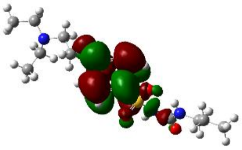
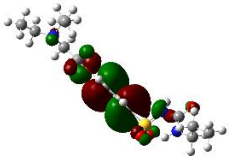
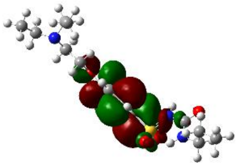
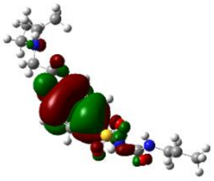
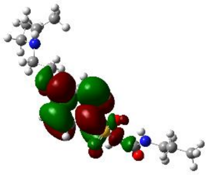
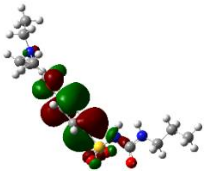
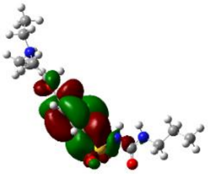
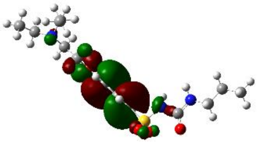
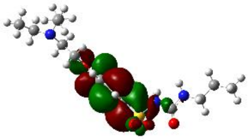
			
FLP-j-r-x3 HOMO	FLP-j-r-x3 LUMO	FLP-j-s-x3′ HOMO	FLP-j-s-x3′ LUMO
			
FLP-j-q-x3′ HOMO	FLP-j-q-x3′ LUMO	FLP-j-r-x3′ HOMO	FLP-j-r-x3′ LUMO
			
FLP-j-s-x3 HOMO	FLP-j-s-x3 LUMO		

Figure 6.72: Shapes of HOMO and LUMO for the calculated conformers of compound FLQ.

			
FLQ-p-q-x2 HOMO	FLQ-p-q-x2 LUMO	FLQ-m-r-x4 HOMO	FLQ-m-r-x4 LUMO
			
FLQ-m-q-x4 HOMO	FLQ-m-q-x4 LUMO	FLQ-p-q-x4 HOMO	FLQ-p-q-x4 LUMO

			
FLQ-m-r-x1 HOMO	FLQ-m-r-x1 LUMO	FLQ-m-q-x1 HOMO	FLQ-m-q-x1 LUMO
			
FLQ-m-q-x1′ HOMO	FLQ-m-q-x1′ LUMO	FLQ-p-r-x4 HOMO	FLQ-p-r-x4 LUMO
			
FLQ-p-r-x4′ HOMO	FLQ-p-r-x4′ LUMO	FLQ-k-q-x4 HOMO	FLQ-k-q-x4 LUMO
			
FLQ-k-q-x1 HOMO	FLQ-k-q-x1 LUMO	FLQ-k-r-x4 HOMO	FLQ-k-r-x4 LUMO
			
FLQ-k-r-x1 HOMO	FLQ-k-r-x1 LUMO	FLQ-j-q-x3 HOMO	FLQ-j-q-x3 LUMO
			
FLQ-j-r-x3 HOMO	FLQ-j-r-x3 LUMO		

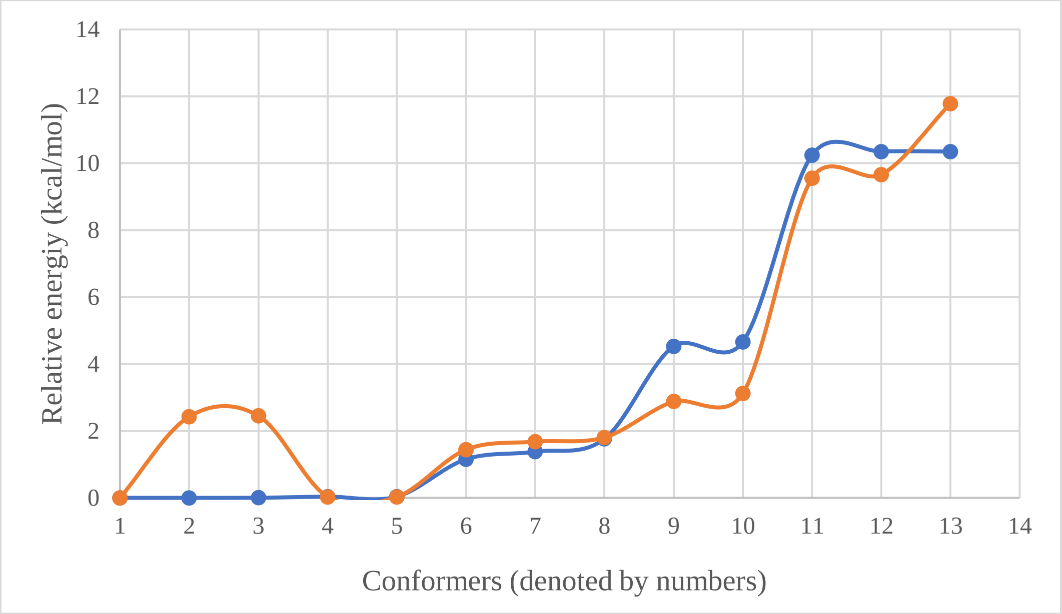
6.3. Figures presenting comparative diagrams for the energy values.

This section presents comparative diagrams of the relative energies of the conformers for each of the compounds considered. The conformers are denoted by numbers along the x-axis, for space reasons; each diagram has an associated table indicating the number (#) representing the individual conformers. All the conformers are listed in order of DFT relative energy. In some of the diagrams, straight line-segments are used instead of curves for clarity reasons and to prevent the curves from extending to the negative section.

6.3.1. Diagrams comparing the HF and DFT relative energies of the calculated conformers of each of the compounds considered.

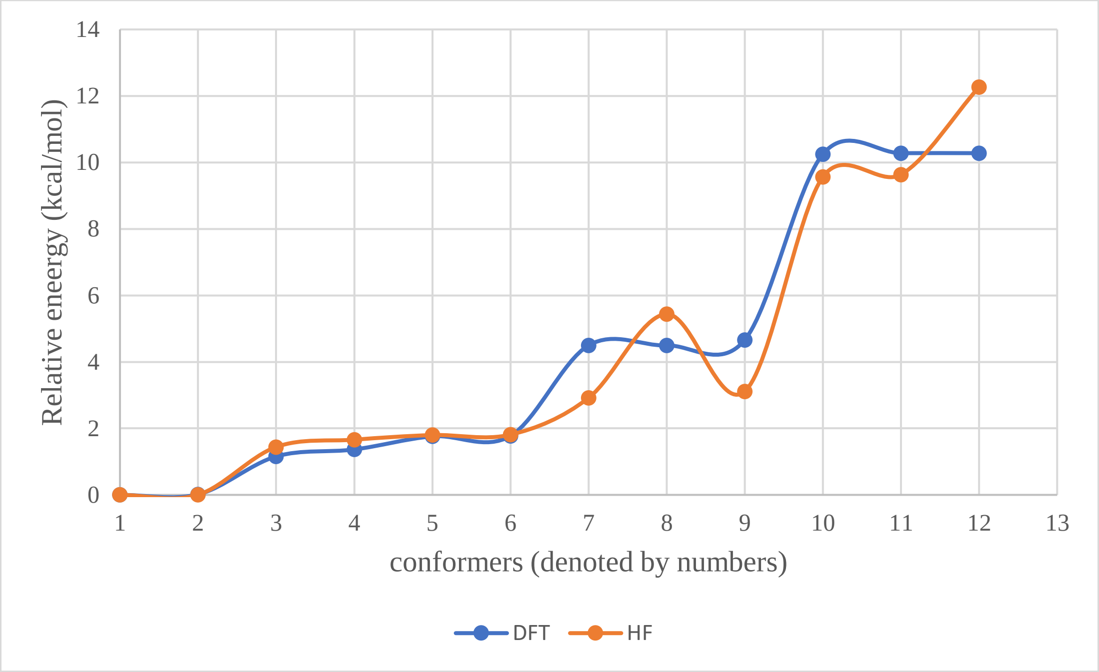
This section presents the diagrams comparing the HF and DFT relative energies of the calculated conformers of each of the compounds considered. The HF and DFT series are represented by different colors: blue for DFT and orange for HF.

Figure 6.73. Diagrams comparing the DFT (—●—) and HF (—●—) relative energies of the calculated conformers of compound AGP.



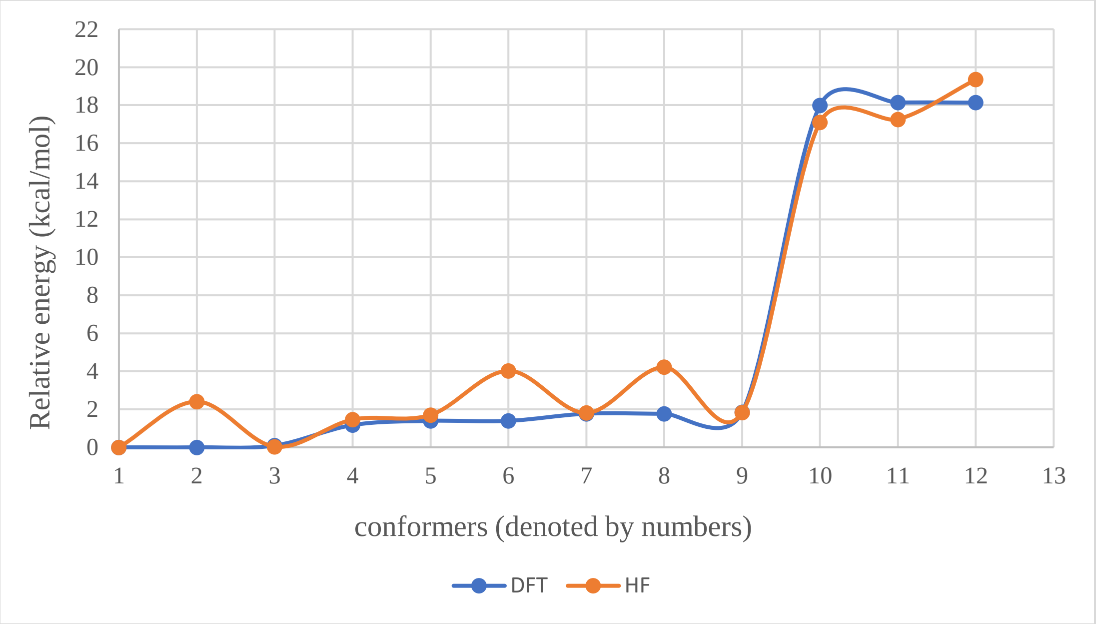
conformers	#	Conformers	#	Conformers	#	Conformers	#
AGP-m-r-u1	1	AGP-p-r-u3	5	AGP-g-r-u3	9	AGP-j-s-u3	13
AGP-m-s-u1	2	AGP-k-q-u1	6	AGP-g-q-u3	10		
AGP-p-t-u3	3	AGP-k-r-u1	7	AGP-j-q-u3	11		
AGP-m-q-u1	4	AGP-m-r-u2	8	AGP-j-r-u3	12		

Figure 6.74. Diagrams comparing the DFT (—●—) and HF (—●—) relative energies of the calculated conformers of compound AGQ.



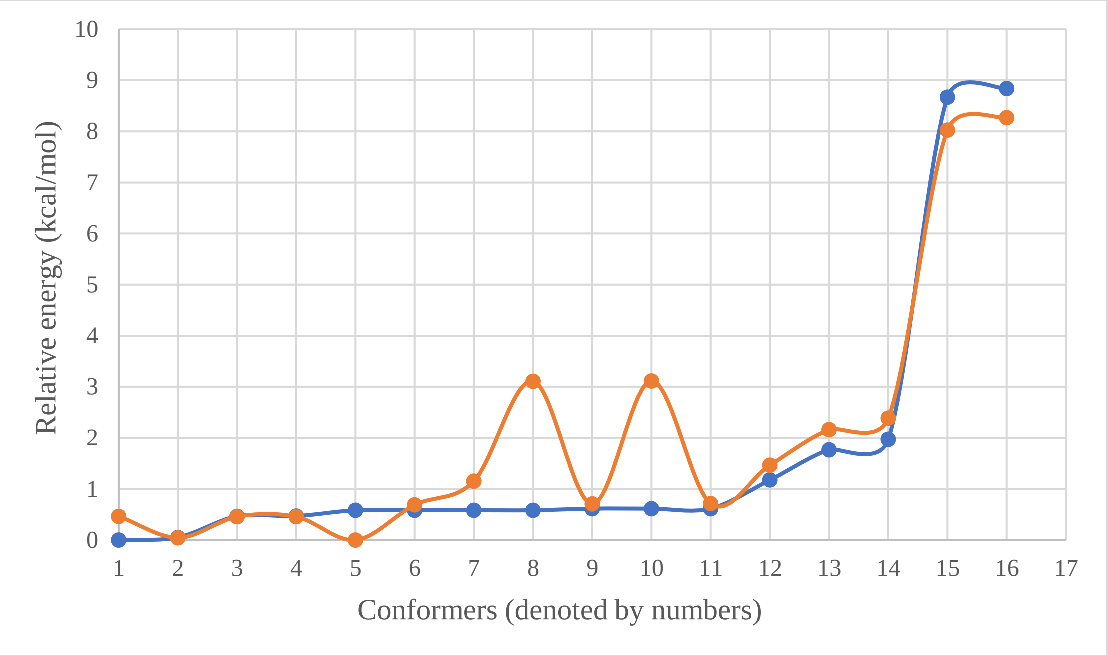
conformer	#	Conformers	#	Conformers	#	Conformers	#
AGQ-m-r-u1	1	AGQ-k-r-u1	4	AGQ-g-r-u3	7	AGQ-j-q-u3	10
AGQ-m-q-u1	2	AGQ-m-r-u2	5	AGQ-g-t-u3	8	AGQ-j-r-u3	11
AGQ-k-q-u1	3	AGQ-m-q-u2	6	AGQ-g-q-u3	9	AGQ-j-t-u3	12

Figure 6.75. Diagrams comparing the DFT (—●—) and HF (—●—) relative energies of the calculated conformers of compound AJP.



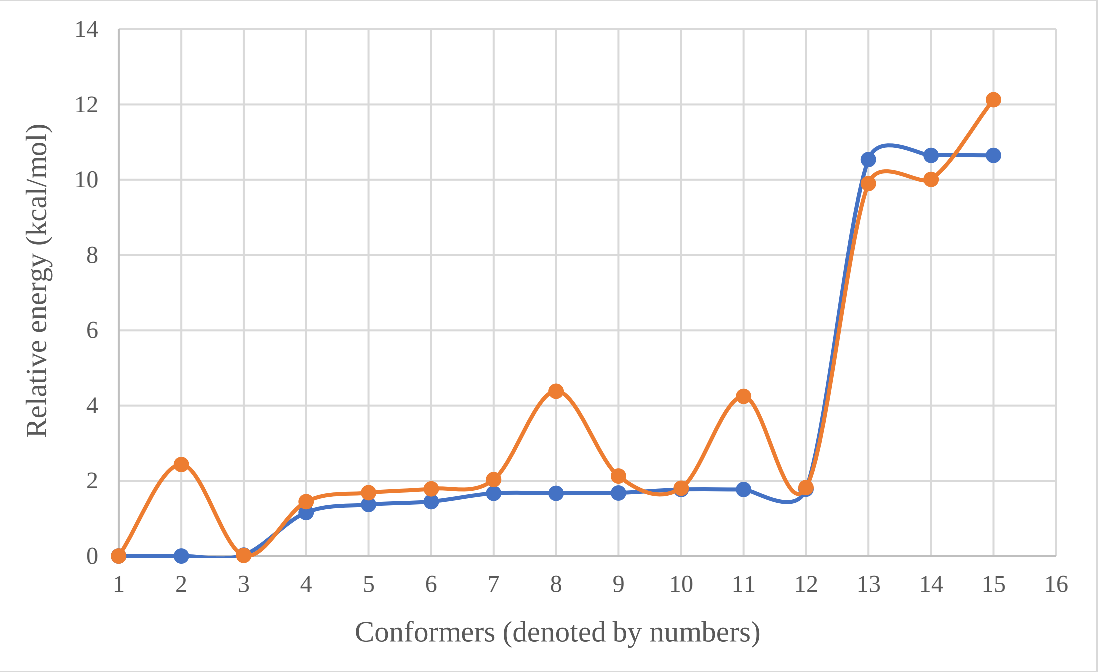
conformer	#	Conformers	#	Conformers	#	Conformers	#
AJP-m-r-u1	1	AJP-k-q-u1	4	AJP-m-r-u2	7	AJP-j-q-u3	10
AJP-m-s-u1	2	AJP-k-r-u1	5	AJP-m-s-u2	8	AJP-j-r-u3	11
AJP-m-q-u1	3	AJP-k-s-u1	6	AJP-m-q-u2	9	AJP-j-s-u3	12

Figure 6.73. Diagrams comparing the DFT (—●—) and HF (—●—) relative energies of the calculated conformers of compound AGP



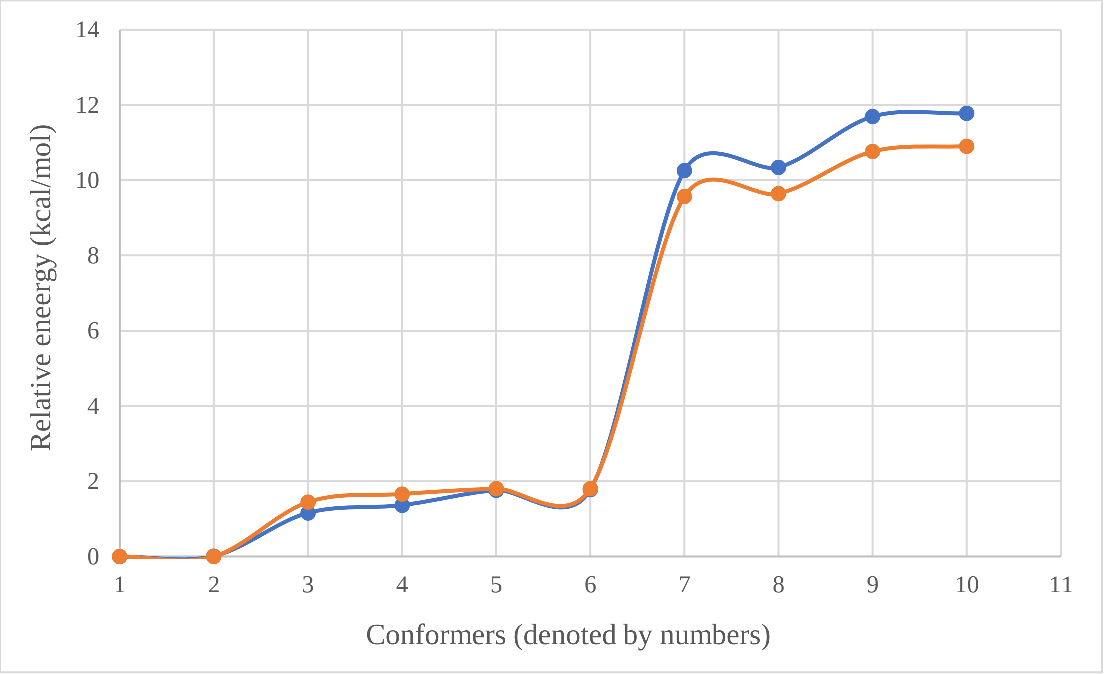
conformer	#	Conformers	#	Conformers	#	Conformers	#
AJQ-p-q-u5	1	AJQ-p-q-u3	5	AJQ-p-r-u3	9	AJQ-k-q-u1′	13
AJQ-m-q-u1	2	AJQ-m-r-u1	6	AJQ-p-s-u3	10	AJQ-k-r-u1	14
AJQ-m-q-u2	3	AJQ-p-q-u5	7	AJQ-m-q-u1	11	AJQ-j-q-u1	15
AJQ-m-r-u2	4	AJQ-m-s-u1	8	AJQ-k-q-u1	12	AJQ-j-r-u1	16

Figure 6.77. Diagrams comparing the DFT (—●—) and HF (—●—) relative energies of the calculated conformers of compound ALP.



conformer	#	Conformers	#	Conformers	#	Conformers	#
ALP-m-r-u1	1	ALP-k-r-u1	5	ALP-k-r-u3	9	ALP-j-q-u3	13
ALP-m-s-u1	2	ALP-k-q-u1′	6	ALP-m-r-u2	10	ALP-j-r-u3	14
ALP-m-q-u1	3	ALP-k-r-u1′	7	ALP-m-s-u2	11	ALP-j-s-u3	15
ALP-k-q-u1	4	ALP-k-s-u1	8	ALP-m-q-u2	12		

Figure 6.78. Diagrams comparing the DFT (—●—) and HF (—●—) relative energies of the calculated conformers of compound ALQ.

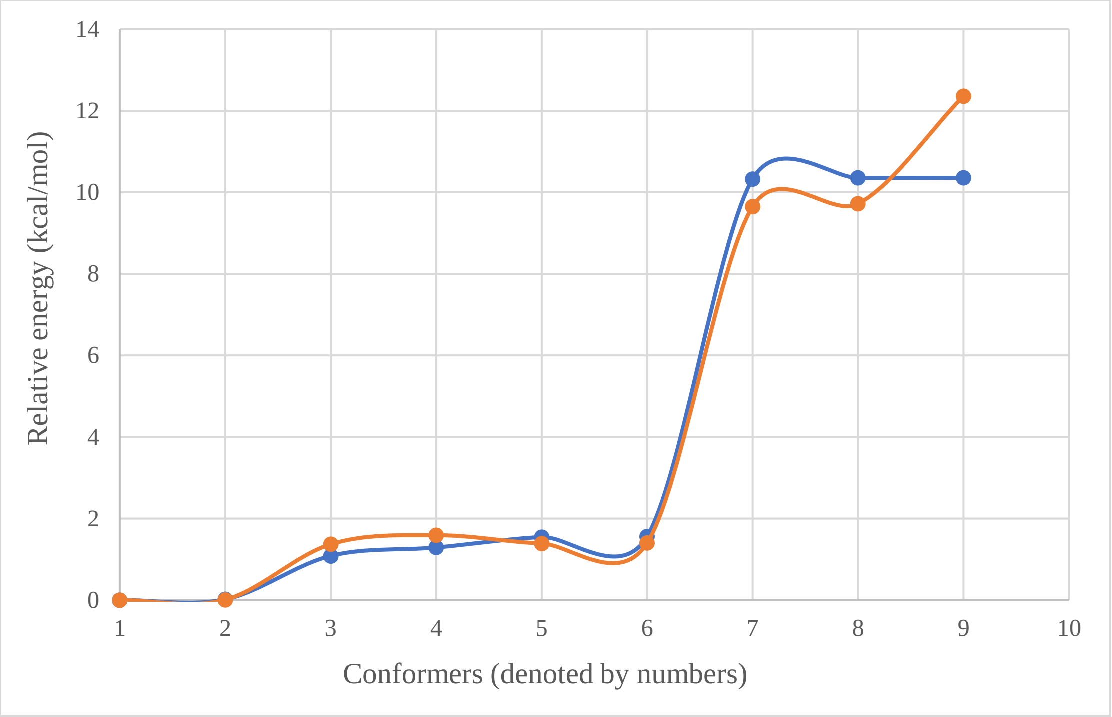


conformer	#	Conformers	#	Conformers	#	Conformers	#
ALQ-m-r-u1	1	ALQ-k-r-u1	4	ALQ-j-q-u3	7	ALQ-j-q-u3	9
ALQ-m-q-u1	2	ALQ-m-r-u2	5	ALQ-j-r-u3	8	ALQ-j-r-u3	10
ALQ-k-q-u1	3	ALQ-m-q-u2	6				

Figure 6.79. Diagrams comparing the DFT (—●—) and HF (—●—) relative energies of the calculated conformers of compound BGP.

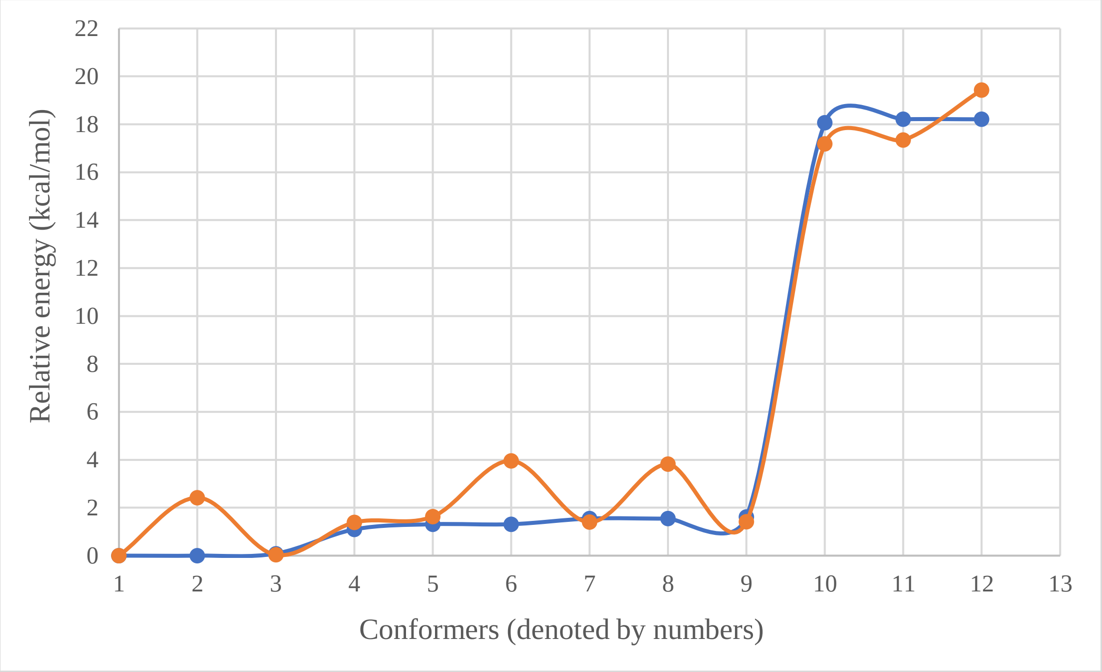
conformer	#	Conformers	#	Conformers	#	Conformers	#
BGP-p-s-v3	1	BGP-m-q-v1	5	BGP-m-r-v2	9	BGP-g-q-v1	13
BGP-p-t-v3	2	BGP-k-q-v3	6	BGP-m-s-v2	10	BGP-j-q-v5	14
BGP-m-r-v1	3	BGP-k-r-v3	7	BGP-m-q-v2	11	BGP-j-r-v5	15
BGP-m-s-v1	4	BGP-k-s-v3	8	BGP-g-r-v1	12	BGP-j-s-v5	16

Figure 6.80. Diagrams comparing the DFT (—●—) and HF (—●—) relative energies of the calculated conformers of compound BGQ.



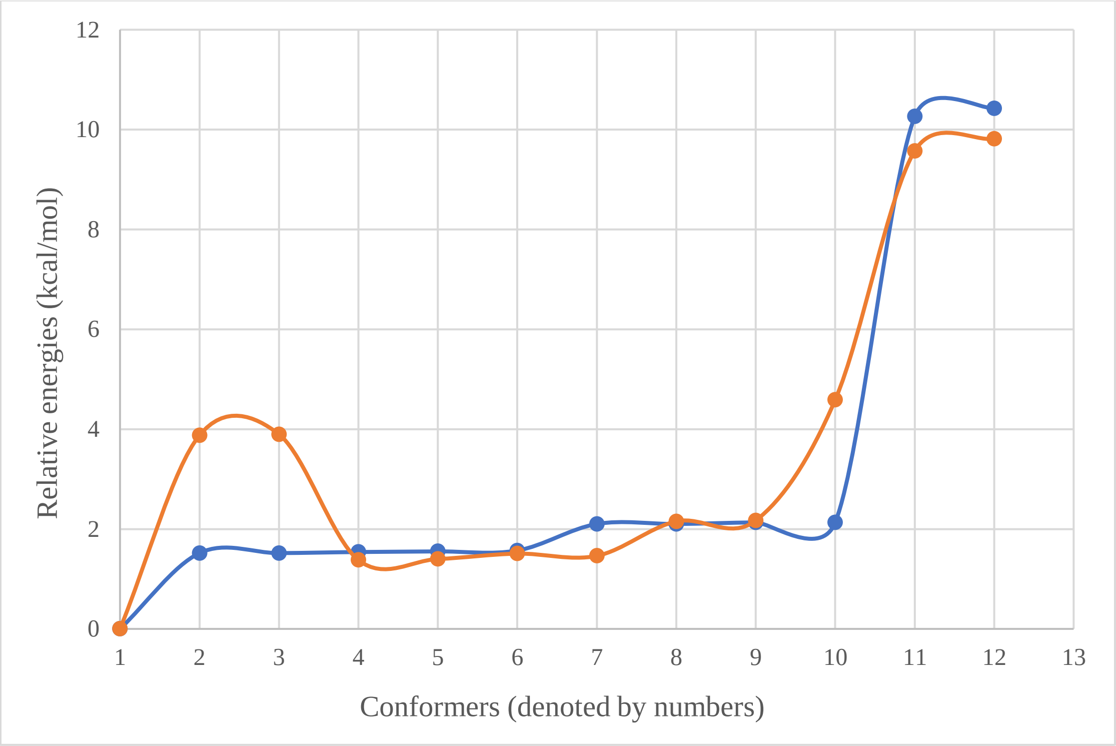
conformer	#	Conformers	#	Conformers	#	Conformers	#
BGQ-m-r-v1	1	BGQ-k-r-v1	4	BGQ-j-q-v3	7	BGQ-j-t-v3	9
BGQ-m-q-v1	2	BGQ-m-r-v2	5	BGQ-j-r-v3	8		
BGQ-k-q-v1	3	BGQ-m-q-v2	6				

Figure 6.81. Diagrams comparing the DFT (—●—) and HF (—●—) relative energies of the calculated conformers of compound BJP.



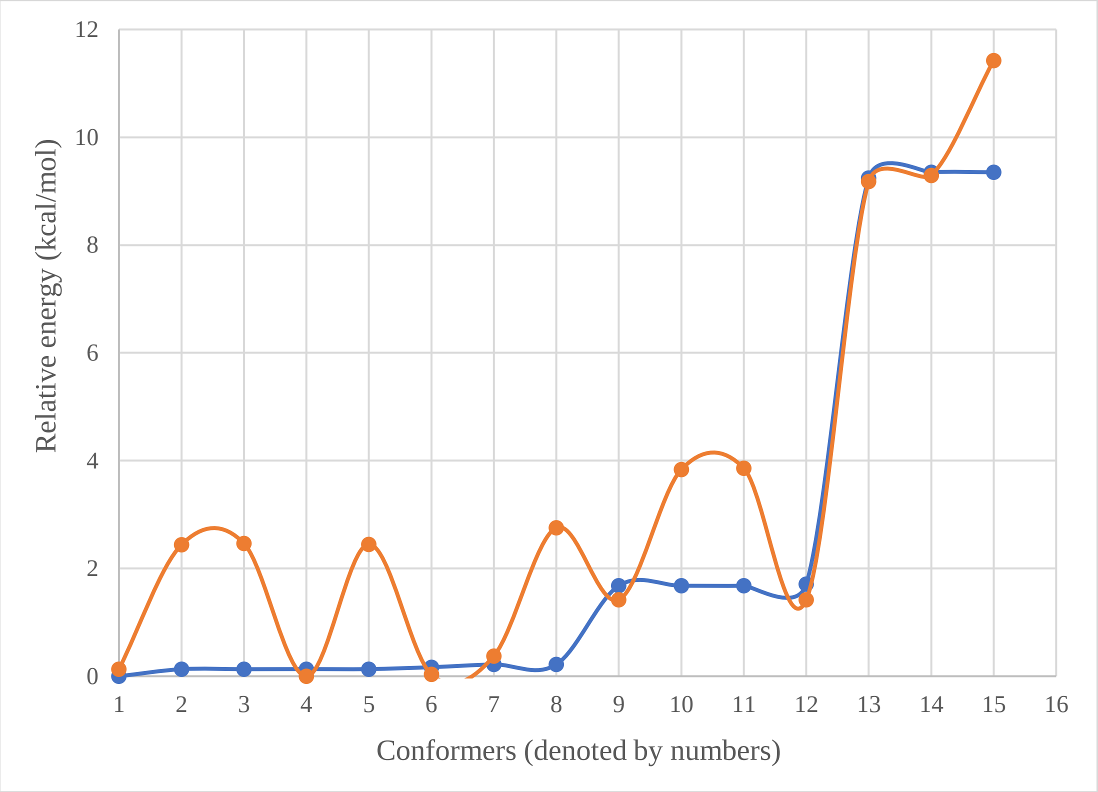
conformer	#	Conformers	#	Conformers	#	Conformers	#
BJP-p-q-v3	1	BJP-k-q-v1	4	BJP-m-r-v2	7	BJP-j-r-v3	10
BJP-p-s-v3	2	BJP-k-r-v1	5	BJP-m-s-v2	8	BJP-j-s-v3	11
BJP-p-r-v3	3	BJP-k-s-v1	6	BJP-m-q-v2	9	BJP-j-q-v3	12

Figure 6.82. Diagrams comparing the DFT (—●—) and HF (—●—) relative energies of the calculated conformers of compound BJQ.



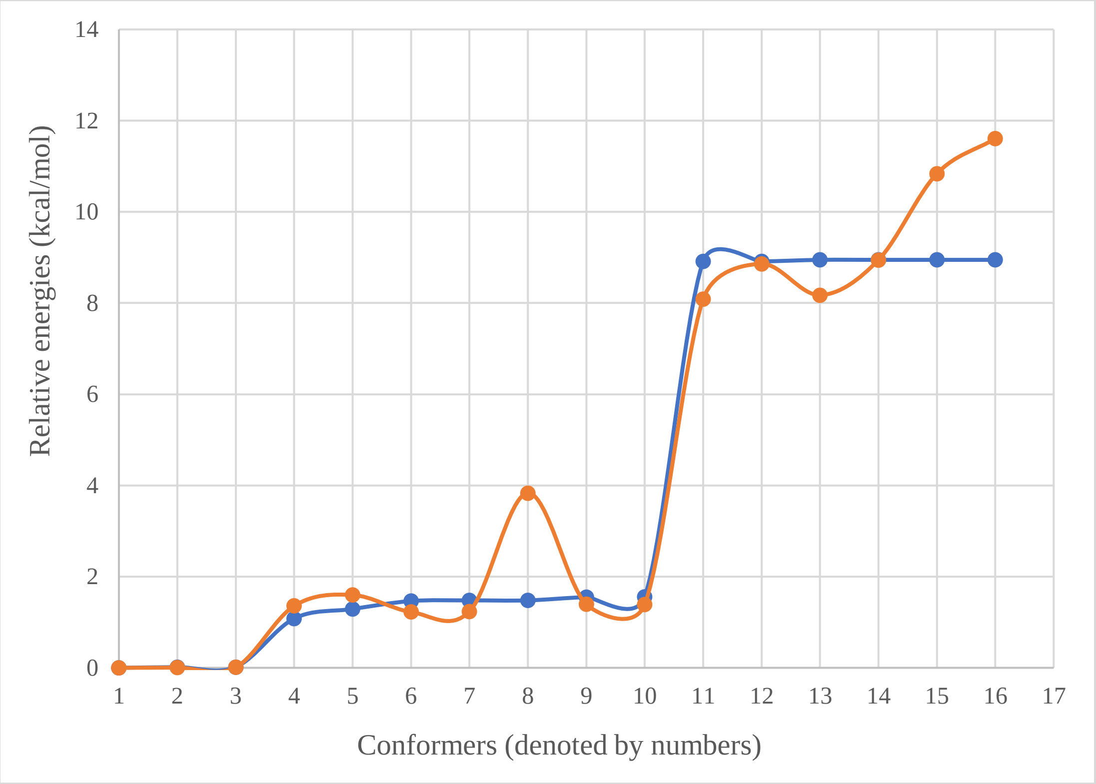
conformer	#	Conformers	#	Conformers	#	Conformers	#
BJQ-p-r-v3	1	BJQ-m-q-v2	4	BJQ-p-q-v3	7	BJQ-p-s-v3	10
BJQ-m-s-v1	2	BJQ-m-r-v2	5	BJQ-p-q-v3′	8	BJQ-j-q-v3	11
BJQ-m-t-v1	3	BJQ-m-q-v1	6	BJQ-p-r-v3	9	BJQ-j-q-v3	12

Figure 6.83. Diagrams comparing the DFT (—●—) and HF (—●—) relative energies of the calculated conformers of compound BLP.



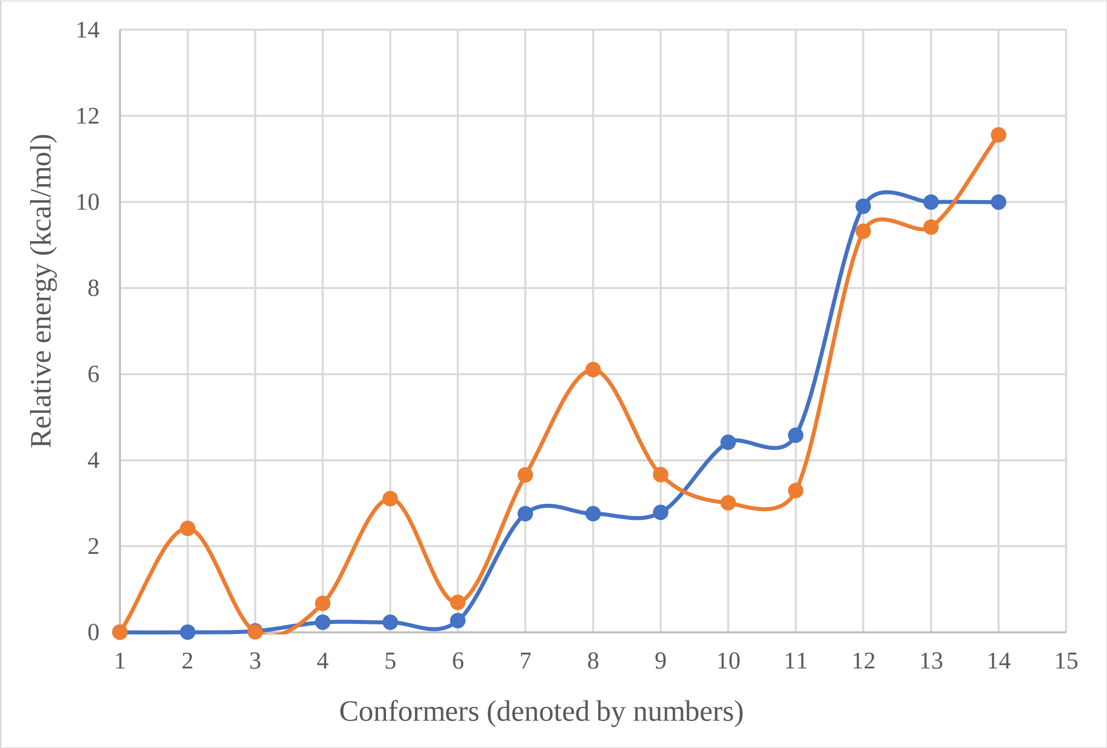
conformer	#	Conformers	#	Conformers	#	Conformers	#
BLP-k-q-v1	1	BLP-m-s-v1	5	BLP-p-q-v4	9	BLP-j-q-v5	13
BLP-p-s-v3	2	BLP-m-r-v1′	6	BLP-p-s-v4	10	BLP-j-r-v5	14
BLP-p-t-v3	3	BLP-k-r-v1	7	BLP-p-t-v4	11	BLP-j-s-v5	15
BLP-m-r-v1	4	BLP-k-s-v1	8	BLP-p-r-v4	12		

Figure 6.84. Diagrams comparing the DFT (—●—) and HF (—●—) relative energies of the calculated conformers of compound BLQ.



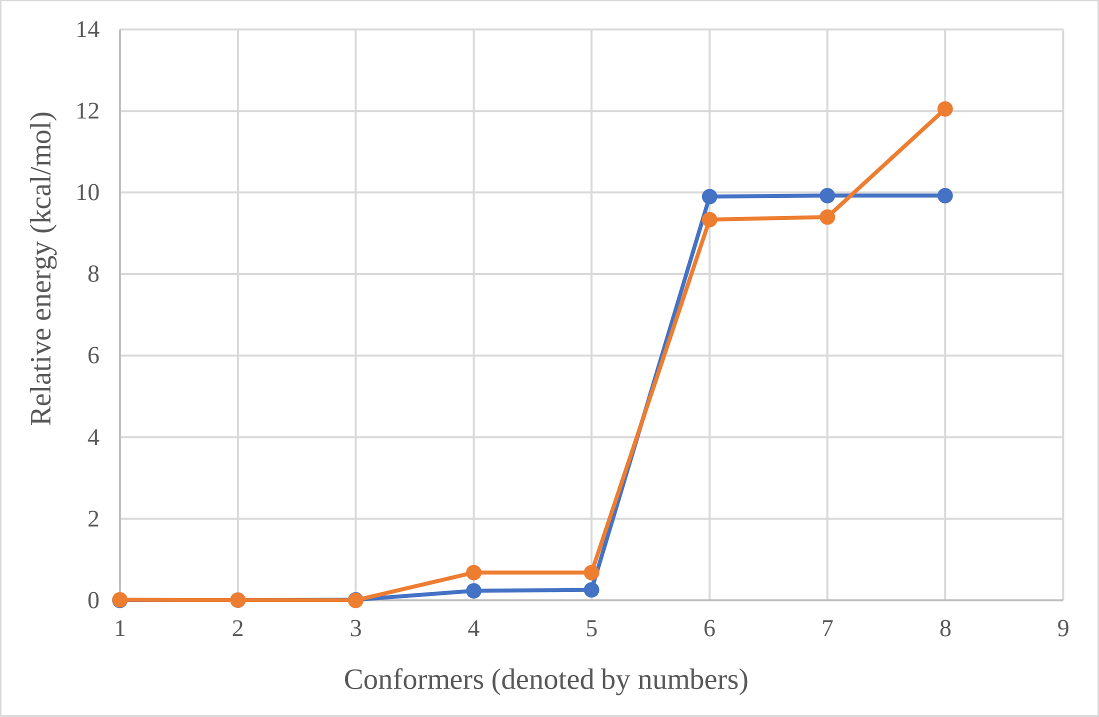
conformer	#	Conformers	#	Conformers	#	Conformers	#
BLQ-p-q-v3	1	BLQ-k-r-v1	5	BLQ-p-q-v4	9	BLQ-j-r-v3	13
BLQ-p-r-v3	2	BLQ-m-r-v1	6	BLQ-p-r-v4	10	BLQ-j-r-v5	14
BLQ-p-r-v3	3	BLQ-m-q-v1	7	BLQ-j-q-v3	11	BLQ-j-t-v3	15
BLQ-k-q-v1	4	BLQ-m-s-v1	8	BLQ-j-q-v5	12	BLQ-j-t-v5	16

Figure 6.85. Diagrams comparing the DFT (─●─) and HF (─●─) relative energies of the calculated conformers of compound CGP.



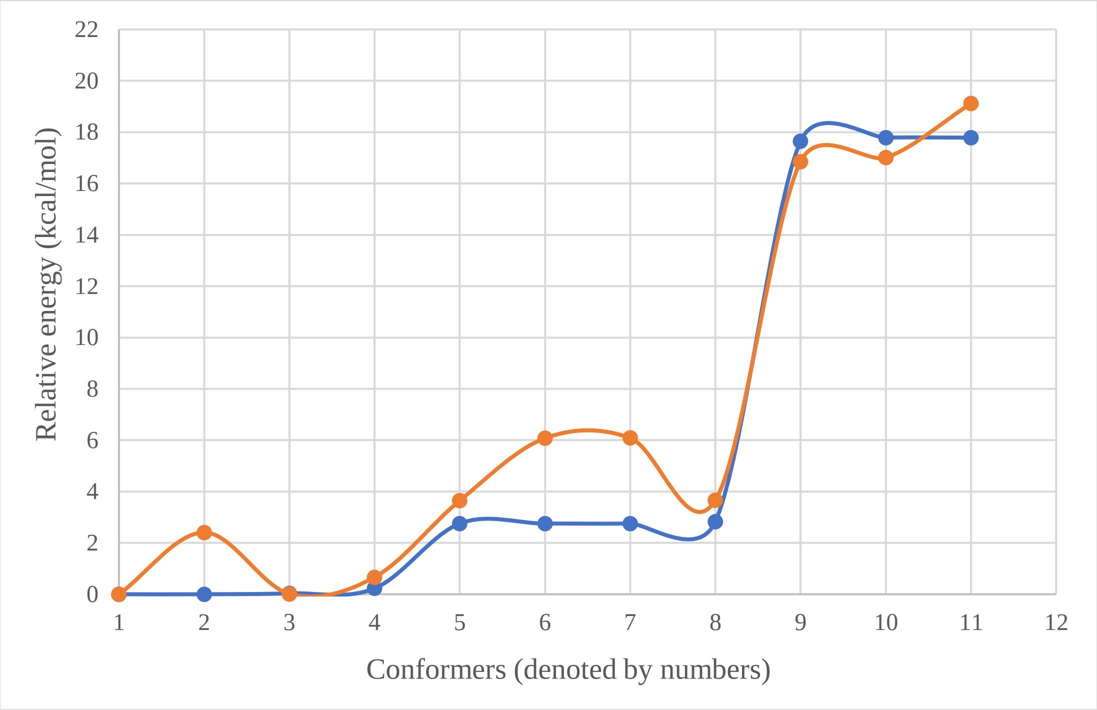
conformer	#	Conformers	#	Conformers	#	Conformers	#
CGP-p-q-w5	1	CGP-m-s-w1	5	CGP-m-q-w2	9	CGP-j-q-w5	12
CGP-p-s-w5	2	CGP-m-q-w1	6	CGP-g-r-w5	10	CGP-j-r-w5	13
CGP-p-r-w5	3	CGP-m-r-w2	7	CGP-g-q-w5	11	CGP-j-s-w5	14
CGP-m-r-w1	4	CGP-m-s-w2	8				

Figure 6.86. Diagrams comparing the DFT (—●—) and HF (—●—) relative energies of the calculated conformers of compound CGQ.



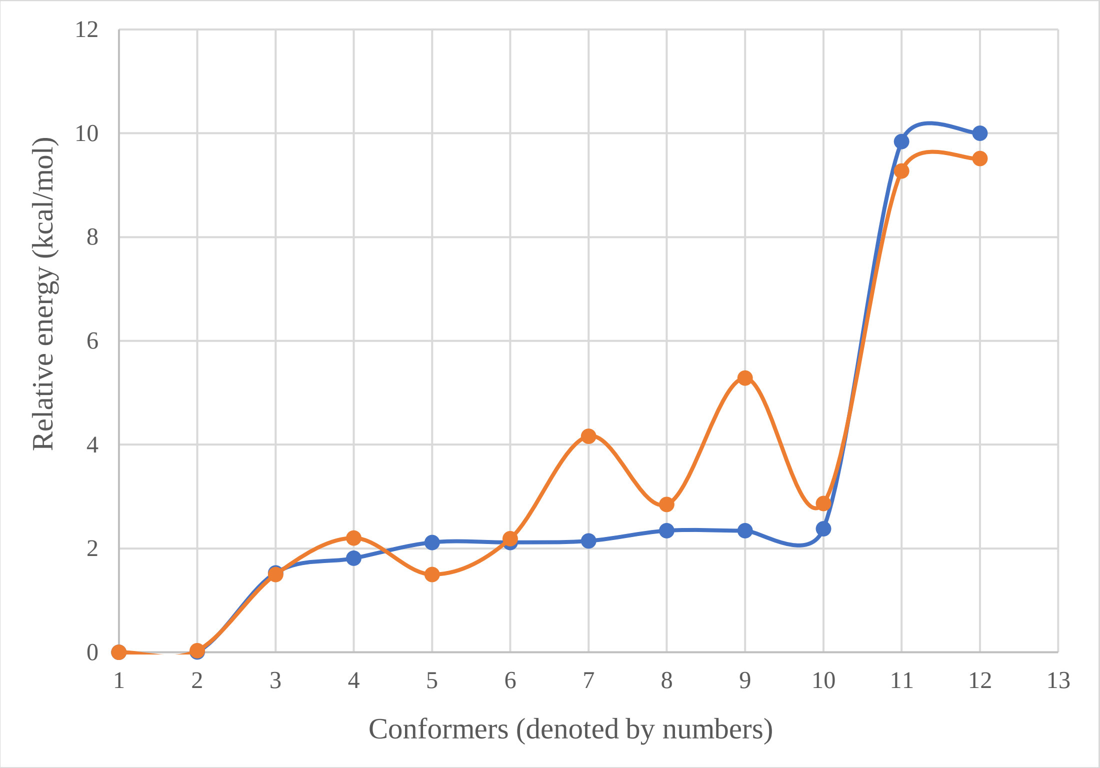
conformer	#	Conformers	#	Conformers	#	Conformers	#
CGQ-p-q-w5	1	CGQ-p-r-w5	3	CGQ-m-q-w1	5	CGQ-j-r-w5	7
CGQ-m-q-w3	2	CGQ-m-r-w1	4	CGQ-j-q-w5	6	CGQ-j-t-w5	8

Figure 6.87. Diagrams comparing the DFT (—●—) and HF (—●—) relative energies of the calculated conformers of compound CJP.



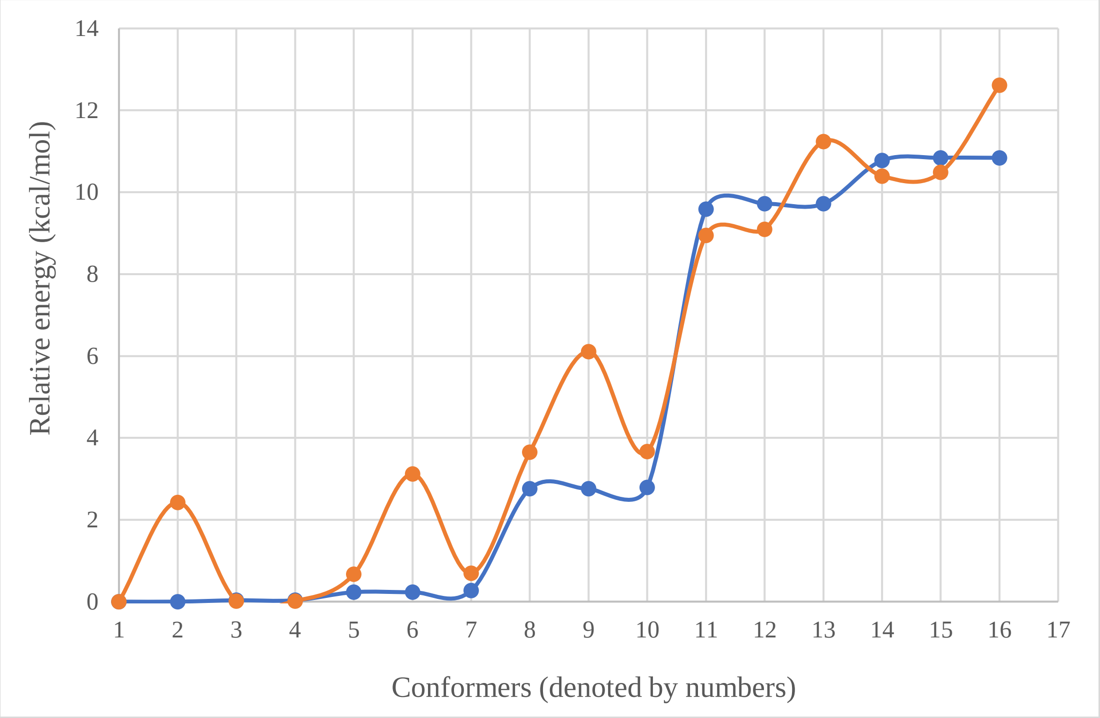
conformer	#	Conformers	#	Conformers	#	Conformers	#
CJP-p-q-w3	1	CJP-m-r-w1	4	CJP-m-t-w2	7	CJP-j-r-w1	10
CJP-p-s-w3	2	CJP-m-r-w2	5	CJP-m-q-w2	8	CJP-j-s-w1	11
CJP-p- r-w3	3	CJP-m-s-w2	6	CJP-j-q-w1	9		

Figure 6.88. Diagrams comparing the DFT (—●—) and HF (—●—) relative energies of the calculated conformers of compound CJQ.



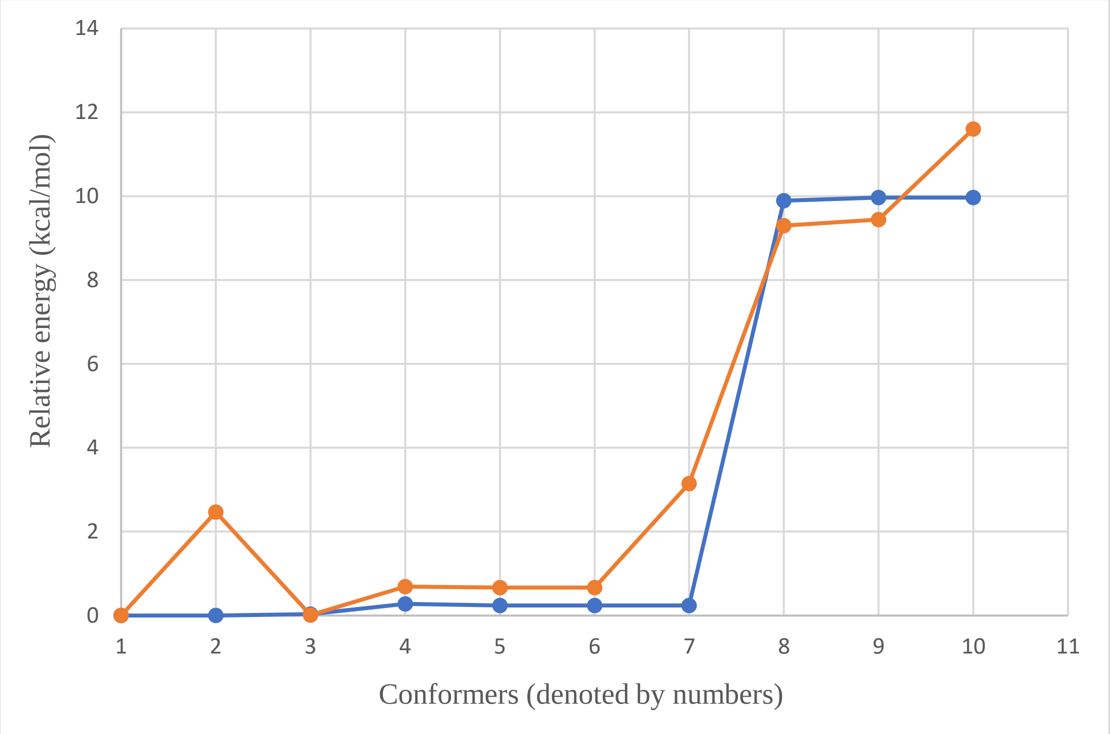
conformer	#	Conformers	#	Conformers	#	Conformers	#
CJQ-m-q-w6	1	CJQ-m-q-w1	4	CJQ-p-s-w5	7	CJQ-m-q-w1′	10
CJQ-m-r-w6	2	CJQ-p-q-w5	5	CJQ-m-r-w1	8	CJQ-j-q-w5	11
CJQ-p-q-w5	3	CJQ-p-q-w5′	6	CJQ-m-s-w1	9	CJQ-j-r-w5	12

Figure 6.89. Diagrams comparing the DFT (—●—) and HF (—●—) relative energies of the calculated conformers of compound CLP.



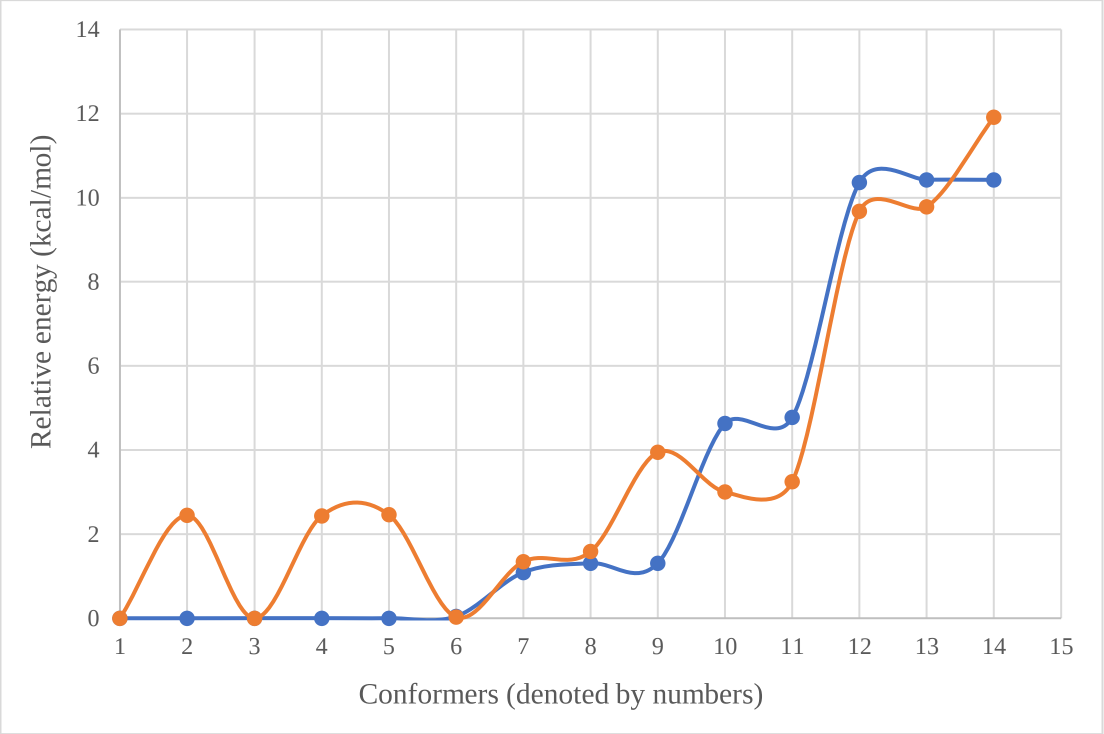
conformer	#	Conformers	#	Conformers	#	Conformers	#
CLP-p-q-w5	1	CLP-m-r-w1	5	CLP-m-s-w2	9	CLP-j-s-w5	13
CLP-p-s-w5	2	CLP-m-s-w1	6	CLP-m-q-w2	10	CLP-j-q-w6	14
CLP-p-r-w5	3	CLP-m-q-w1	7	CLP-j-q-w5	11	CLP-j-r-w6	15
CLP-p-r-w5′	4	CLP-m-q-w2	8	CLP-j-r-w5	12	CLP-j-s-w6	16

Figure 6.90. Diagrams comparing the DFT (—●—) and HF (—●—) relative energies of the calculated conformers of compound CLQ.



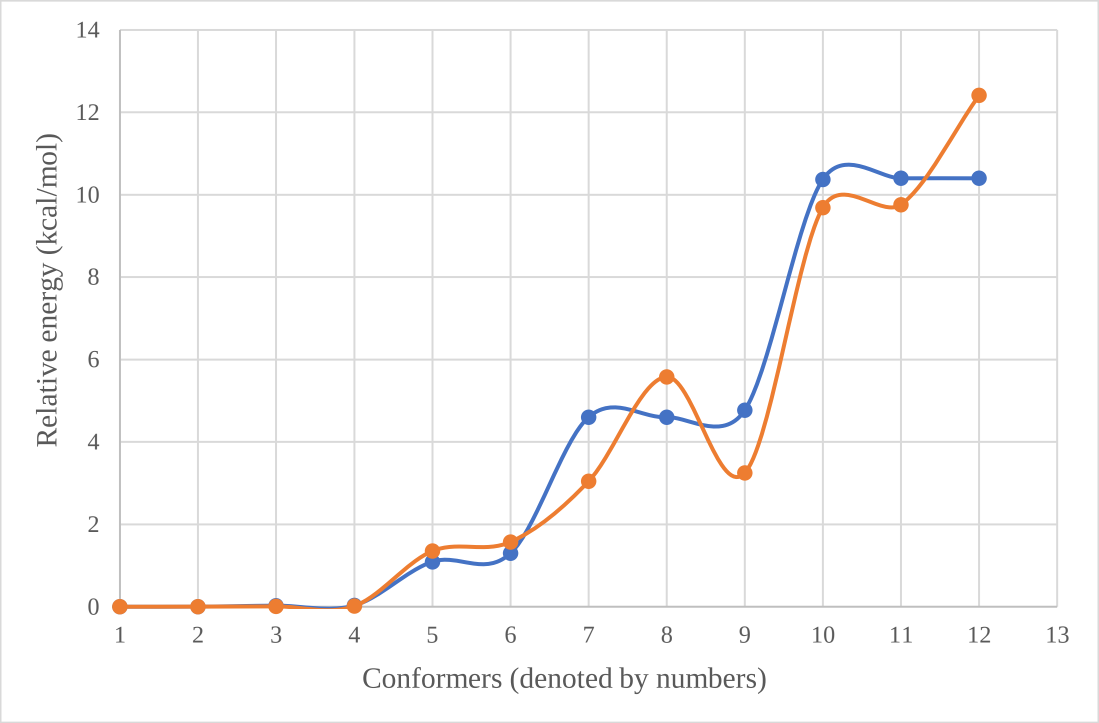
conformer	#	Conformers	#	Conformers	#	Conformers	#
CLQ-p-q-w5	1	CLQ-m-r-w1′	4	CLQ-m-q-w1′	7	CLQ-j-r-w5	9
CLQ-p-s-w5	2	CLQ-m-r-w1	5	CLQ-j-q-w5	8	CLQ-j-s-w6	10
CLQ-m-q-w1	3	CLQ-m-s-w1	6				

Figure 6.91. Diagrams comparing the DFT (—●—) and HF (—●—) relative energies of the calculated conformers of compound DGP.



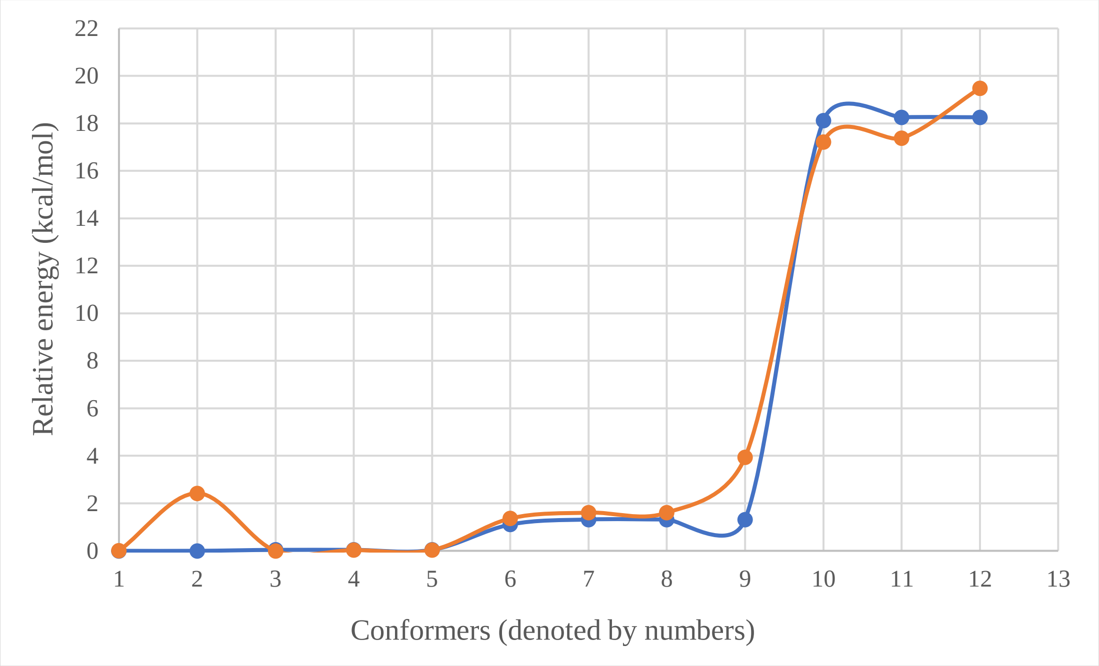
conformer	#	Conformers	#	Conformers	#	Conformers	#
DGP-m-r	1	DGP-p-t	5	DGP-k-s	9	DGP-j-q	12
DGP-m-s	2	DGP-m-q	6	DGP-g-r	10	DGP-j-r	13
DGP-p-q	3	DGP-k-q	7	DGP-g-q	11	DGP-j-s	14
DGP-p-s	4	DGP-k-r	8				

Figure 6.92. Diagrams comparing the DFT (—●—) and HF (—●—) relative energies of the calculated conformers of compound DGQ.



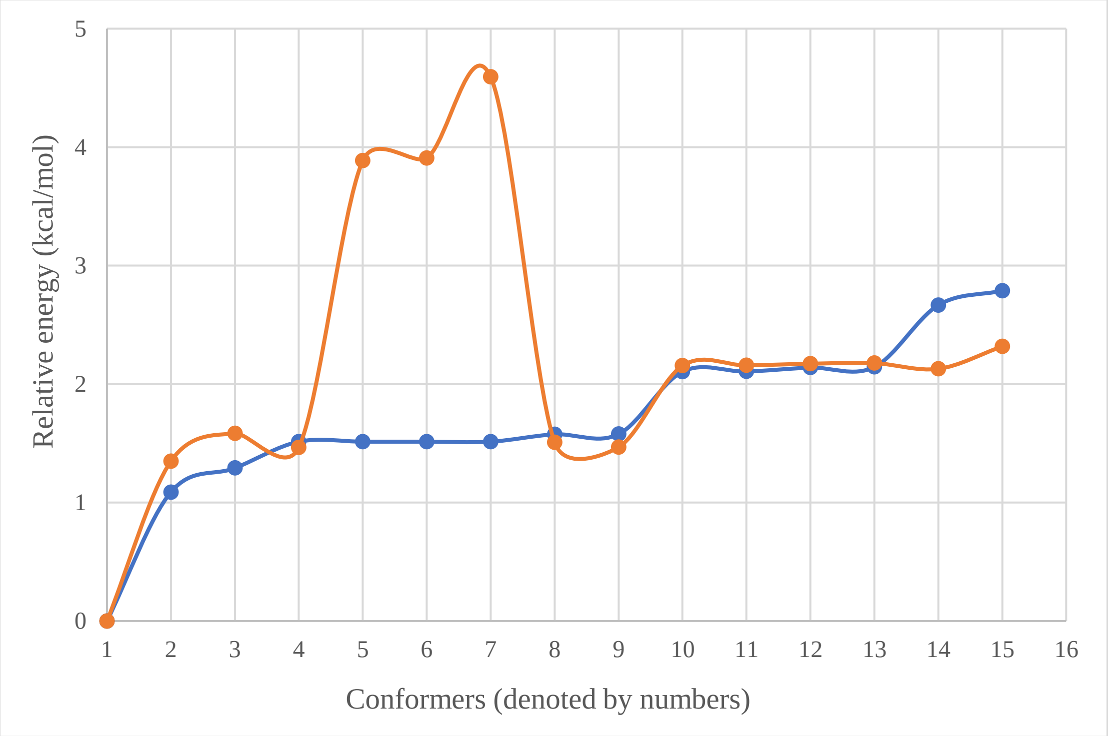
conformer	#	Conformers	#	Conformers	#	Conformers	#
DGQ-m-r	1	DGQ-m-q′	4	DGQ-g-r	7	DGQ-j-q	10
DGQ-p-q	2	DGQ-k-q	5	DGQ-g-t	8	DGQ-j-r	11
DGQ-m-q	3	DGQ-k-r	6	DGQ-g-q	9	DGQ-j-t	12

Figure 6.93. Diagrams comparing the DFT (—●—) and HF (—●—) relative energies of the calculated conformers of compound DJP.



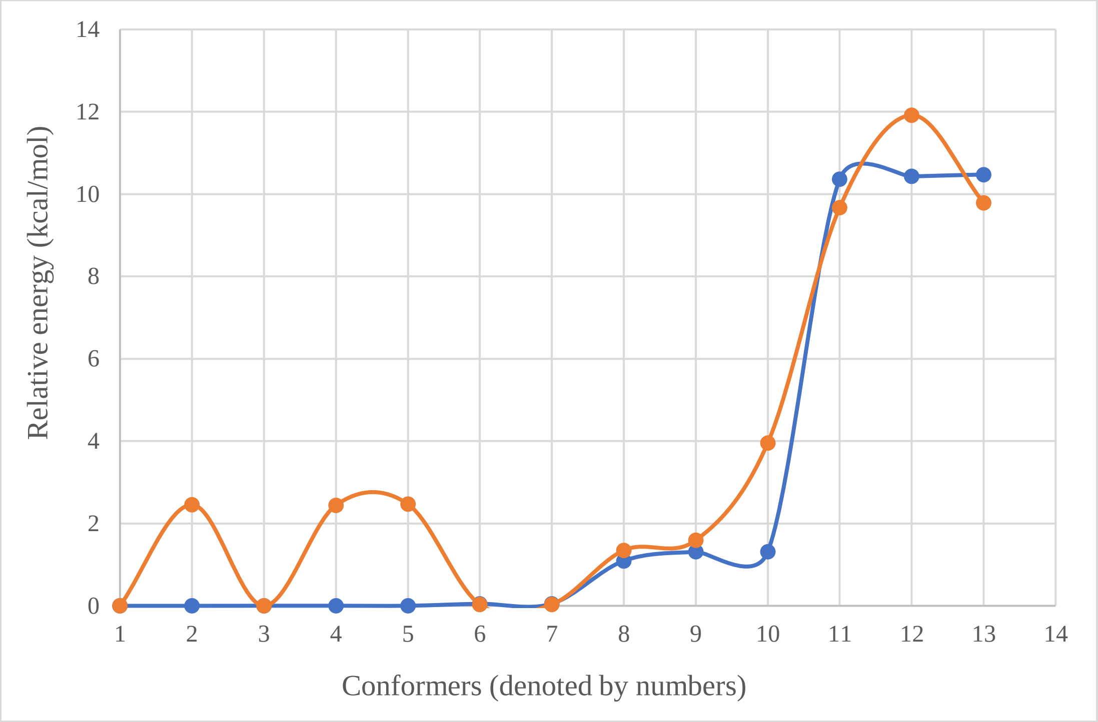
conformer	#	Conformers	#	Conformers	#	Conformers	#
DJP-m-r	1	DJP-m-q	4	DJP-k-r	7	DJP-j-q	10
DJP-p-s	2	DJP-p-r	5	DJP-k-r′	8	DJP-j-s	11
DJP-p-q	3	DJP-k-q	6	DJP-k-s	9	DJP-j-r	12

Figure 6.94. Diagrams comparing the DFT (—●—) and HF (—●—) relative energies of the calculated conformers of compound DJQ.



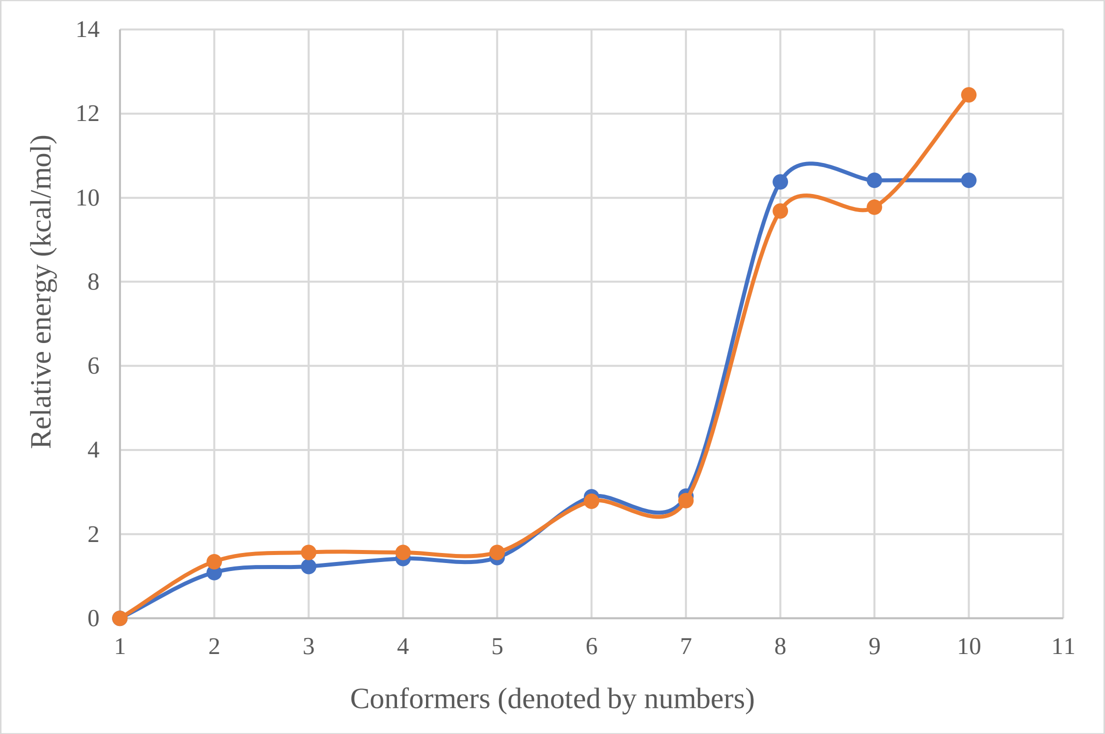
conformer	#	Conformers	#	Conformers	#	Conformers	#
DJQ-m-q	1	DJQ-m-s	5	DJQ-p-q	9	DJQ-m-q	13
DJQ-k-q	2	DJQ-m-t	6	DJQ-m-r′	10	DJQ-j-q	14
DJQ-k-r	3	DJQ-m-s′	7	DJQ-p-q′	11	DJQ-j-r	15
DJQ-m-r	4	DJQ-m-q	8	DJQ-p-r	12		

Figure 6.95. Diagrams comparing the DFT (—●—) and HF (—●—) relative energies of the calculated conformers of compound DLP.



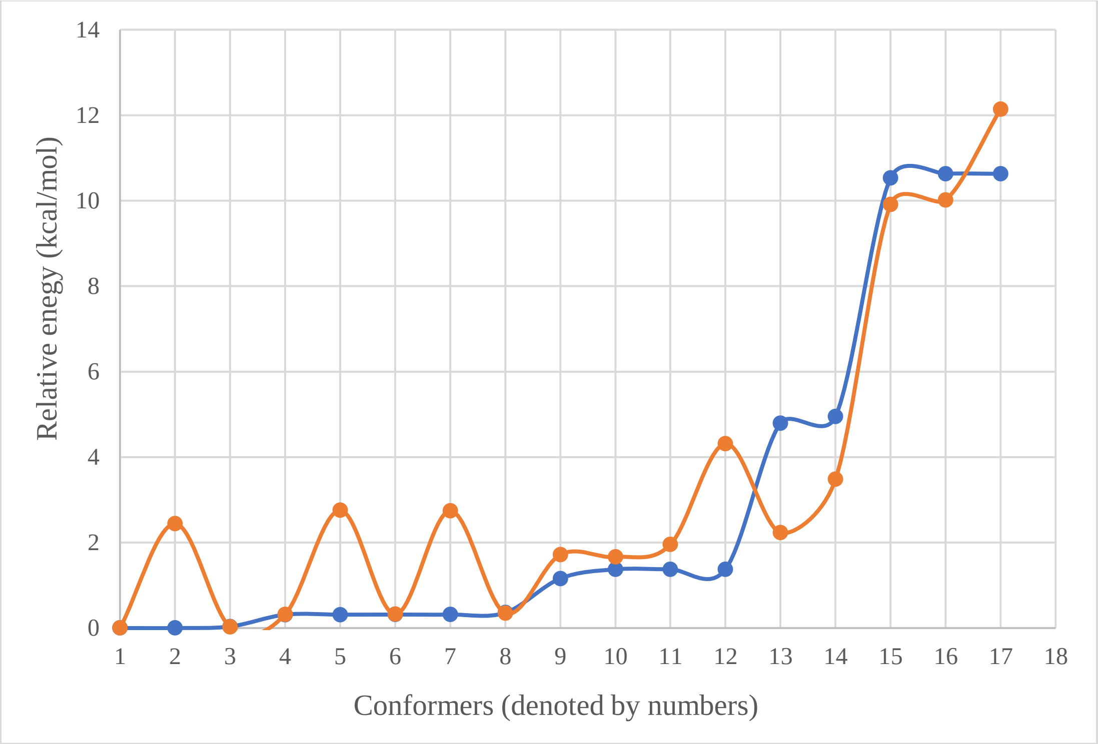
conformer	#	Conformers	#	Conformers	#	Conformers	#
DLP-m-r	1	DLP-p-t	5	DLP-k-r	9	DLP-j-s	12
DLP-m-s	2	DLP-m-q	6	DLP-k-s	10	DLP-j-r	13
DLP-p-q	3	DLP-p-r	7	DLP-j-q	11		
DLP-p-s	4	DLP-k-q	8				

Figure 6.96. Diagrams comparing the DFT (—●—) and HF (—●—) relative energies of the calculated conformers of compound DLQ.



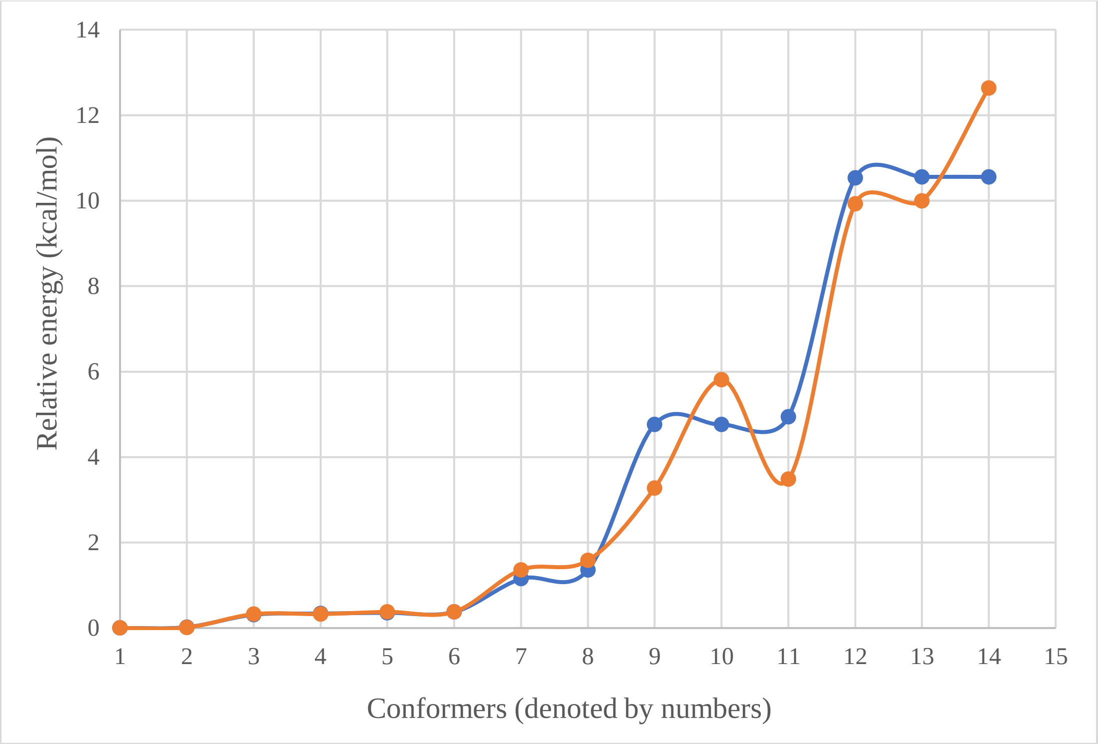
conformer	#	Conformers	#	Conformers	#	Conformers	#
DLQ-p-q	1	DLQ-m-r	4	DLQ-m-q′	7	DLQ-j-r	9
DLQ-k-q	2	DLQ-m-q	5	DLQ-j-q	8	DLQ-j-t	10
DLQ-k-r	3	DLQ-m-r′	6				

Figure 6.97. Diagrams comparing the DFT (─●─) and HF (─●─) relative energies of the calculated conformers of compound EGP.



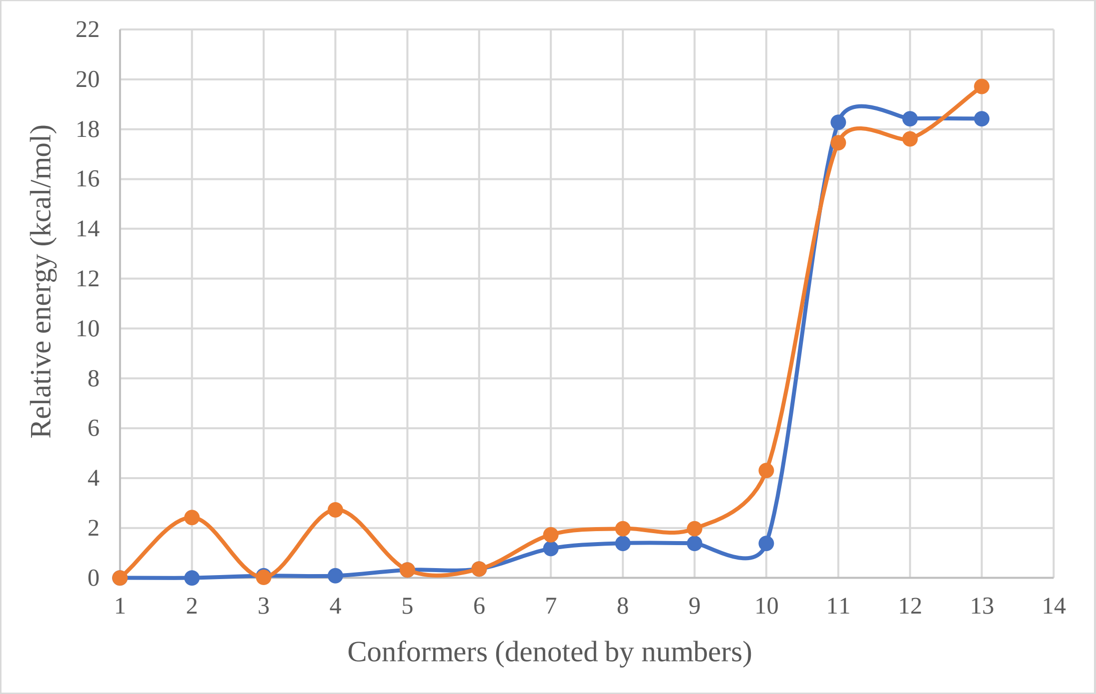
conformer	#	Conformers	#	Conformers	#	Conformers	#
EGP-m-r-x4	1	EGP-p-q-x3	6	EGP-k-q-x1	11	EGP-j-q-x3	15
EGP-m-s-x4	2	EGP-p-s-x3	7	EGP-k-s-x1	12	EGP-j-r-x3	16
EGP-m-q-x4	3	EGP-m-q-x1	8	EGP-g-r-x1	13	EGP-j-s-x3	17
EGP-m-r-x1	4	EGP-k-q-x1	9	EGP-g-q-x1	14		
EGP-m-s-x1	5	EGP-k-r-x2	10				

Figure 6.98. Diagrams comparing the DFT (—●—) and HF (—●—) relative energies of the calculated conformers of compound EGQ.



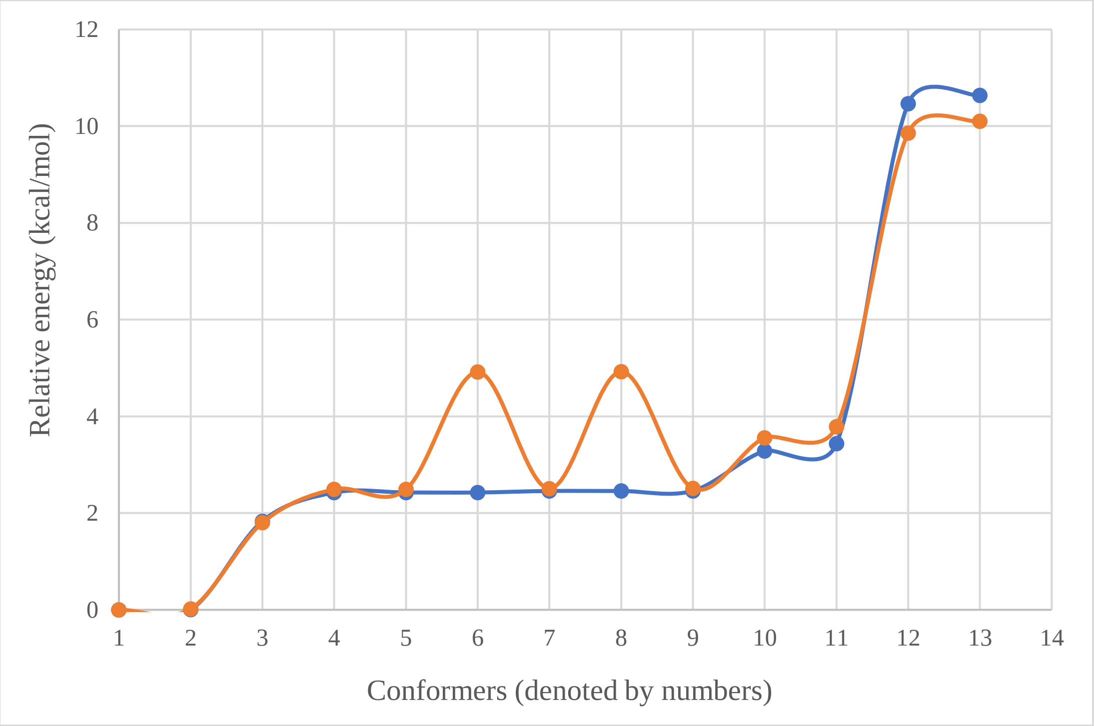
conformer	#	Conformers	#	Conformers	#	Conformers	#
EGQ-m-r-x4	1	EGQ-p-q-x3	5	EGQ-g-r-x1	9	EGQ-j-q-x3	12
EGQ-m-q-x4	2	EGQ-p-r-x3	6	EGQ-g-t-x1	10	EGQ-j-r-x3	13
EGQ-m-r-x1	3	EGQ-k-q-x4	7	EGQ-g-q-x1	11	EGQ-j-t-x3	14
EGQ-m-q-x1	4	EGQ-k-r-x4	8				

Figure 6.99. Diagrams comparing the DFT (—●—) and HF (—●—) relative energies of the calculated conformers of compound EJP.



conformer	#	Conformers	#	Conformers	#	Conformers	#
EJP-m-s-x4	1	EJP-p-q-x4	5	EJP-k-r-x1′	9	EJP-j-r-x3	12
EJP-m-r-x4	2	EJP-p-r-x4	6	EJP-k-s-x1	10	EJP-j-s-x3	13
EJP-m-q-x4	3	EJP-k-q-x1	7	EJP-j-q-x3	11		
EJP-p-s-x4	4	EJP-k-r-x1	8				

Figure 6.100. Diagrams comparing the DFT (—●—) and HF (—●—) relative energies of the calculated conformers of compound EJQ.

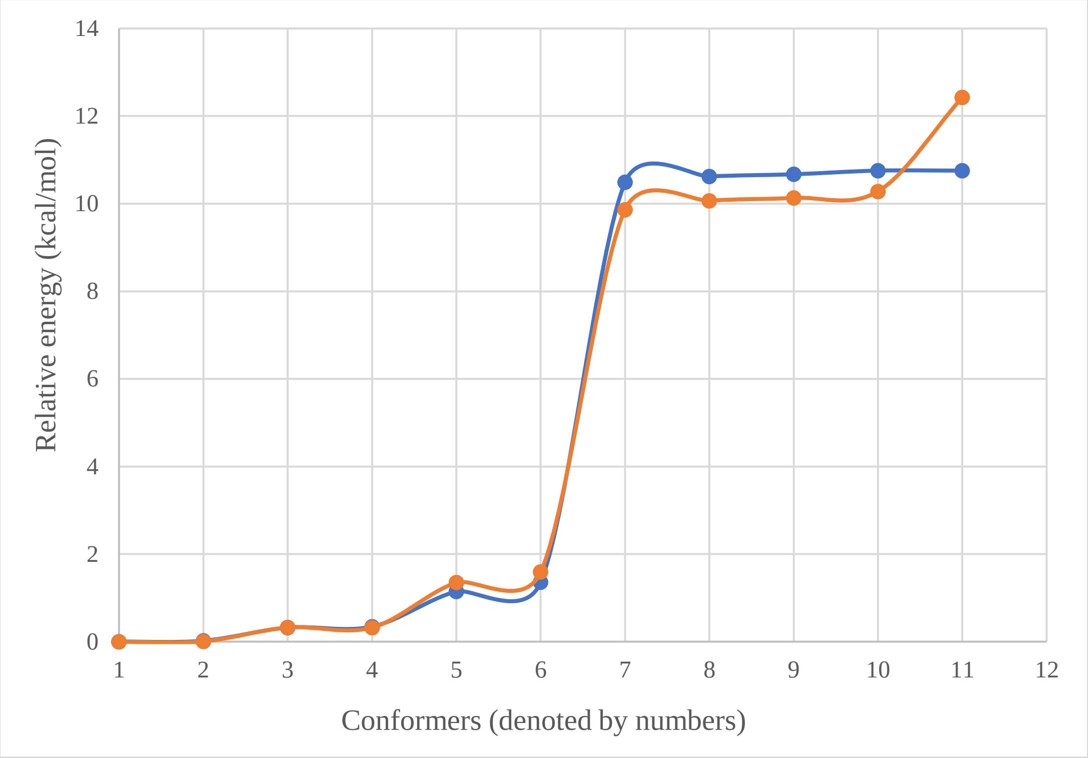


conformer	#	Conformers	#	Conformers	#	Conformers	#
EJQ-m-q-x4	1	EJQ-m-r-x1	5	EJQ-m-q-x1	9	EJQ-j-q-x3	12
EJQ-m-r-x4	2	EJQ-m-s-x1	6	EJQ-k-q-x4	10	EJQ-j-r-x3	13
EJQ-p-q-x4	3	EJQ-p-r-x4	7	EJQ-k-r-x4	11		
EJQ-p-q-x4′	4	EJQ-p-s-x4	8				

Figure 6.101. Diagrams comparing the DFT (—●—) and HF (—●—) relative energies of the calculated conformers of compound ELP.

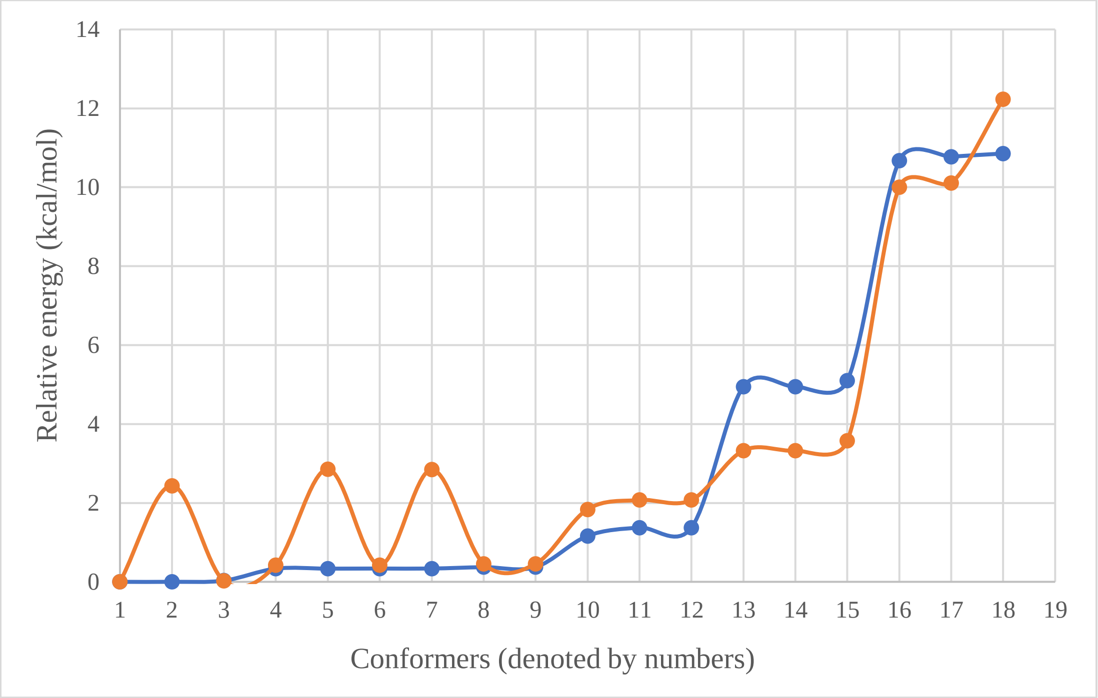
conformer	#	Conformers	#	Conformers	#	Conformers	#
ELP-m-s-x4	1	ELP-p-s-x4	6	ELP-k-s-x1	11	ELP-j-q-x3′	15
ELP-m-q-x4	2	ELP-p-s-x4′	7	ELP-j-q-x3	12	ELP-j-r-x3′	16
ELP-m-q-x4	3	ELP-m-q-x1	8	ELP-j-r-x3	13	ELP-j-s-x3′	17
ELP-m-r-x1	4	ELP-k-q-x1	9	ELP-j-s-x3	14		
ELP-m-s-x1	5	ELP-k-r-x1	10				

Figure 6.102. Diagrams comparing the DFT (—●—) and HF (—●—) relative energies of the calculated conformers of compound ELQ.



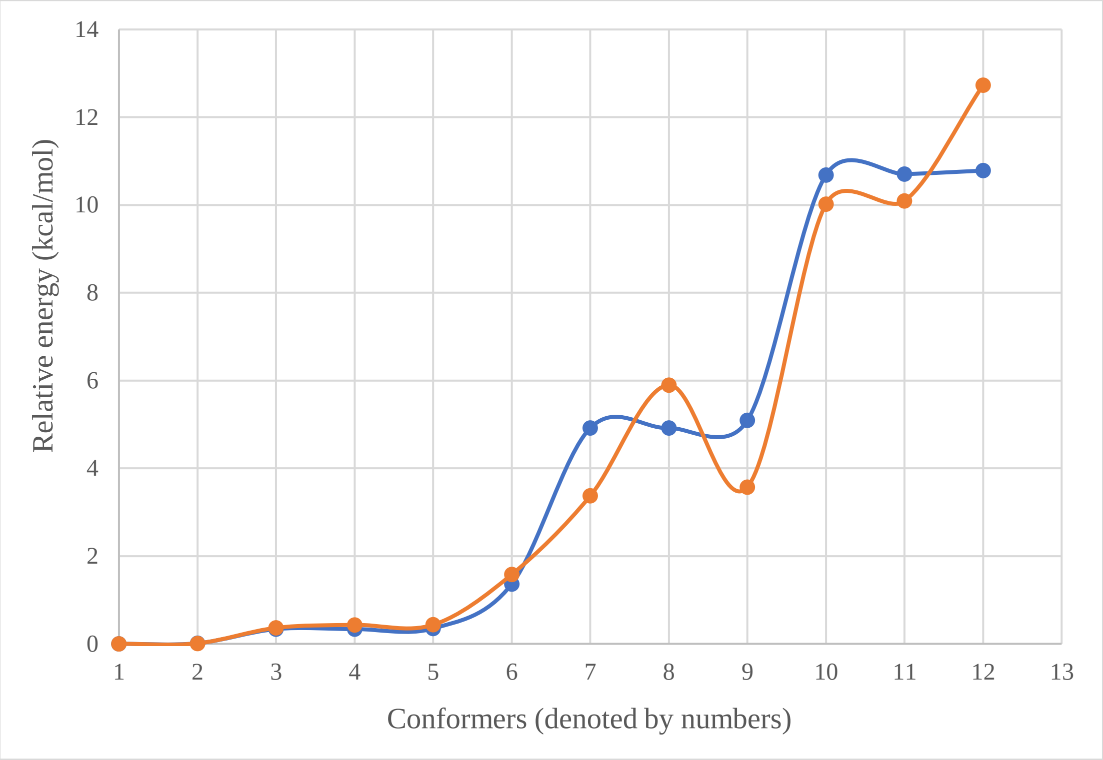
conformer	#	Conformers	#	Conformers	#	Conformers	#
ELQ-m-r-x4	1	ELQ-m-q-x1	4	ELQ-j-q-x3	7	ELQ-j-r-x3′	10
ELQ-m-q-x4	2	ELQ-k-q-x4	5	ELQ-j-r-x3	8	ELQ-j-s-x3	11
ELQ-m-r-x1	3	ELQ-k-r-x4	6	ELQ-j-q-x3′	9		

Figure 6.103. Diagrams comparing the DFT (–●–) and HF (–●–) relative energies of the calculated conformers of compound FGP.



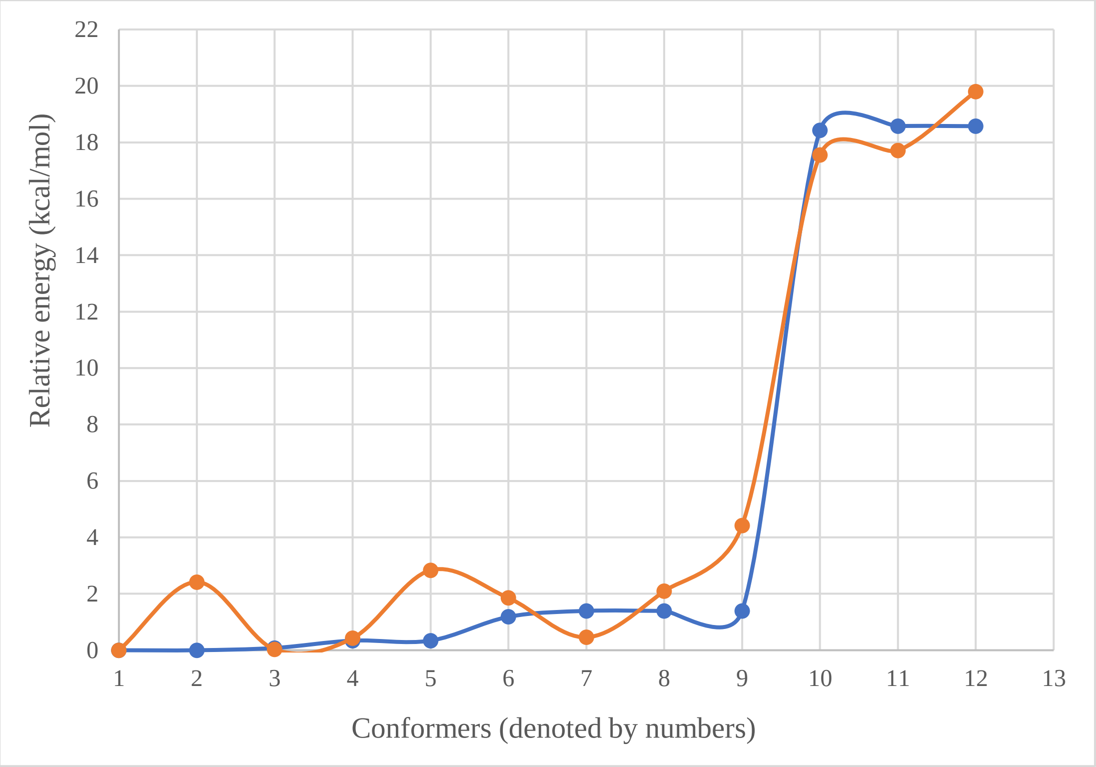
conformer	#	Conformers	#	Conformers	#	Conformers	#
FGP-m-r-x4	1	FGP-p-q-x4	6	FGP-k-r-x1	11	FGP-g-q-x1	15
FGP-m-s-x4	2	FGP-p-s-x4	7	FGP-k-r-x1	12	FGP-j-q-x3	16
FGP-m-q-x4	3	FGP-m-q-x1	8	FGP-g-r-x1	13	FGP-j-r-x3	17
FGP-m-r-x1	4	FGP-p-r-x4	9	FGP-g-r-x1′	14	FGP-j-s-x3	18
FGP-m-s-x1	5	FGP-k-q-x1	10				

Figure 6.104. Diagrams comparing the DFT (—●—) and HF (—●—) relative energies of the calculated conformers of compound FGQ.



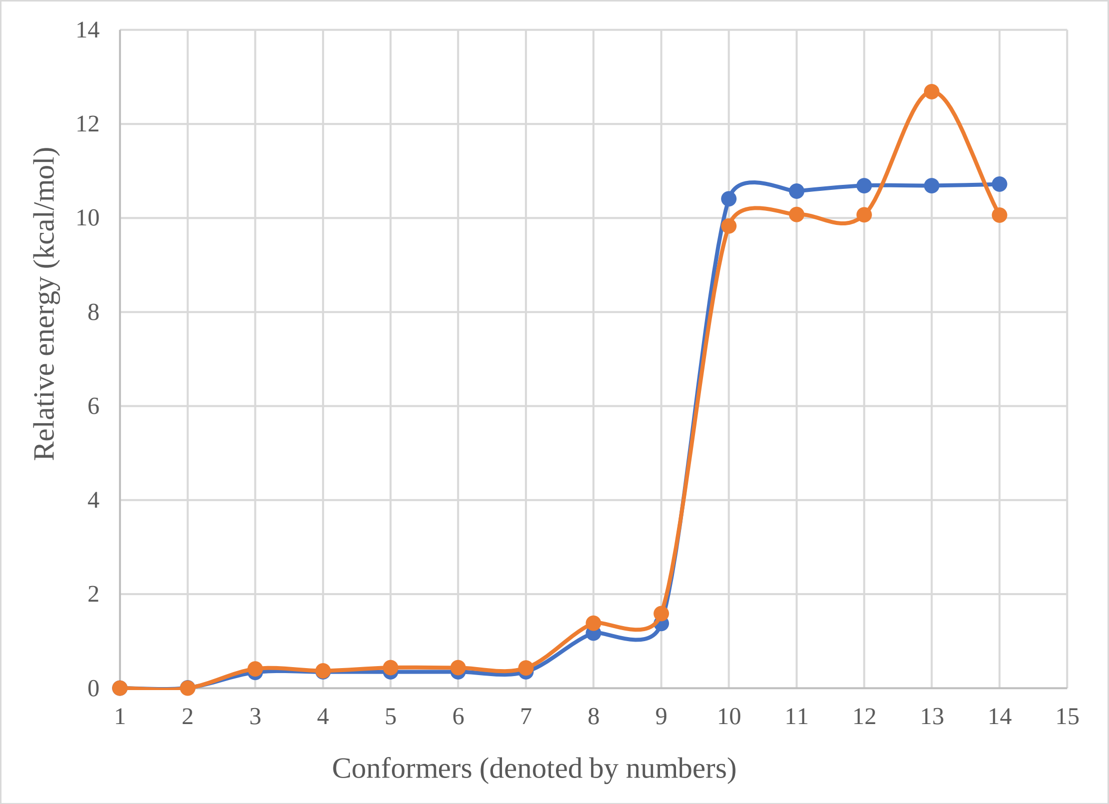
conformer	#	Conformers	#	Conformers	#	Conformers	#
FGQ-m-r-x4	1	FGQ-m-r-x1	4	FGQ-g-r-x1	7	FGQ-j-q-x3	10
FGQ-m-q-x4	2	FGQ-m-q-x1	5	FGQ-g-t-x1	8	FGQ-j-r-x3	11
FGQ-p-q-x4	3	FGQ-k-r-x4	6	FGQ-g-q-x1	9	FGQ-j-t-x3	12

Figure 6.105. Diagrams comparing the DFT (—●—) and HF (—●—) relative energies of the calculated conformers of compound FJP.



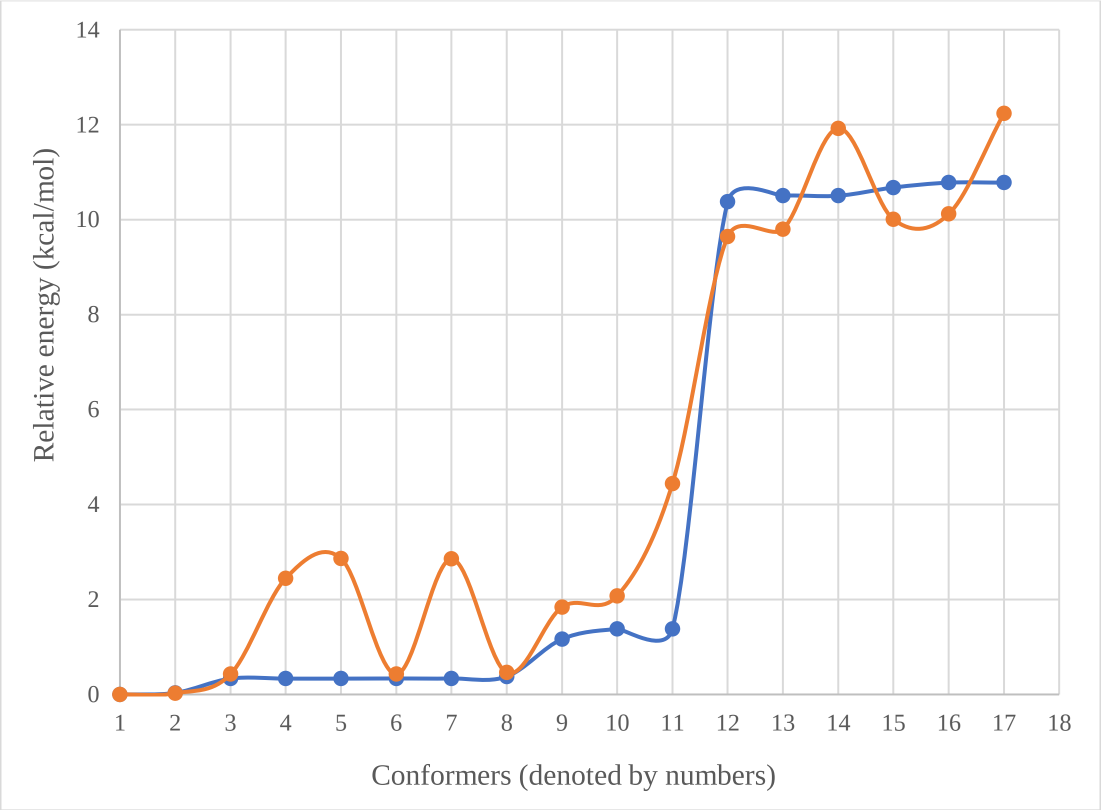
conformer	#	Conformers	#	Conformers	#	Conformers	#
FJP-m-r-x4	1	FJP-p-q-x4	4	FJP-p-r-x1	7	FJP-j-q-x3	10
FJP-m-s-x4	2	FJP-p-s-x4	5	FJP-k-r-x1	8	FJP-j-r-x3	11
FJP-m-q-x4	3	FJP-k-q-x1	6	FJP-k-s-x1	9	FJP-j-s-x3	12

Figure 6.106. Diagrams comparing the DFT (—●—) and HF (—●—) relative energies of the calculated conformers of compound FJQ.



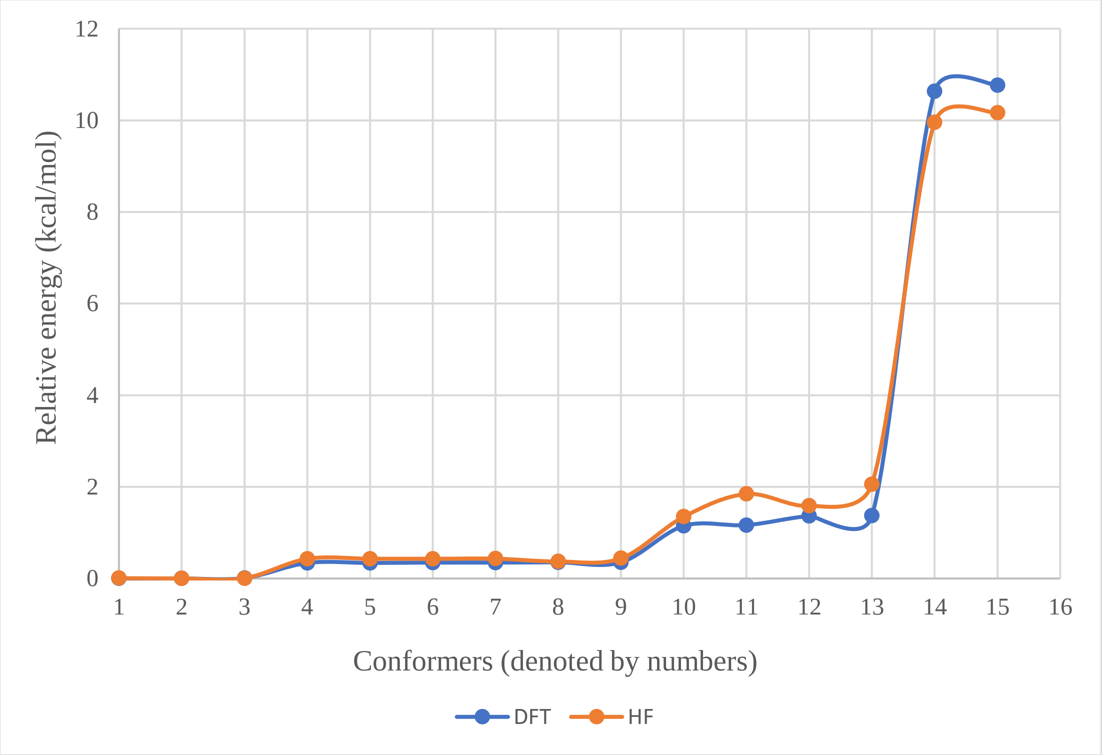
conformer	#	Conformers	#	Conformers	#	Conformers	#
FJQ-m-q-x4	1	FJQ-p-q-x4′	5	FJQ-k-r-x4	9	FJQ-j-r-x3′	12
FJQ-m-r-x4	2	FJQ-m-q-x1	6	FJQ-j-q-x3	10	FJQ-j-t-x3	13
FJQ-p-r-x4	3	FJQ-m-r-x1	7	FJQ-j-r-x3	11	FJQ-j-q-x3′	14
FJQ-p-q-x4	4	FJQ-k-q-x4	8				

Figure 6.107. Diagrams comparing the DFT (—●—) and HF (—●—) relative energies of the calculated conformers of compound FLP.



conformer	#	Conformers	#	Conformers	#	Conformers	#
FLP-m-r-x4	1	FLP-p-q-x4	6	FLP-k-s-x1	11	FLP-j-q-x3′	15
FLP-m-q-x4	2	FLP-p-s-x4	7	FLP-j-q-x3	12	FLP-j-r-x3′	16
FLP-m-r-x1	3	FLP-m-q-x1	8	FLP-j-r-x3	13	FLP-j-s-x3	17
FLP-m-s-x4	4	FLP-k-q-x1	9	FLP-j-s-x3′	14		
FLP-m-s-x1	5	FLP-k-r-x1	10				

Figure 6.108. Diagrams comparing the DFT (—●—) and HF (—●—) relative energies of the calculated conformers of compound FLQ.



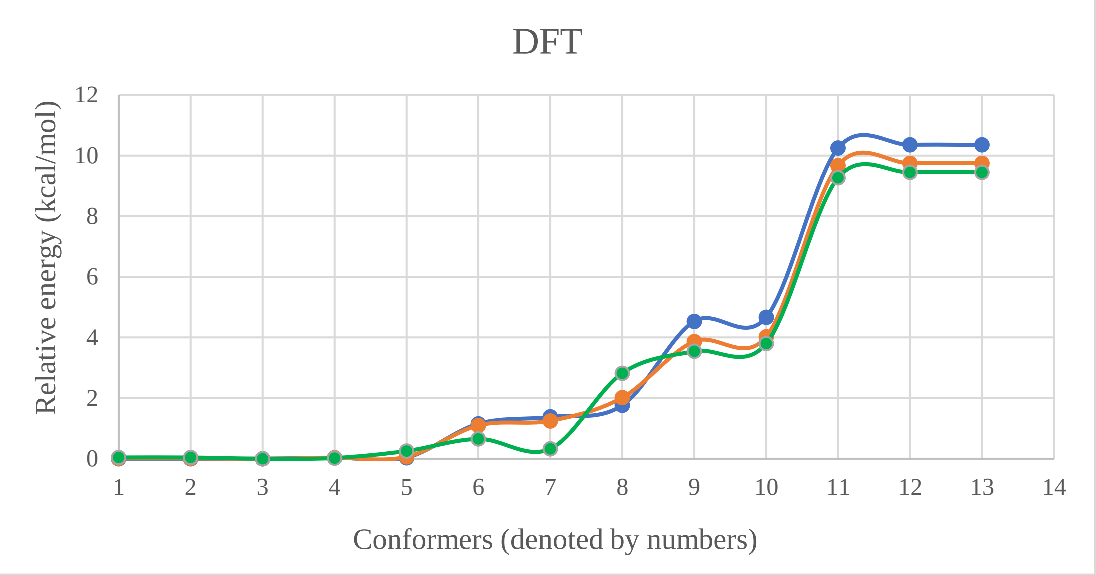
conformer	#	Conformers	#	Conformers	#	Conformers	#
FLQ-p-q-x2	1	FLQ-m-r-x1	5	FLQ-p-r-x4′	9	FLQ-k-r-x1	13
FLQ-m-r-x4	2	FLQ-m-q-x1	6	FLQ-k-q-x4	10	FLQ-j-q-x3	14
FLQ-m-q-x4	3	FLQ-m-q-x1′	7	FLQ-k-q-x1	11	FLQ-j-r-x3	15
FLQ-p-q-x4	4	FLQ-p-r-x4	8	FLQ-k-r-x4	12		

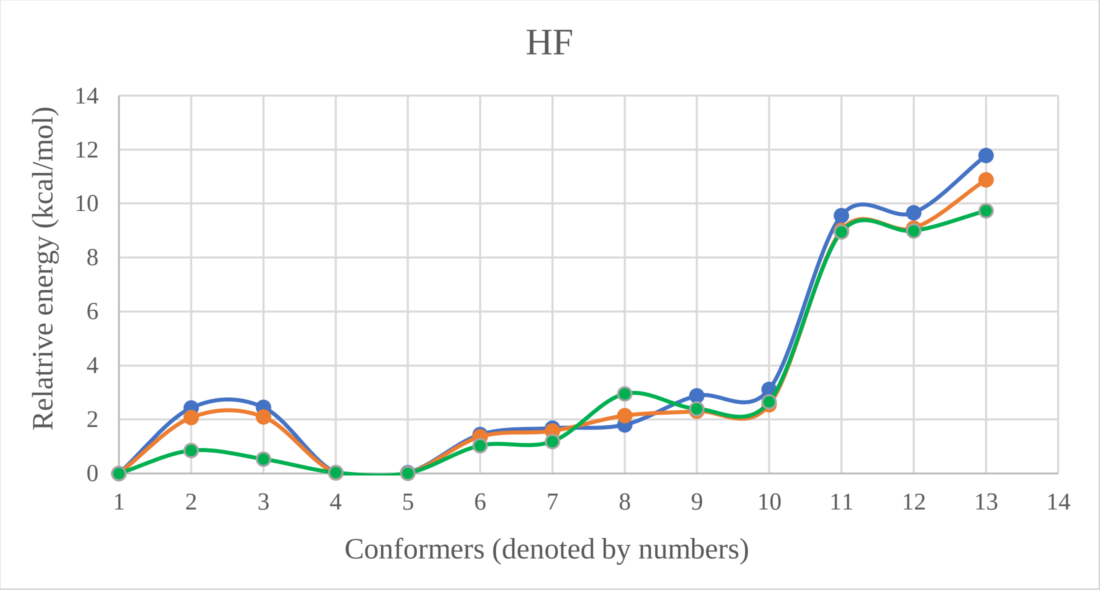
6.3.2. Diagrams comparing the uncorrected relative energy (ΔE), relative energy corrected for ZPE ($\Delta E_{corrected}$) and Gibbs free energy (ΔG) of the conformers of each of the compounds considered.

This section presents diagrams comparing the uncorrected relative energies (ΔE), relative energies corrected for ZPE (sum of electronic and zero-point energies, $\Delta E_{corrected}$) and Gibbs free energies (sum of electronic and thermal free energies, ΔG). The energy series are represented by different colours: blue for ΔE, orange for $\Delta E_{corrected}$ and green for ΔG.

For each compound, separated diagrams are made for the DFT and HF results (respectively denoted as DFT and HF and indicated on top of each diagrams). In both HF and DFT diagrams, the conformers are listed in order of increasing DFT relative energies; for this reason, there might be cases in which the HF results show apparently abnormal behaviour (not always increasing; for example, figures 6.112 and 6.115), when there are discrepancies in the relative energy sequence between the DFT and HF results.

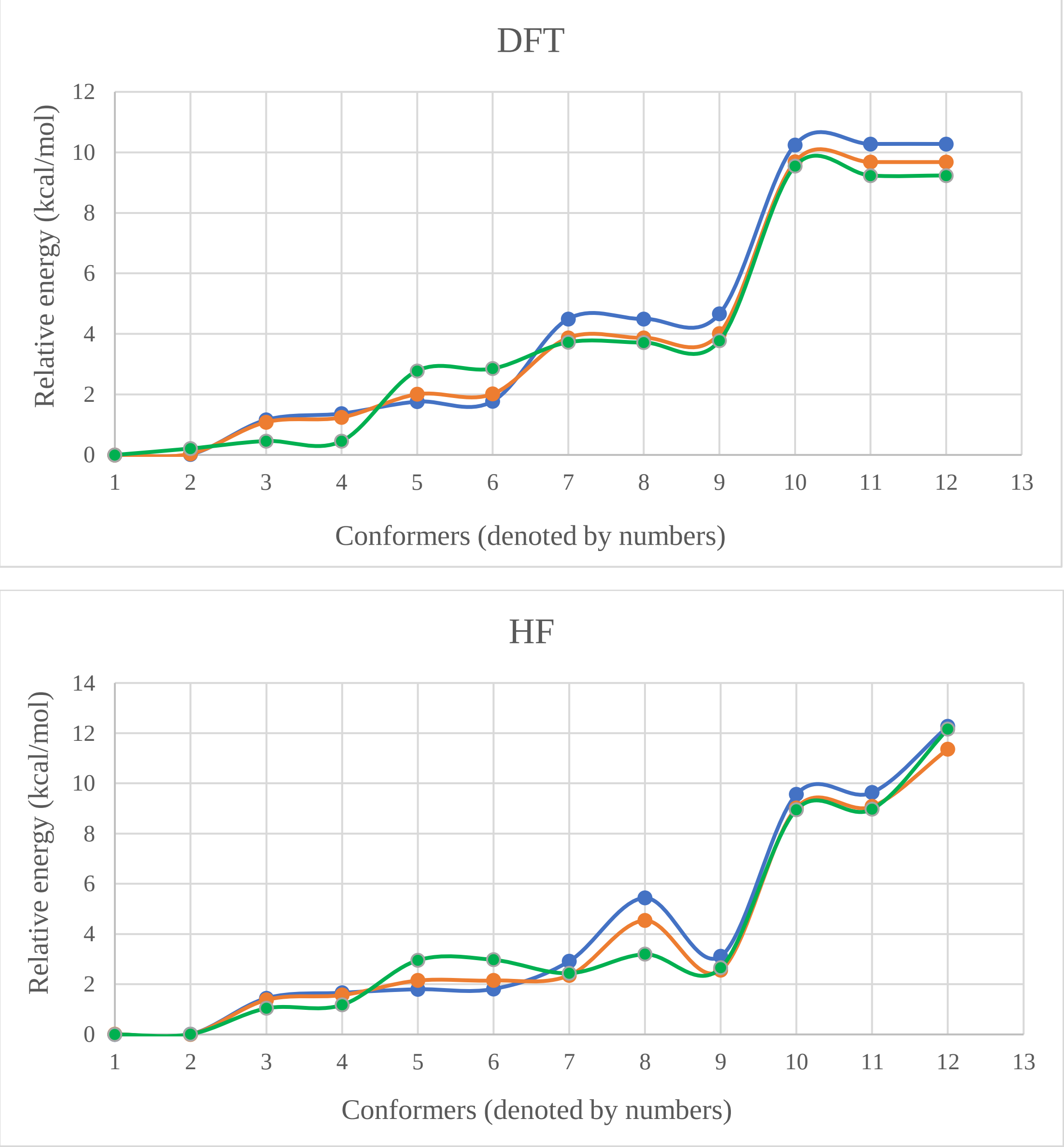
Figure 6.109. Diagrams comparing the uncorrected relative energies (—●—), relative energies corrected for ZPE (—●—) and Gibbs free energies (—●—) of the calculated conformers of compound AGP.





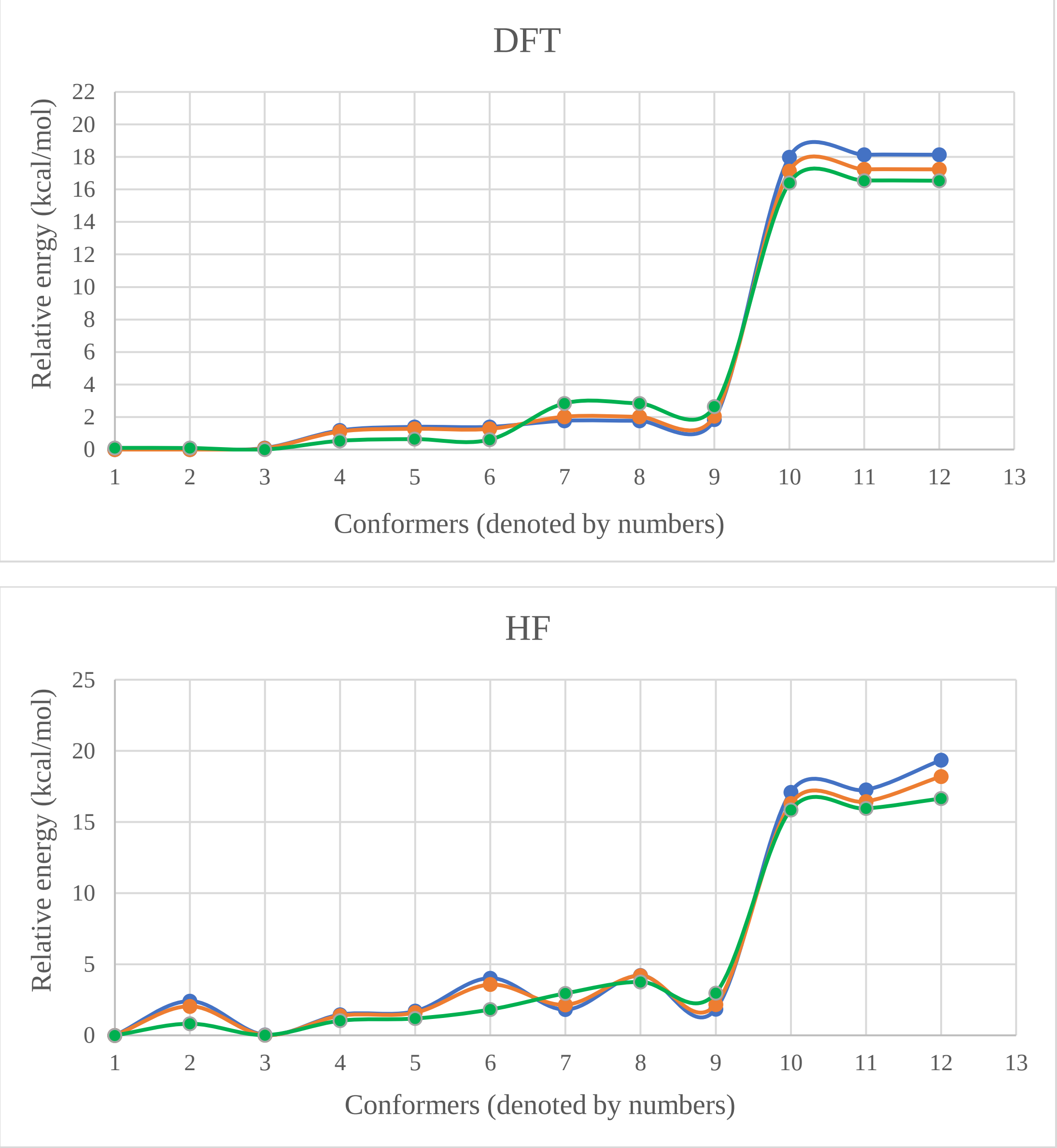
conformers	#	Conformers	#	Conformers	#	Conformers	#
AGP-m-r-u1	1	AGP-p-r-u3	5	AGP-g-r-u3	9	AGP-j-s-u3	13
AGP-m-s-u1	2	AGP-k-q-u1	6	AGP-g-q-u3	10		
AGP-p-t-u3	3	AGP-k-r-u1	7	AGP-j-q-u3	11		
AGP-m-q-u1	4	AGP-m-r-u2	8	AGP-j-r-u3	12		

Figure 6.110. Diagrams comparing the uncorrected relative energies (—●—), relative energies corrected for ZPE (—●—) and Gibbs free energies (—●—) of the calculated conformers of compound AGQ.



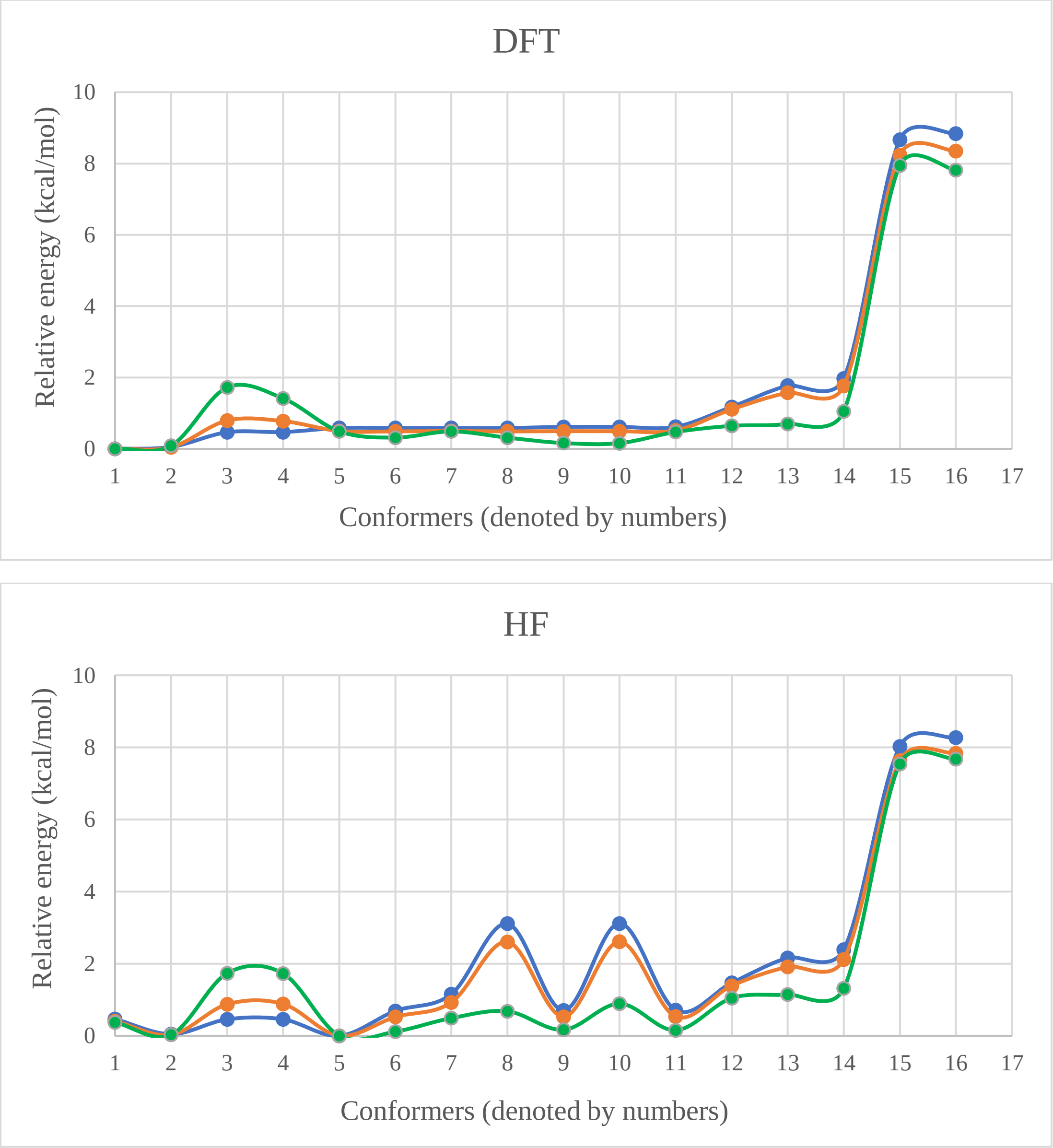
conformer	#	Conformers	#	Conformers	#	Conformers	#
AGQ-m-r-u1	1	AGQ-k-r-u1	4	AGQ-g-r-u3	7	AGQ-j-q-u3	10
AGQ-m-q-u1	2	AGQ-m-r-u2	5	AGQ-g-t-u3	8	AGQ-j-r-u3	11
AGQ-k-q-u1	3	AGQ-m-q-u2	6	AGQ-g-q-u3	9	AGQ-j-t-u3	12

Figure 6.111. Diagrams comparing the uncorrected relative energies (—●—), relative energies corrected for ZPE (—●—) and Gibbs free energies (—●—) of the calculated conformers of compound AJP.



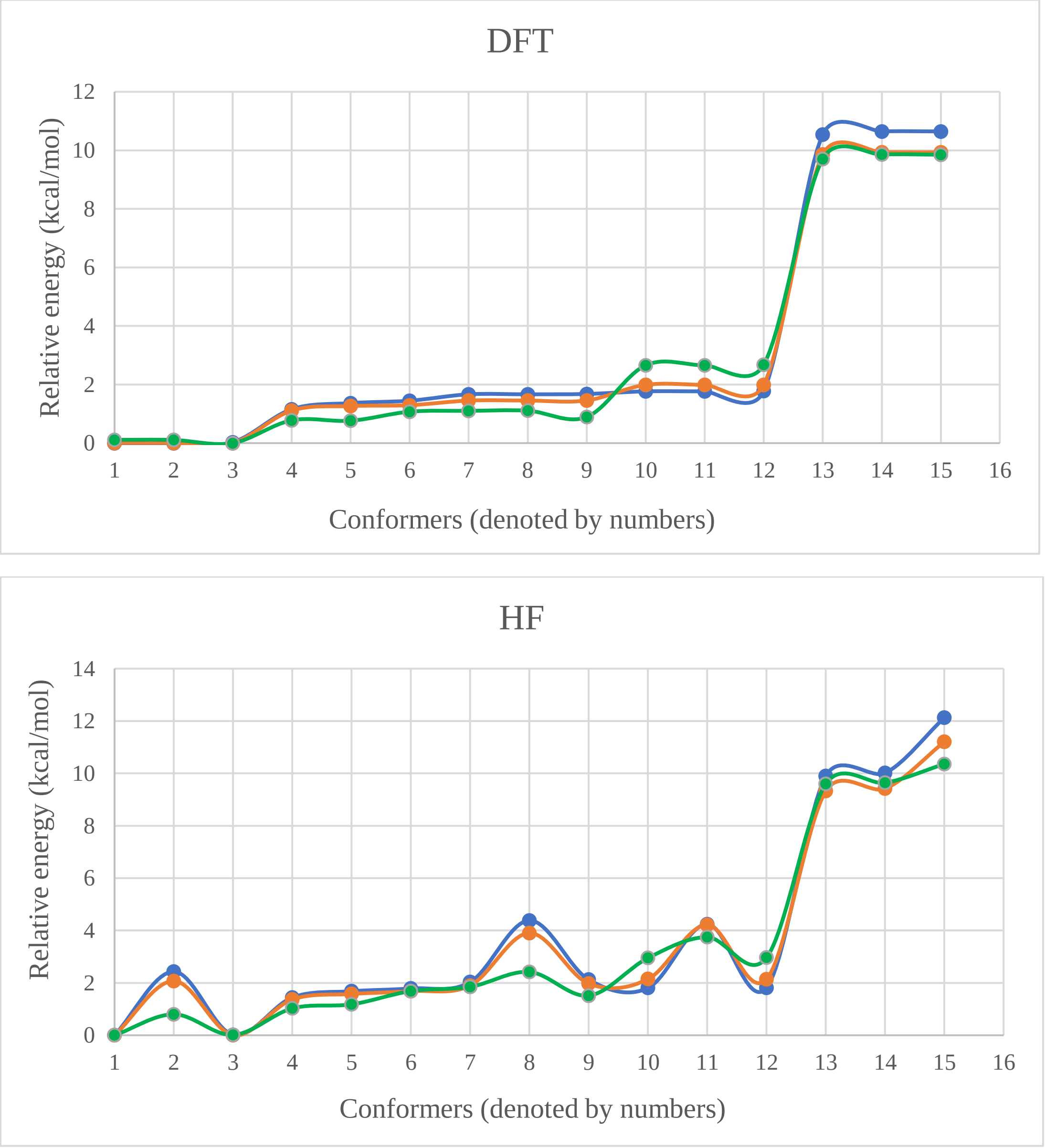
conformer	#	Conformers	#	Conformers	#	Conformers	#
AJP-m-r-u1	1	AJP-k-q-u1	4	AJP-m-r-u2	7	AJP-j-q-u3	10
AJP-m-s-u1	2	AJP-k-r-u1	5	AJP-m-s-u2	8	AJP-j-r-u3	11
AJP-m-q-u1	3	AJP-k-s-u1	6	AJP-m-q-u2	9	AJP-j-s-u3	12

Figure 6.112. Diagrams comparing the uncorrected relative energies (—●—), relative energies corrected for ZPE (—●—) and Gibbs free energies (—●—) of the calculated conformers of compound AJQ.



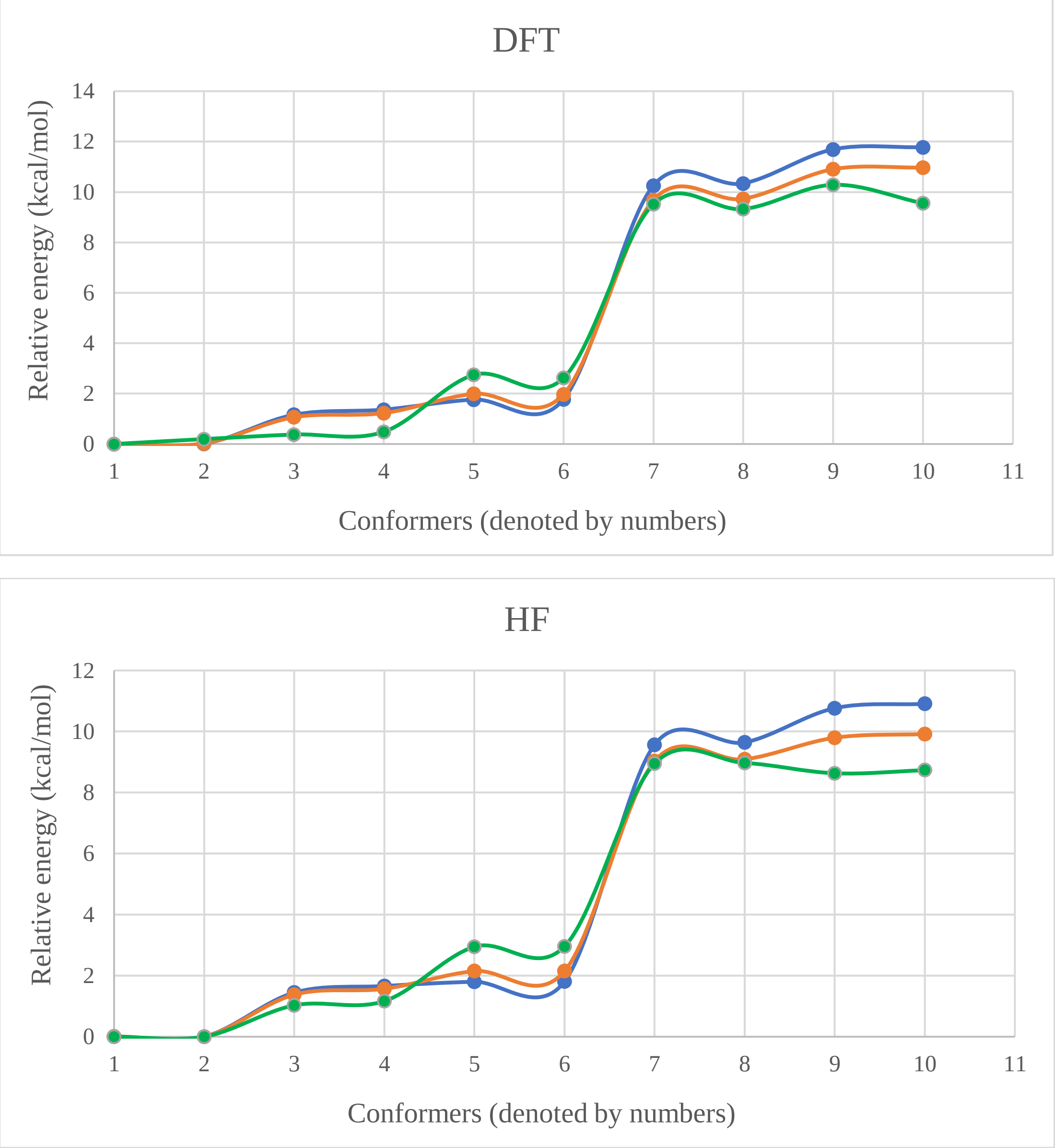
conformer	#	Conformers	#	Conformers	#	Conformers	#
AJQ-p-q-u5	1	AJQ-p-q-u3	5	AJQ-p-r-u3	9	AJQ-k-q-u1′	13
AJQ-m-q-u1	2	AJQ-m-r-u1	6	AJQ-p-s-u3	10	AJQ-k-r-u1	14
AJQ-m-q-u2	3	AJQ-p-q-u5	7	AJQ-m-q-u1	11	AJQ-j-q-u1	15
AJQ-m-r-u2	4	AJQ-m-s-u1	8	AJQ-k-q-u1	12	AJQ-j-r-u1	16

Figure 6.113. Diagrams comparing the uncorrected relative energies (—●—), relative energies corrected for ZPE (—●—) and Gibbs free energies (—●—) of the calculated conformers of compound ALP.



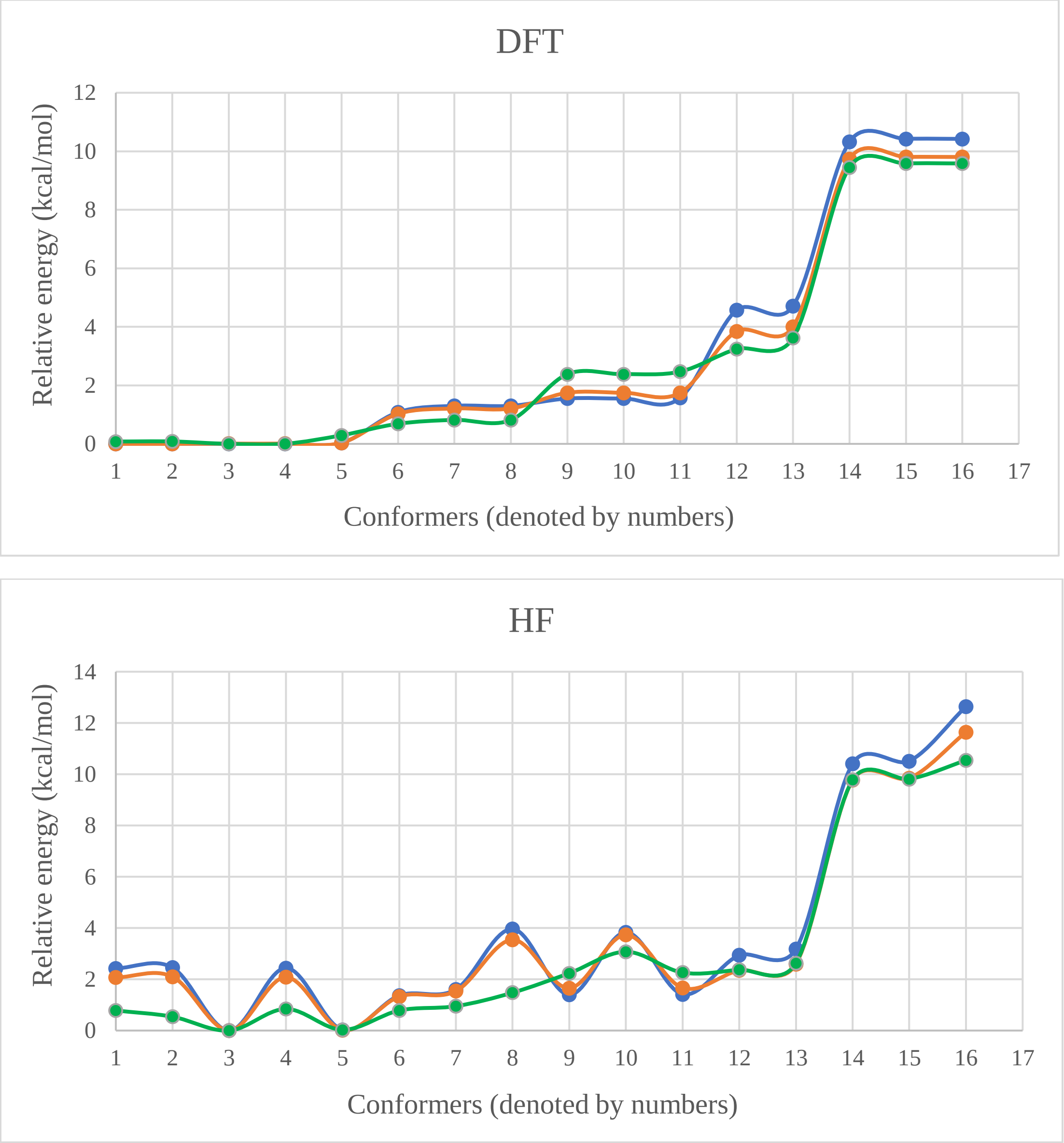
conformer	#	Conformers	#	Conformers	#	Conformers	#
ALP-m-r-u1	1	ALP-k-r-u1	5	ALP-k-r-u3	9	ALP-j-q-u3	13
ALP-m-s-u1	2	ALP-k-q-u1′	6	ALP-m-r-u2	10	ALP-j-r-u3	14
ALP-m-q-u1	3	ALP-k-r-u1′	7	ALP-m-s-u2	11	ALP-j-s-u3	15
ALP-k-q-u1	4	ALP-k-s-u1	8	ALP-m-q-u2	12		

Figure 6.114. Diagrams comparing the uncorrected relative energies (—●—), relative energies corrected for ZPE (—●—) and Gibbs free energies (—●—) of the calculated conformers of compound ALQ.



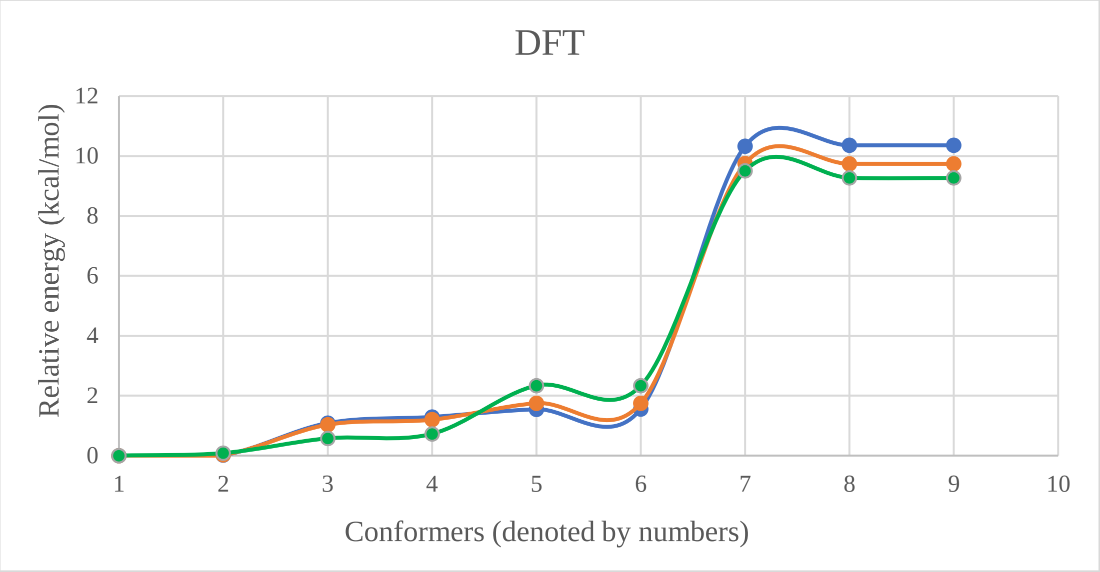
conformer	#	Conformers	#	Conformers	#	Conformers	#
ALQ-m-r-u1	1	ALQ-k-r-u1	4	ALQ-j-q-u3	7	ALQ-j-q-u3	9
ALQ-m-q-u1	2	ALQ-m-r-u2	5	ALQ-j-r-u3	8	ALQ-j-r-u3	10
ALQ-k-q-u1	3	ALQ-m-q-u2	6				

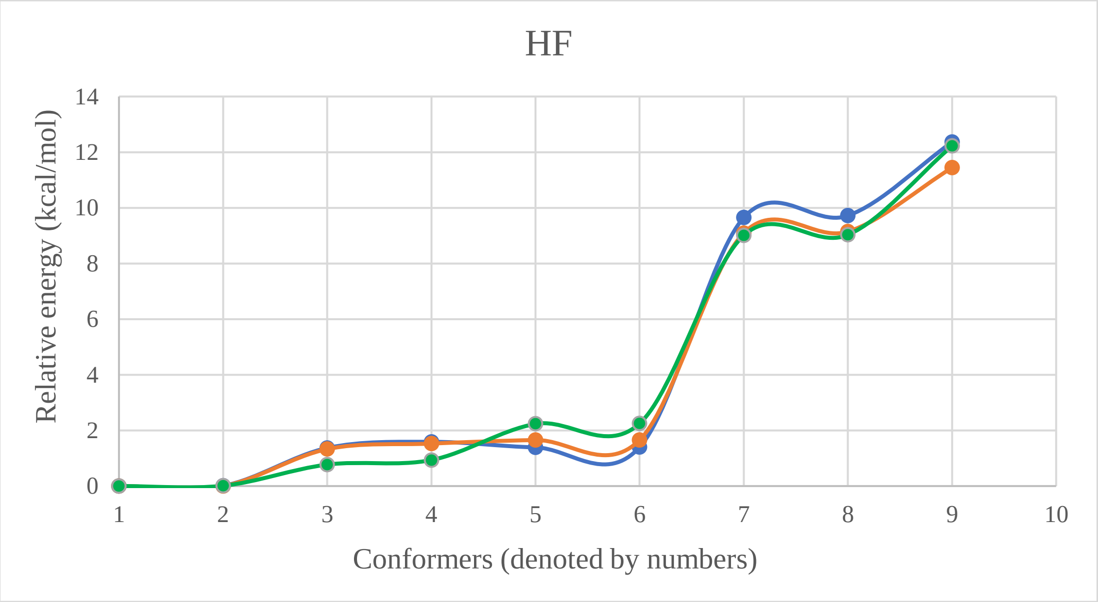
Figure 6.115. Diagrams comparing the uncorrected relative energies (—●—), relative energies corrected for ZPE (—●—) and Gibbs free energies (—●—) of the calculated conformers of compound BGP.



conformer	#	Conformers	#	Conformers	#	Conformers	#
BGP-p-s-v3	1	BGP-m-q-v1	5	BGP-m-r-v2	9	BGP-g-q-v1	13
BGP-p-t-v3	2	BGP-k-q-v3	6	BGP-m-s-v2	10	BGP-j-q-v5	14
BGP-m-r-v1	3	BGP-k-r-v3	7	BGP-m-q-v2	11	BGP-j-r-v5	15
BGP-m-s-v1	4	BGP-k-s-v3	8	BGP-g-r-v1	12	BGP-j-s-v5	16

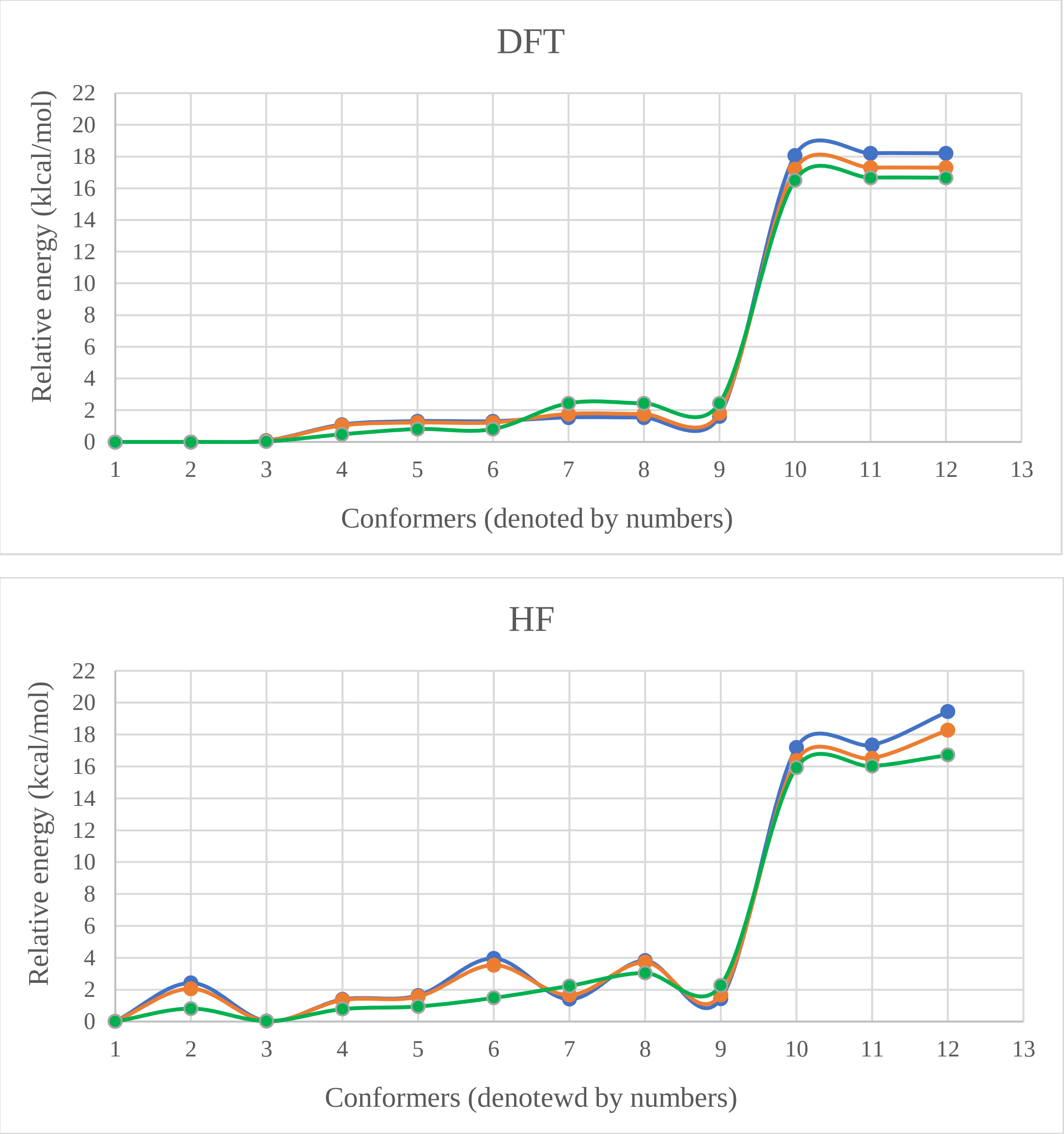
Figure 6.116. Diagrams comparing the uncorrected relative energies (—●—), relative energies corrected for ZPE (—●—) and Gibbs free energies (—●—) of the calculated conformers of compound BGQ.





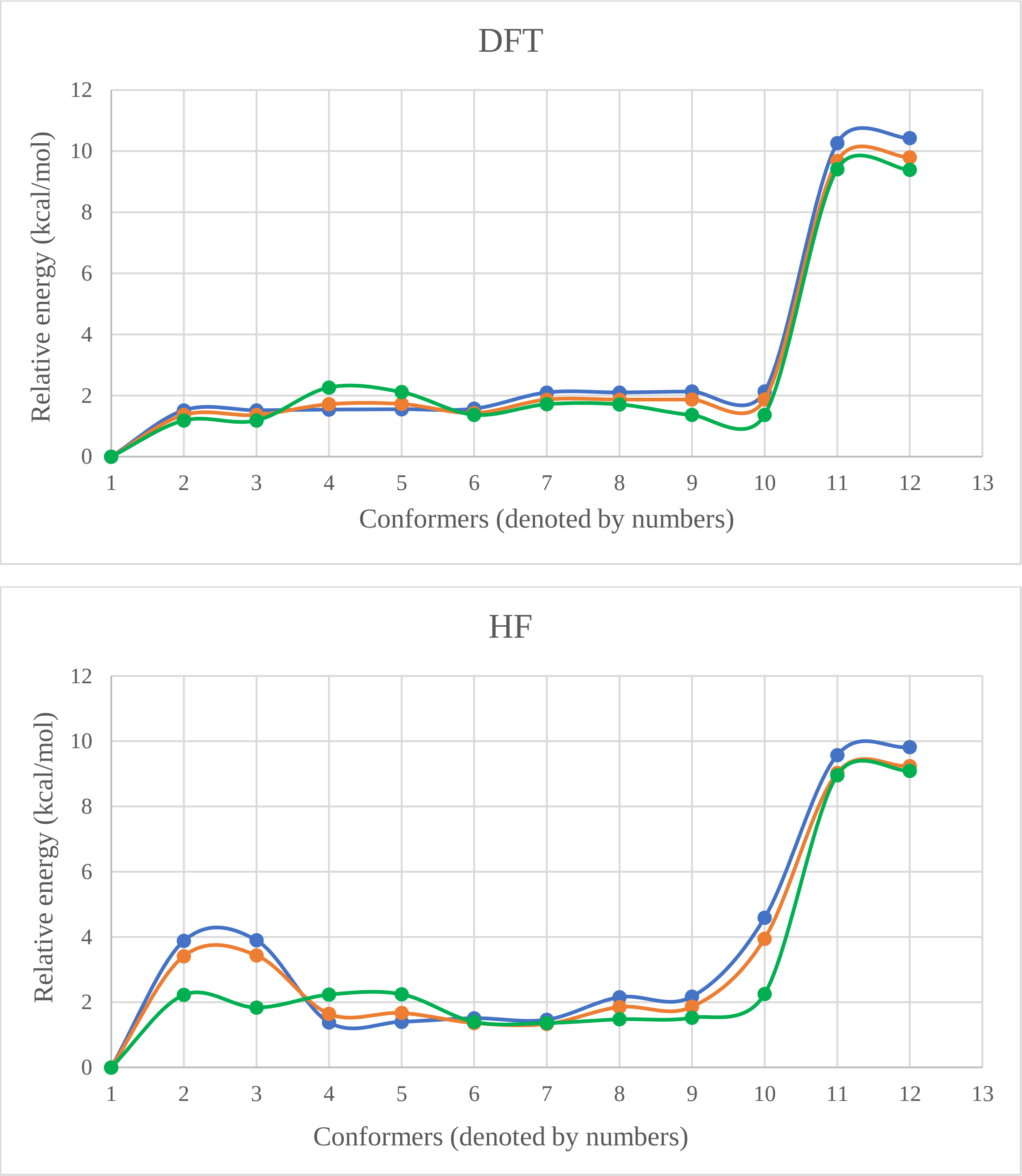
conformer	#	Conformers	#	Conformers	#	Conformers	#
BGQ-m-r-v1	1	BGQ-k-r-v1	4	BGQ-j-q-v3	7	BGQ-j-t-v3	9
BGQ-m-q-v1	2	BGQ-m-r-v2	5	BGQ-j-r-v3	8		
BGQ-k-q-v1	3	BGQ-m-q-v2	6				

Figure 6.117. Diagrams comparing the uncorrected relative energies (—●—), relative energies corrected for ZPE (—●—) and Gibbs free energies (—●—) of the calculated conformers of compound BJP.



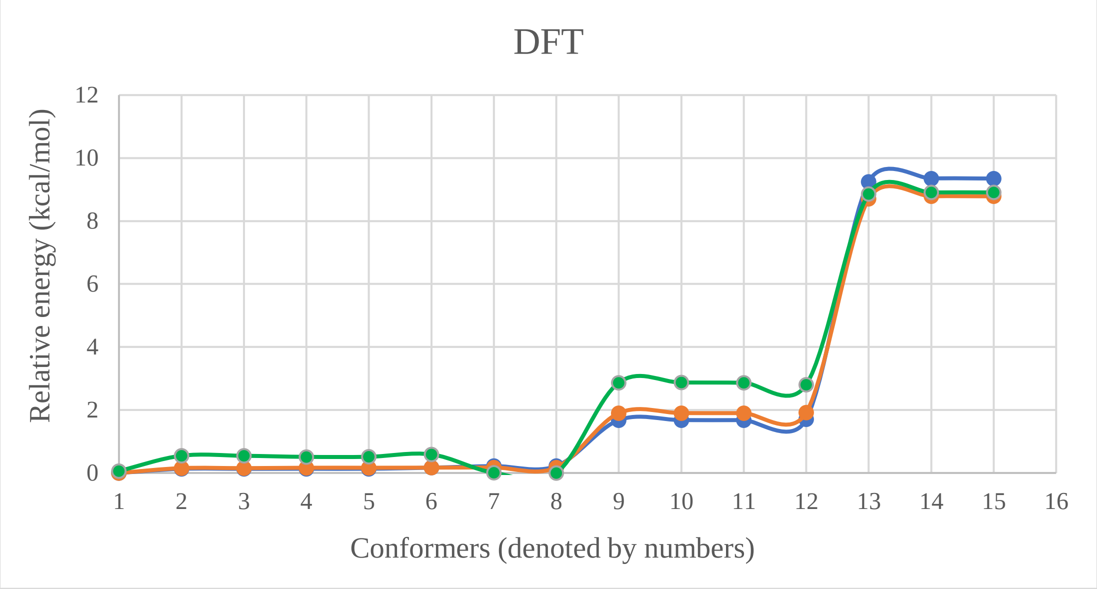
conformer	#	Conformers	#	Conformers	#	Conformers	#
BJP-p-q-v3	1	BJP-k-q-v1	4	BJP-m-r-v2	7	BJP-j-r-v3	10
BJP-p-s-v3	2	BJP-k-r-v1	5	BJP-m-s-v2	8	BJP-j-s-v3	11
BJP-p-r-v3	3	BJP-k-s-v1	6	BJP-m-q-v2	9	BJP-j-q-v3	12

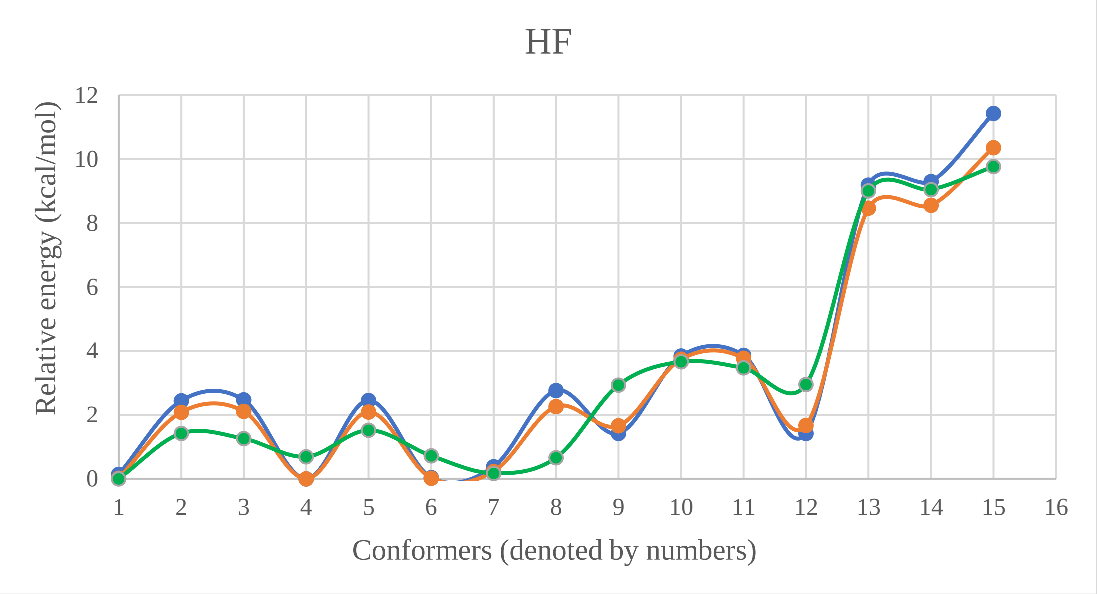
Figure 6.118. Diagrams comparing the uncorrected relative energies (—●—), relative energies corrected for ZPE (—●—) and Gibbs free energies (—●—) of the calculated conformers of compound BJQ.



conformer	#	Conformers	#	Conformers	#	Conformers	#
BJQ-p-r-v3	1	BJQ-m-q-v2	4	BJQ-p-q-v3	7	BJQ-p-s-v3	10
BJQ-m-s-v1	2	BJQ-m-r-v2	5	BJQ-p-q-v3′	8	BJQ-j-q-v3	11
BJQ-m-t-v1	3	BJQ-m-q-v1	6	BJQ-p-r-v3	9	BJQ-j-q-v3	12

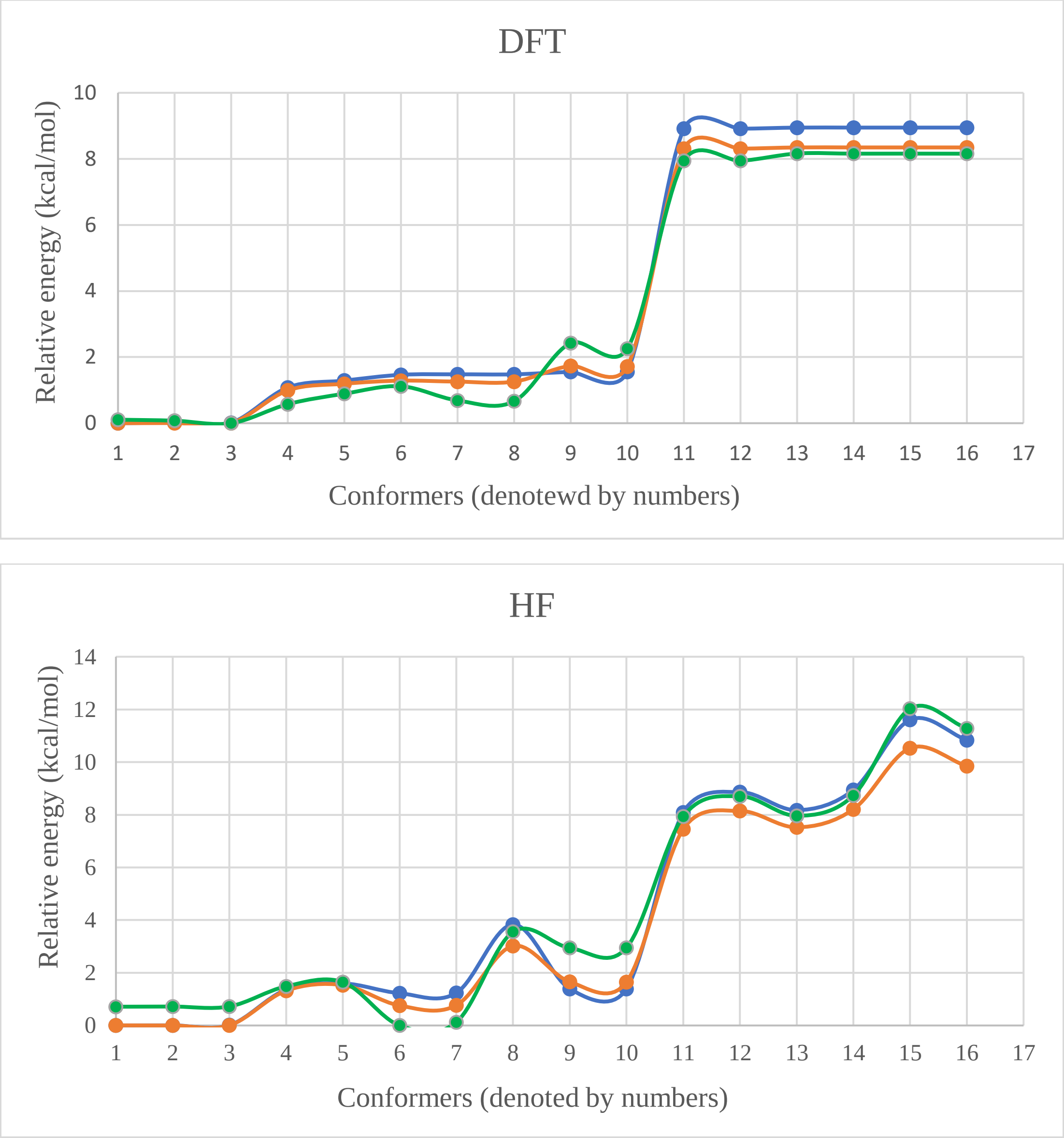
Figure 6.119. Diagrams comparing the uncorrected relative energies (—●—), relative energies corrected for ZPE (—●—) and Gibbs free energies (—●—) of the calculated conformers of compound BLP.





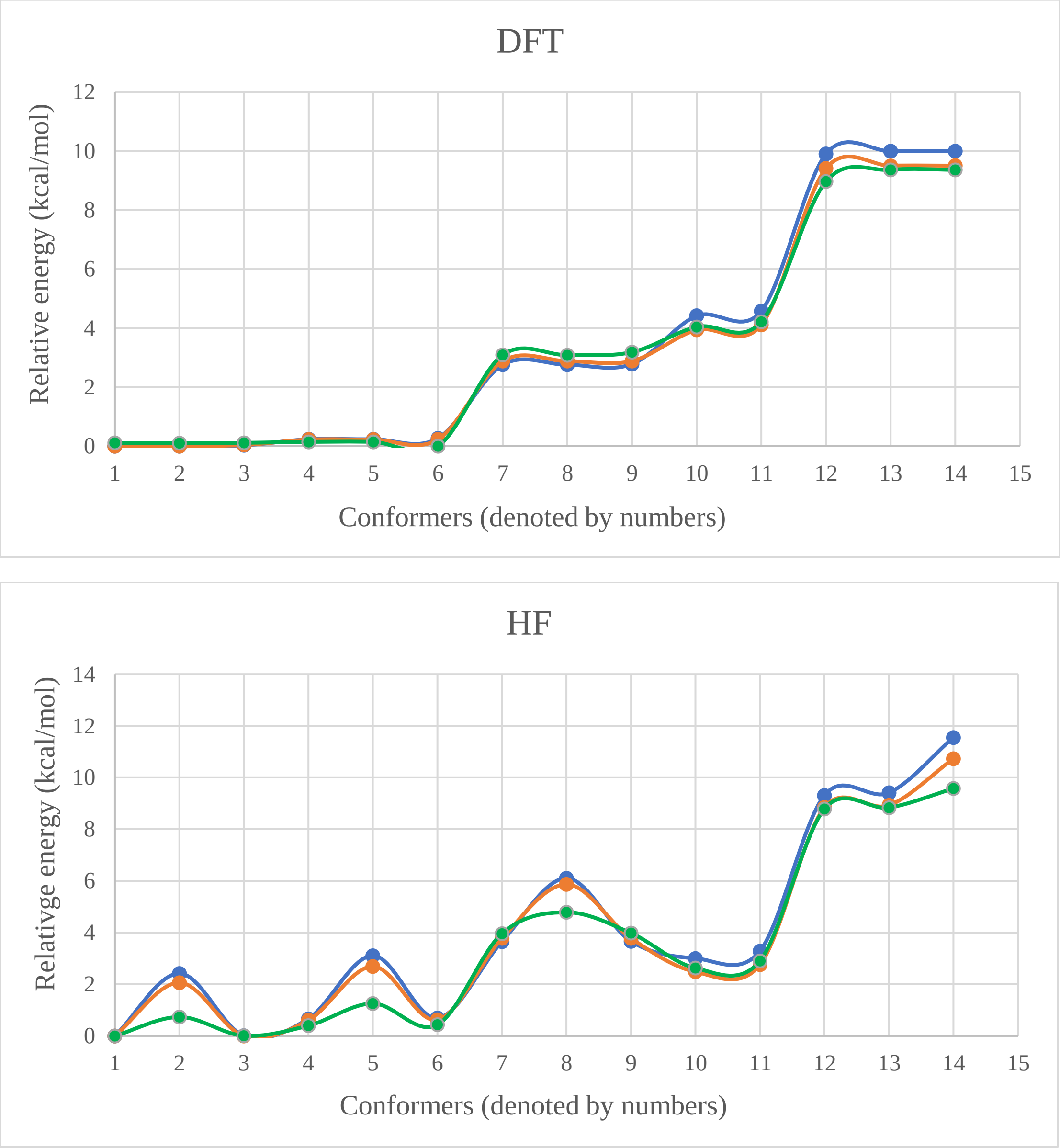
conformer	#	Conformers	#	Conformers	#	Conformers	#
BLP-k-q-v1	1	BLP-m-s-v1	5	BLP-p-q-v4	9	BLP-j-q-v5	13
BLP-p-s-v3	2	BLP-m-r-v1′	6	BLP-p-s-v4	10	BLP-j-r-v5	14
BLP-p-t-v3	3	BLP-k-r-v1	7	BLP-p-t-v4	11	BLP-j-s-v5	15
BLP-m-r-v1	4	BLP-k-s-v1	8	BLP-p-r-v4	12		

Figure 6.120. Diagrams comparing the uncorrected relative energies (—●—), relative energies corrected for ZPE (—●—) and Gibbs free energies (—●—) of the calculated conformers of compound BLQ.



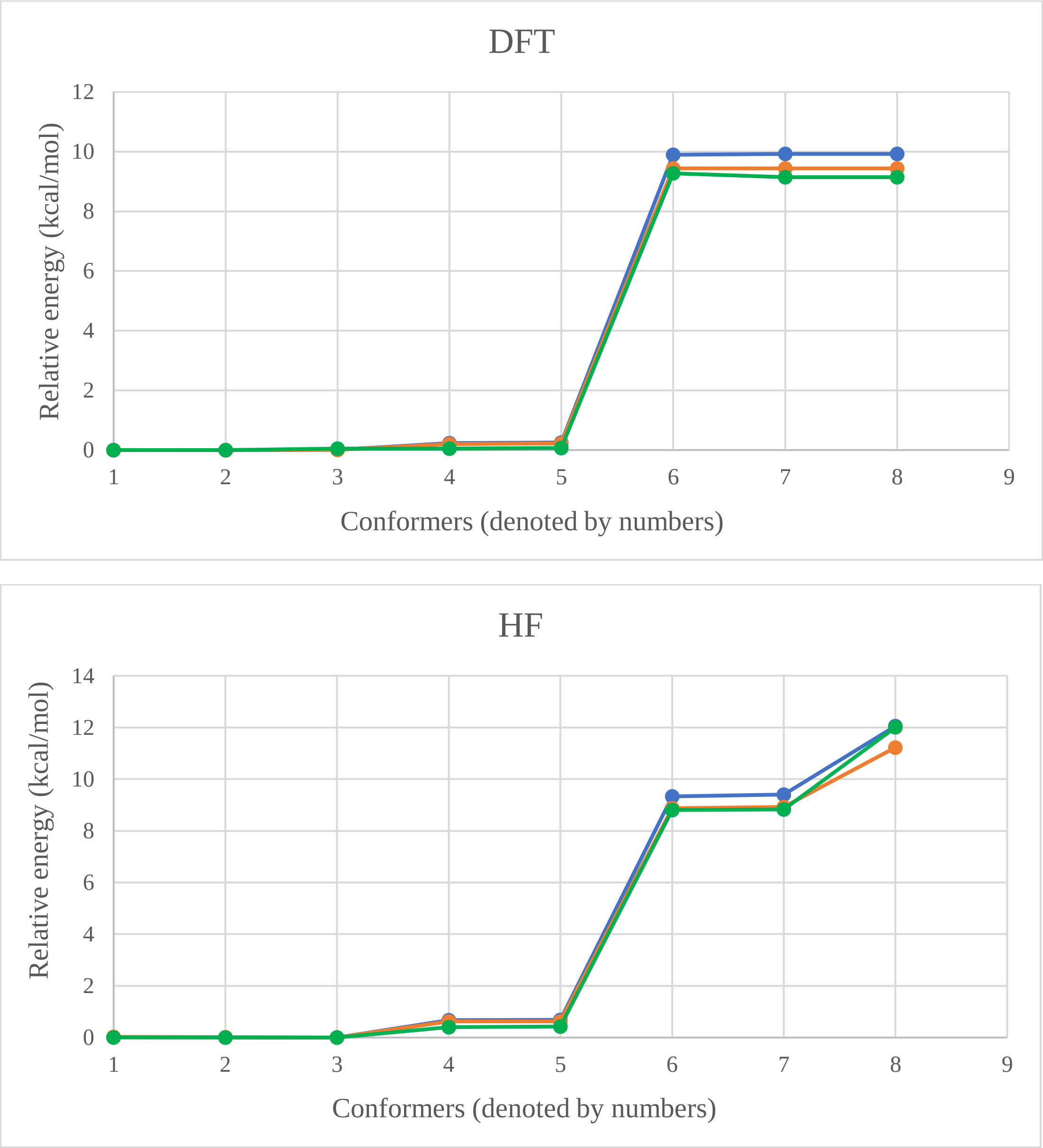
conformer	#	Conformers	#	Conformers	#	Conformers	#
BLQ-p-q-v3	1	BLQ-k-r-v1	5	BLQ-p-q-v4	9	BLQ-j-r-v3	13
BLQ-p-r-v3	2	BLQ-m-r-v1	6	BLQ-p-r-v4	10	BLQ-j-r-v5	14
BLQ-p-r-v3	3	BLQ-m-q-v1	7	BLQ-j-q-v3	11	BLQ-j-t-v3	15
BLQ-k-q-v1	4	BLQ-m-s-v1	8	BLQ-j-q-v5	12	BLQ-j-t-v5	16

Figure 6.121. Diagrams comparing the uncorrected relative energies (—●—), relative energies corrected for ZPE (—●—) and Gibbs free energies (—●—) of the calculated conformers of compound CGP.



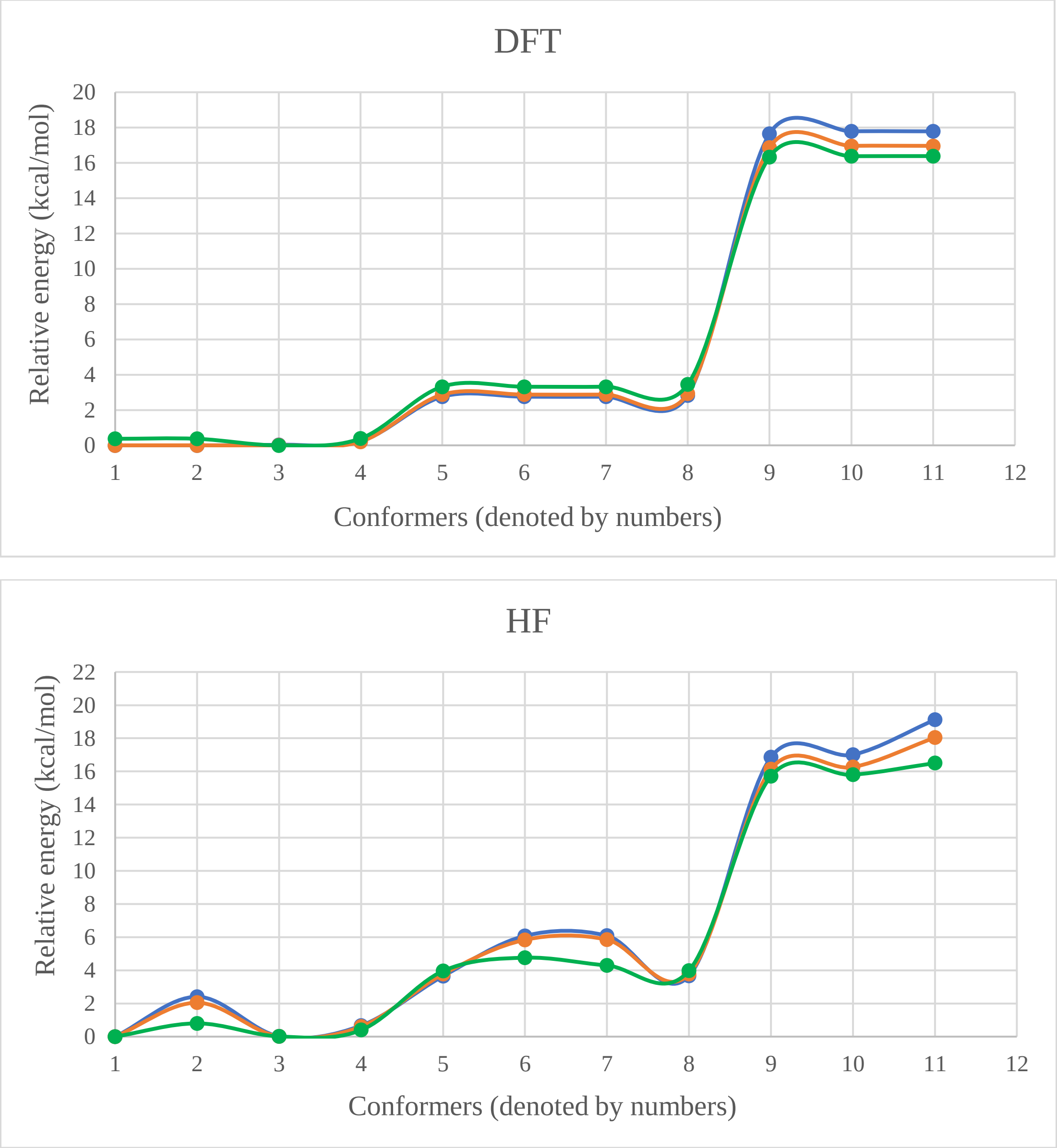
conformer	#	Conformers	#	Conformers	#	Conformers	#
CGP-p-q-w5	1	CGP-m-s-w1	5	CGP-m-q-w2	9	CGP-j-q-w5	12
CGP-p-s-w5	2	CGP-m-q-w1	6	CGP-g-r-w5	10	CGP-j-r-w5	13
CGP-p-r-w5	3	CGP-m-r-w2	7	CGP-g-q-w5	11	CGP-j-s-w5	14
CGP-m-r-w1	4	CGP-m-s-w2	8				

Figure 6.122. Diagrams comparing the uncorrected relative energies (—●—), relative energies corrected for ZPE (—●—) and Gibbs free energies (—●—) of the calculated conformers of compound CGQ.



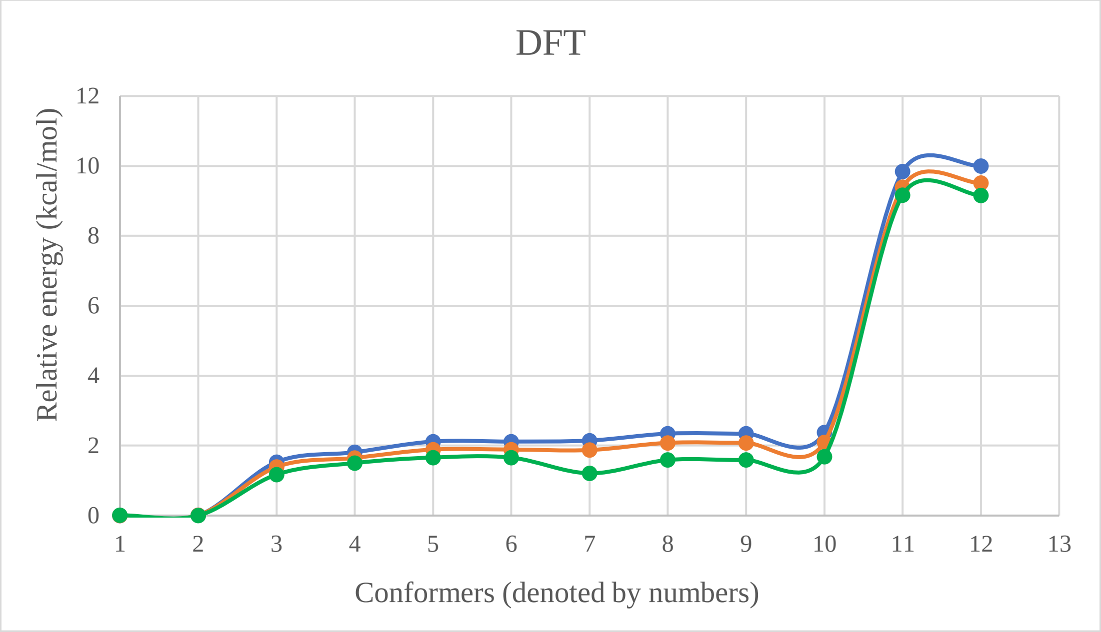
conformer	#	Conformers	#	Conformers	#	Conformers	#
CGQ-p-q-w5	1	CGQ-p-r-w5	3	CGQ-m-q-w1	5	CGQ-j-r-w5	7
CGQ-m-q-w3	2	CGQ-m-r-w1	4	CGQ-j-q-w5	6	CGQ-j-t-w5	8

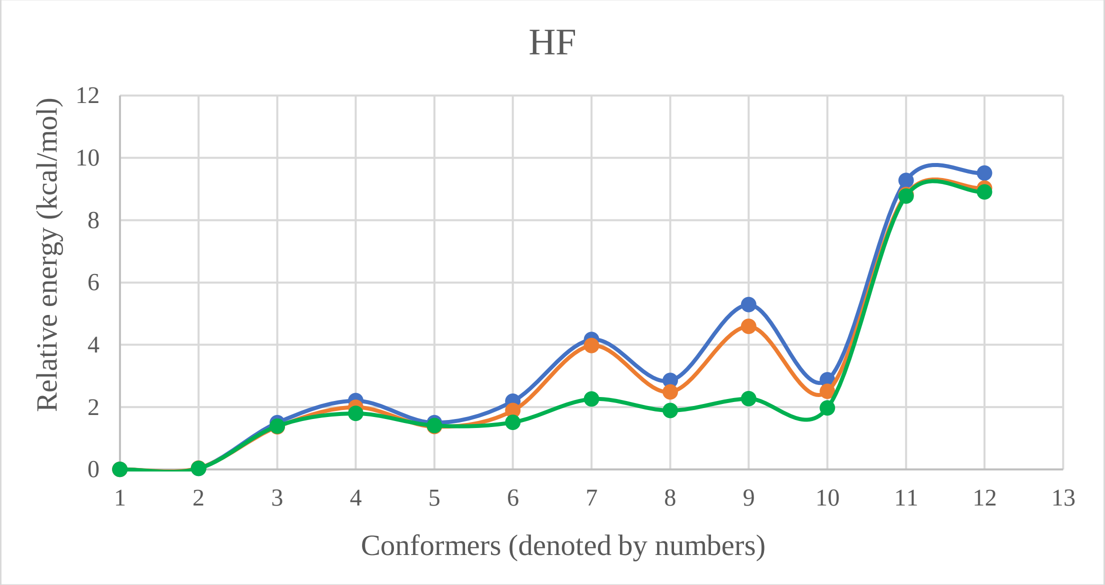
Figure 6.123. Diagrams comparing the uncorrected relative energies (—●—), relative energies corrected for ZPE (—●—) and Gibbs free energies (—●—) of the calculated conformers of compound CJP.



conformer	#	Conformers	#	Conformers	#	Conformers	#
CJP-p-q-w3	1	CJP-m-r-w1	4	CJP-m-t-w2	7	CJP-j-r-w1	10
CJP-p-s-w3	2	CJP-m-r-w2	5	CJP-m-q-w2	8	CJP-j-s-w1	11
CJP-p- r-w3	3	CJP-m-s-w2	6	CJP-j-q-w1	9		

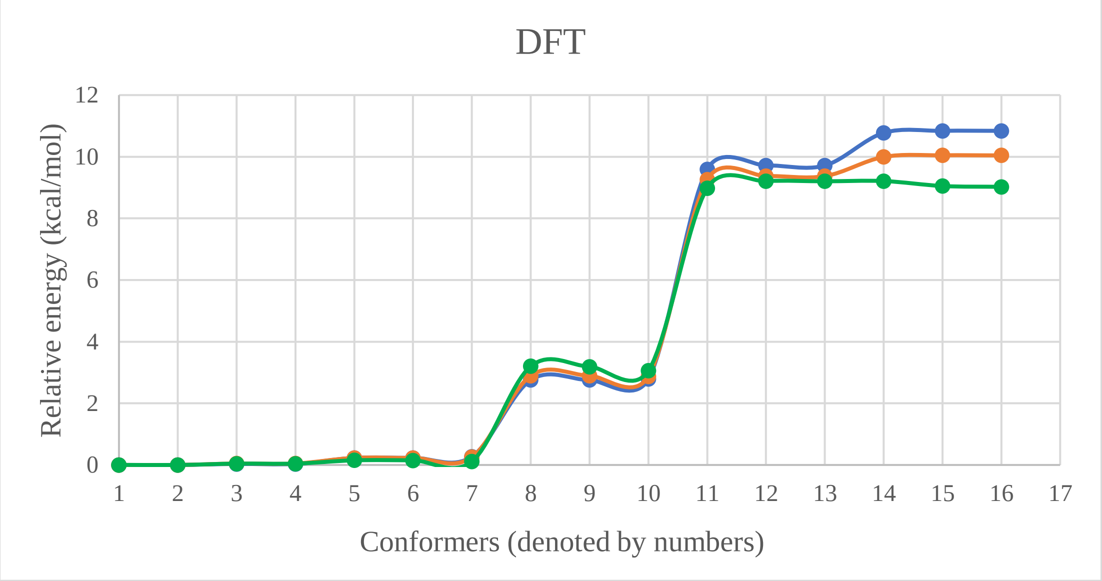
Figure 6.124. Diagrams comparing the uncorrected relative energies (—●—), relative energies corrected for ZPE (—●—) and Gibbs free energies (—●—) of the calculated conformers of compound CJQ.

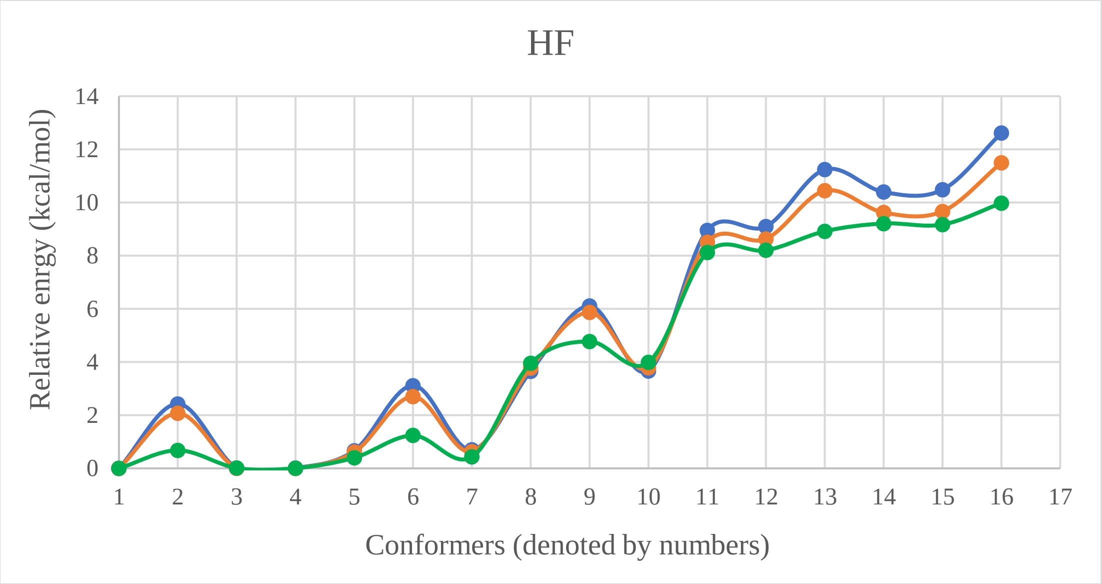




conformer	#	Conformers	#	Conformers	#	Conformers	#
CJQ-m-q-w6	1	CJQ-m-q-w1	4	CJQ-p-s-w5	7	CJQ-m-q-w1′	10
CJQ-m-r-w6	2	CJQ-p-q-w5	5	CJQ-m-r-w1	8	CJQ-j-q-w5	11
CJQ-p-q-w5	3	CJQ-p-q-w5′	6	CJQ-m-s-w1	9	CJQ-j-r-w5	12

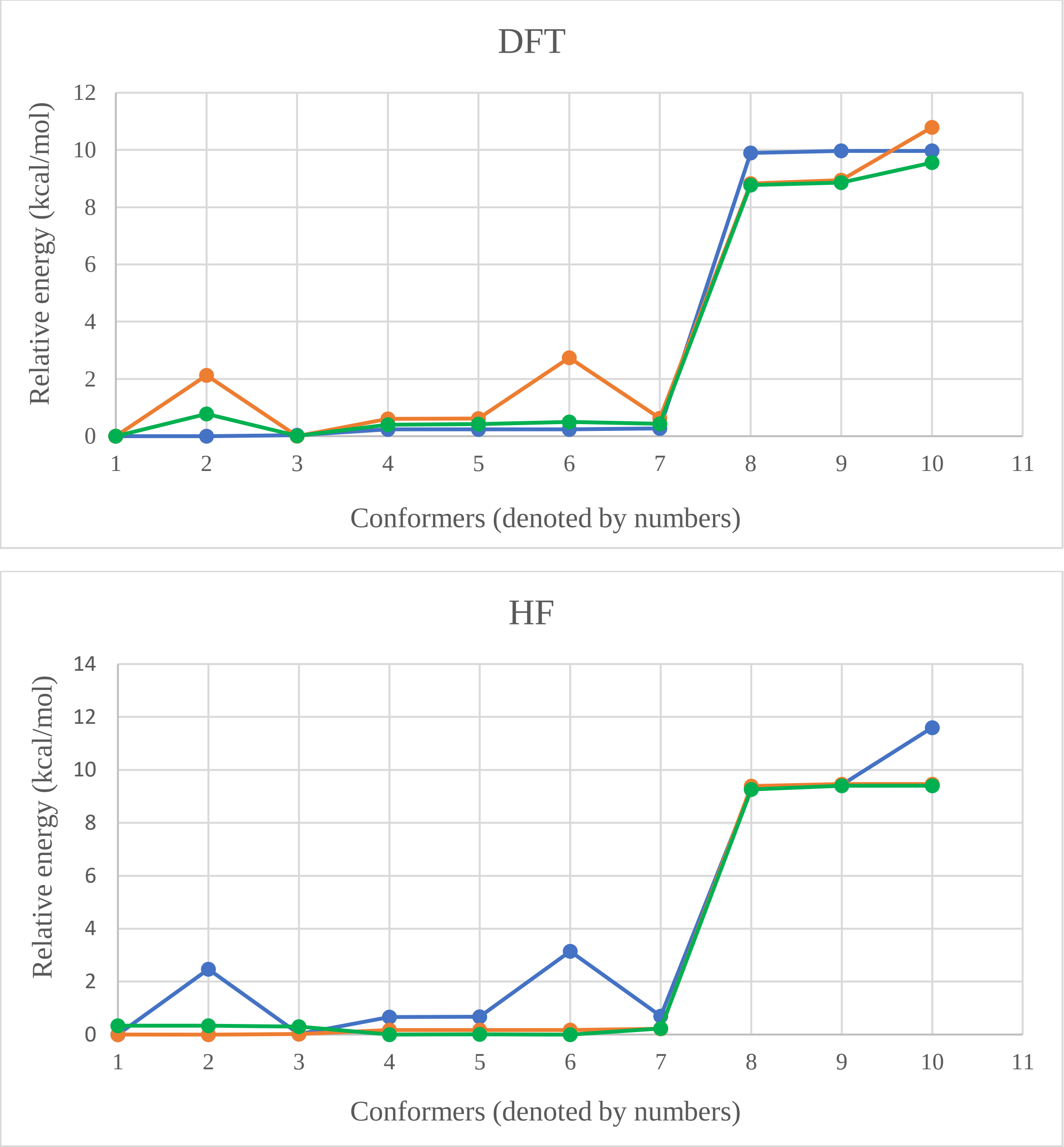
Figure 6.125. Diagrams comparing the uncorrected relative energies (—●—), relative energies corrected for ZPE (—●—) and Gibbs free energies (—●—) of the calculated conformers of compound CLP.





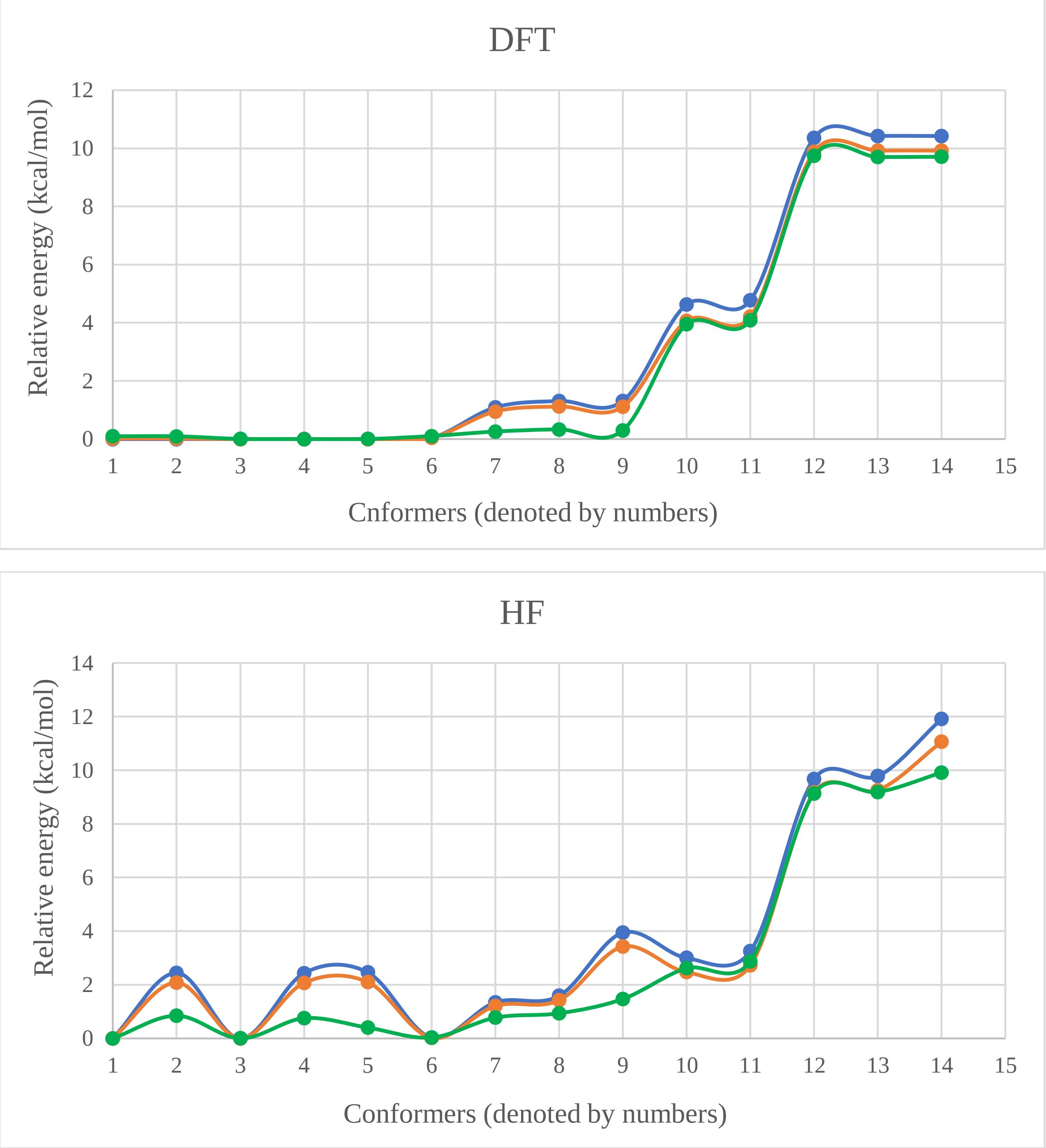
conformer	#	Conformers	#	Conformers	#	Conformers	#
CLP-p-q-w5	1	CLP-m-r-w1	5	CLP-m-s-w2	9	CLP-j-s-w5	13
CLP-p-s-w5	2	CLP-m-s-w1	6	CLP-m-q-w2	10	CLP-j-q-w6	14
CLP-p-r-w5	3	CLP-m-q-w1	7	CLP-j-q-w5	11	CLP-j-r-w6	15
CLP-p-r-w5′	4	CLP-m-q-w2	8	CLP-j-r-w5	12	CLP-j-s-w6	16

Figure 6.126. Diagrams comparing the uncorrected relative energies (—●—), relative energies corrected for ZPE (—●—) and Gibbs free energies (—●—) of the calculated conformers of compound CLQ.



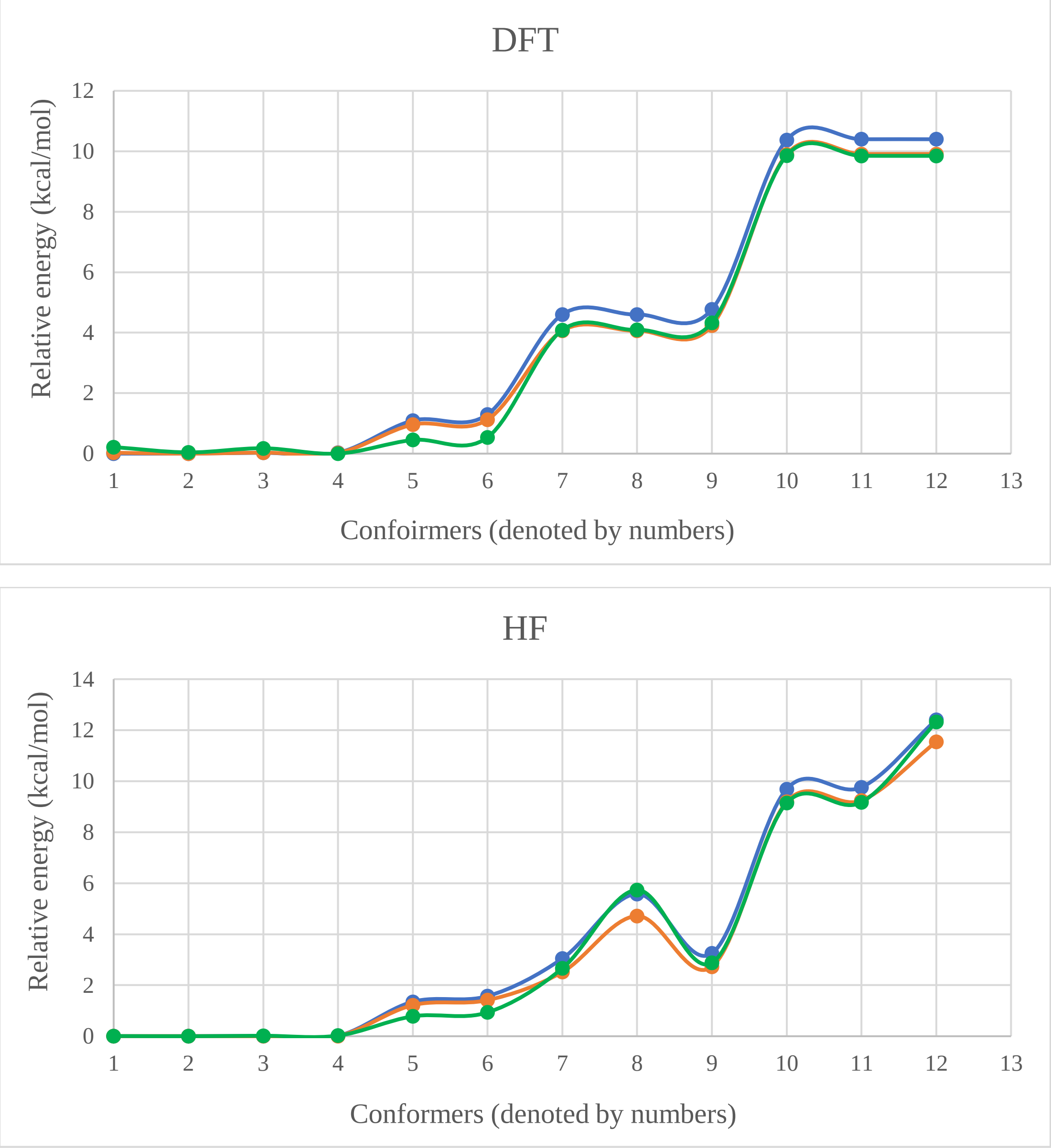
conformer	#	Conformers	#	Conformers	#	Conformers	#
CLQ-p-q-w5	1	CLQ-m-r-w1′	4	CLQ-m-q-w1′	7	CLQ-j-r-w5	9
CLQ-p-s-w5	2	CLQ-m-r-w1	5	CLQ-j-q-w5	8	CLQ-j-s-w6	10
CLQ-m-q-w1	3	CLQ-m-s-w1	6				

Figure 6.127. Diagrams comparing the uncorrected relative energies (—●—), relative energies corrected for ZPE (—●—) and Gibbs free energies (—●—) of the calculated conformers of compound DGP.



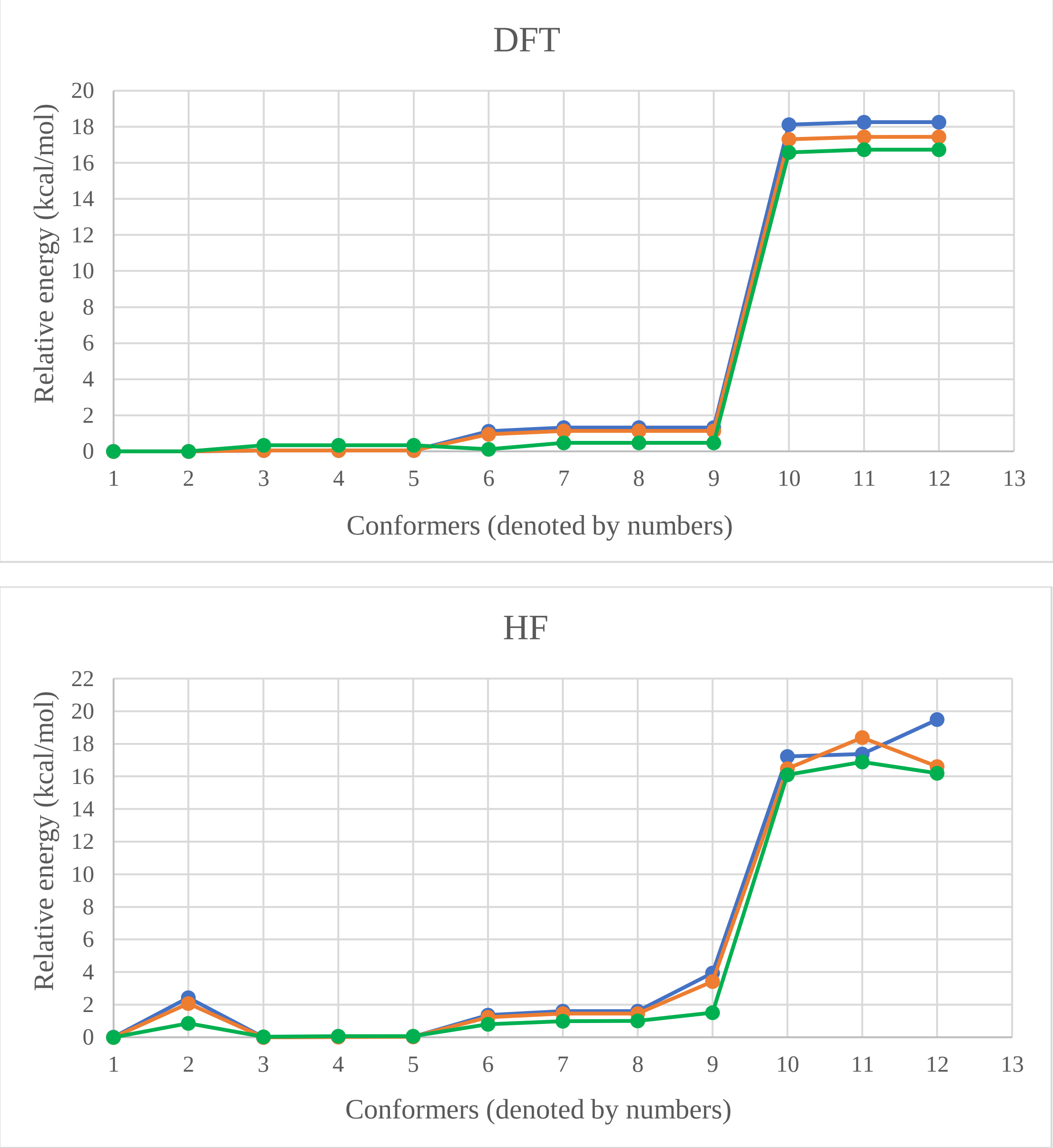
conformer	#	Conformers	#	Conformers	#	Conformers	#
DGP-m-r	1	DGP-p-t	5	DGP-k-s	9	DGP-j-q	12
DGP-m-s	2	DGP-m-q	6	DGP-g-r	10	DGP-j-r	13
DGP-p-q	3	DGP-k-q	7	DGP-g-q	11	DGP-j-s	14
DGP-p-s	4	DGP-k-r	8				

Figure 6.128. Diagrams comparing the uncorrected relative energies (—●—), relative energies corrected for ZPE (—●—) and Gibbs free energies (—●—) of the calculated conformers of compound DGQ.



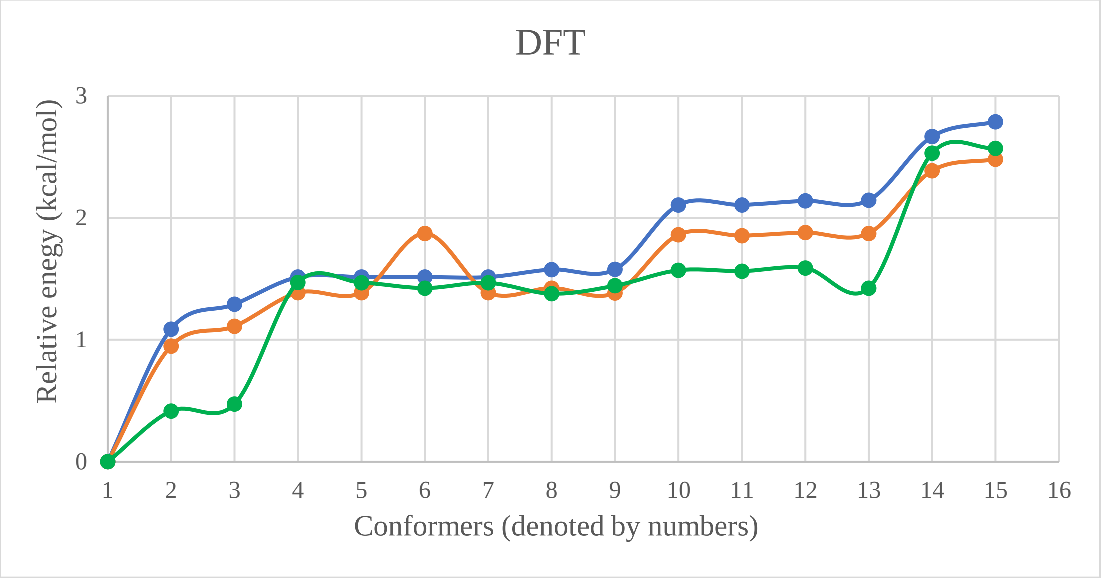
conformer	#	Conformers	#	Conformers	#	Conformers	#
DGQ-m-r	1	DGQ-m-q′	4	DGQ-g-r	7	DGQ-j-q	10
DGQ-p-q	2	DGQ-k-q	5	DGQ-g-t	8	DGQ-j-r	11
DGQ-m-q	3	DGQ-k-r	6	DGQ-g-q	9	DGQ-j-t	12

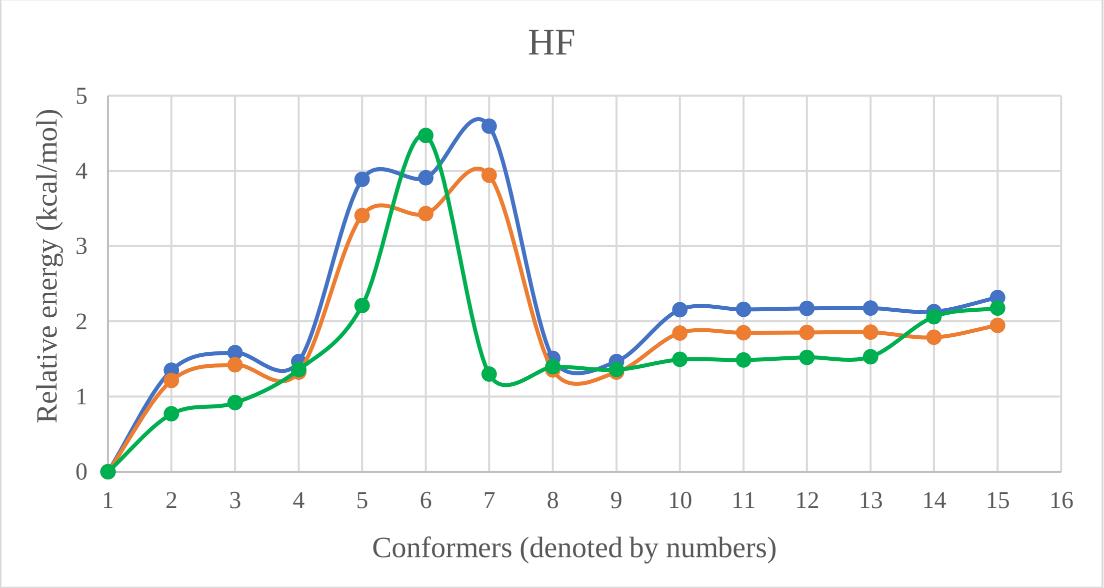
Figure 6.129. Diagrams comparing the uncorrected relative energies (—●—), relative energies corrected for ZPE (—●—) and Gibbs free energies (—●—) of the calculated conformers of compound DJP.



conformer	#	Conformers	#	Conformers	#	Conformers	#
DJP-m-r	1	DJP-m-q	4	DJP-k-r	7	DJP-j-q	10
DJP-p-s	2	DJP-p-r	5	DJP-k-r′	8	DJP-j-s	11
DJP-p-q	3	DJP-k-q	6	DJP-k-s	9	DJP-j-r	12

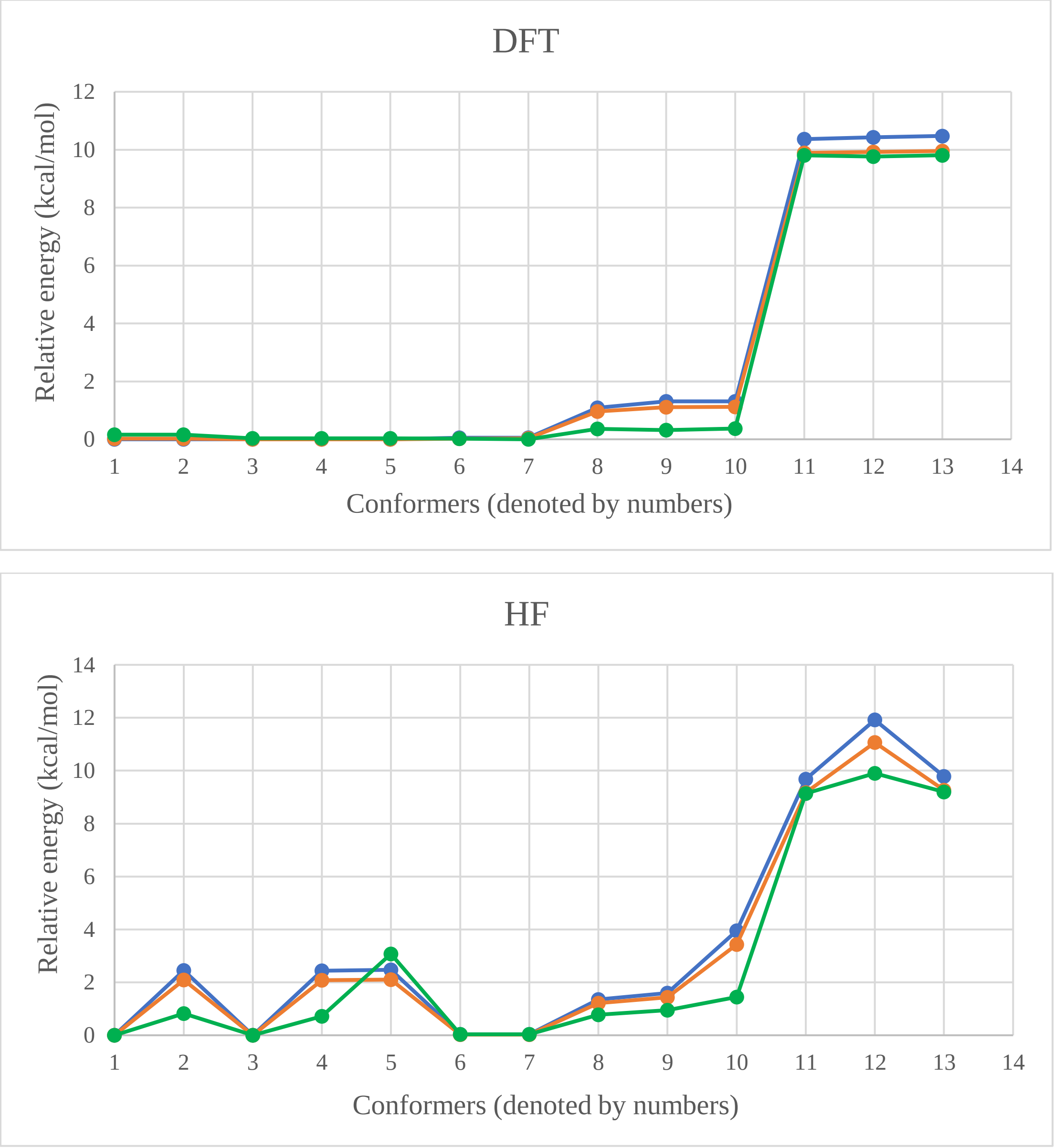
Figure 6.130. Diagrams comparing the uncorrected relative energies (—●—), relative energies corrected for ZPE (—●—) and Gibbs free energies (—●—) of the calculated conformers of compound DJQ.





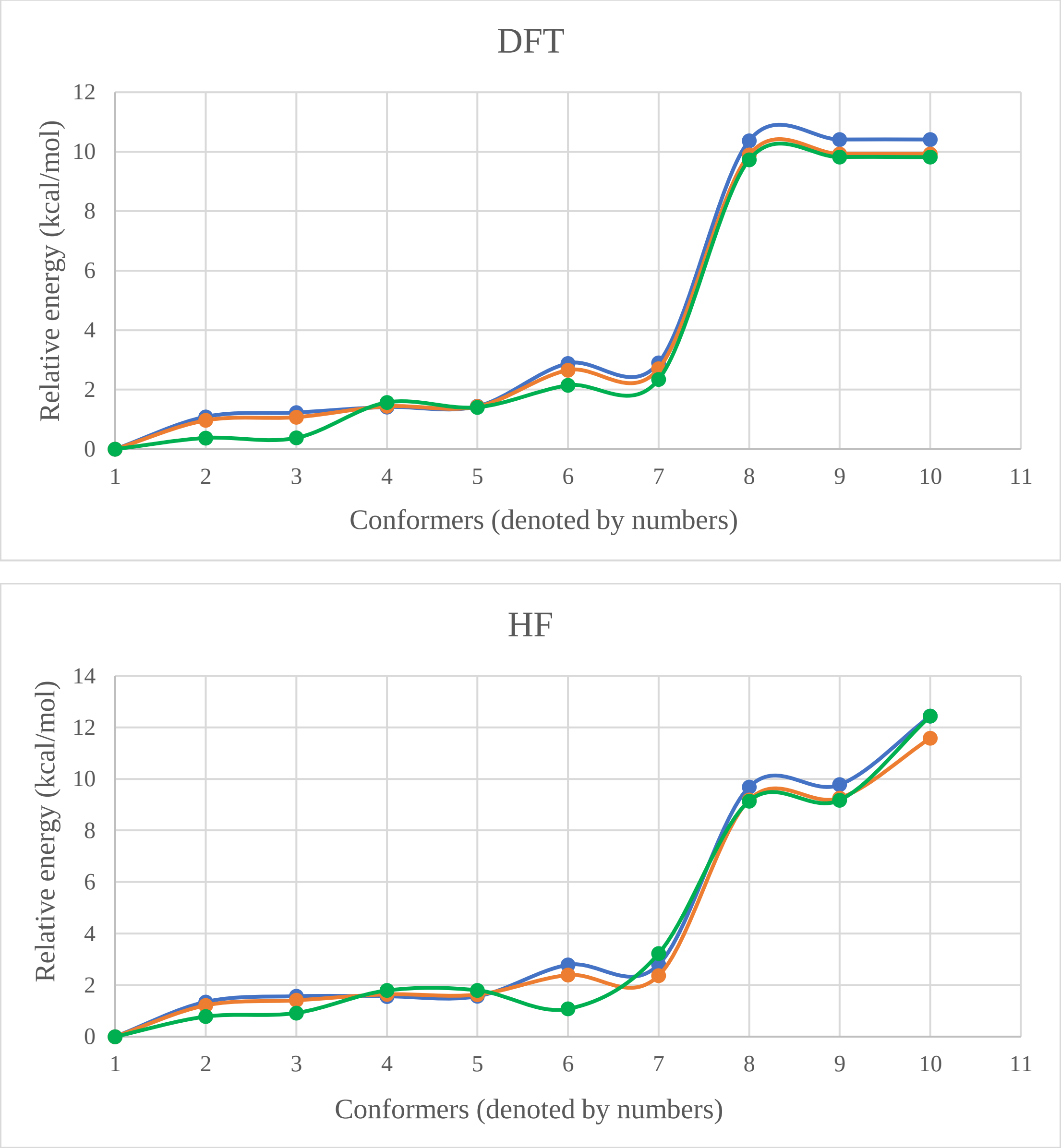
conformer	#	Conformers	#	Conformers	#	Conformers	#
DJQ-m-q	1	DJQ-m-s	5	DJQ-p-q	9	DJQ-m-q	13
DJQ-k-q	2	DJQ-m-t	6	DJQ-m-r′	10	DJQ-j-q	14
DJQ-k-r	3	DJQ-m-s′	7	DJQ-p-q′	11	DJQ-j-r	15
DJQ-m-r	4	DJQ-m-q	8	DJQ-p-r	12		

Figure 6.131. Diagrams comparing the uncorrected relative energies (—●—), relative energies corrected for ZPE (—●—) and Gibbs free energies (—●—) of the calculated conformers of compound DLP.



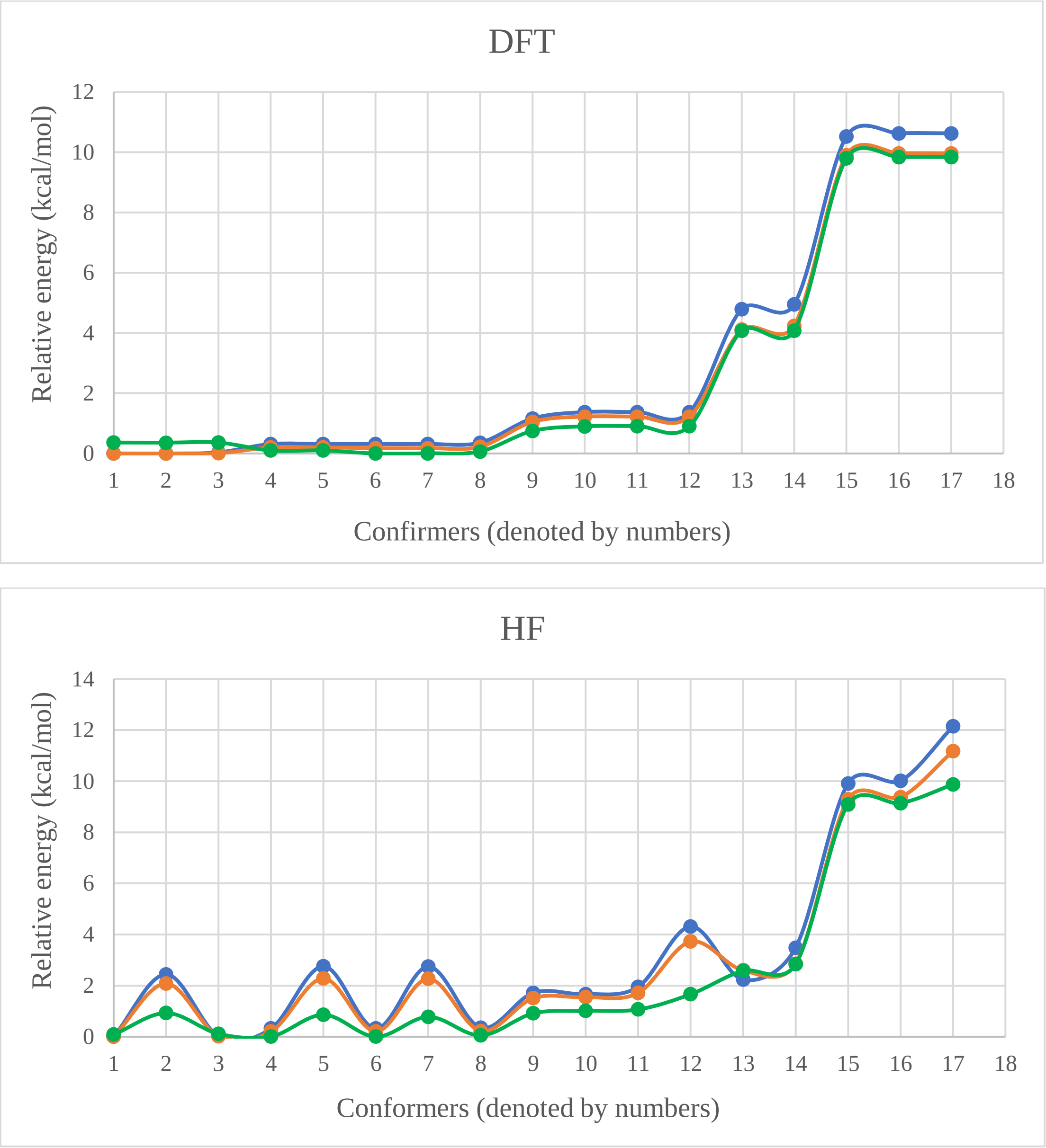
conformer	#	Conformers	#	Conformers	#	Conformers	#
DLP-m-r	1	DLP-p-t	5	DLP-k-r	9	DLP-j-s	12
DLP-m-s	2	DLP-m-q	6	DLP-k-s	10	DLP-j-r	13
DLP-p-q	3	DLP-p-r	7	DLP-j-q	11		
DLP-p-s	4	DLP-k-q	8				

Figure 6.132. Diagrams comparing the uncorrected relative energies (●), relative energies corrected for ZPE (●) and Gibbs free energies (●) of the calculated conformers of compound DLQ.



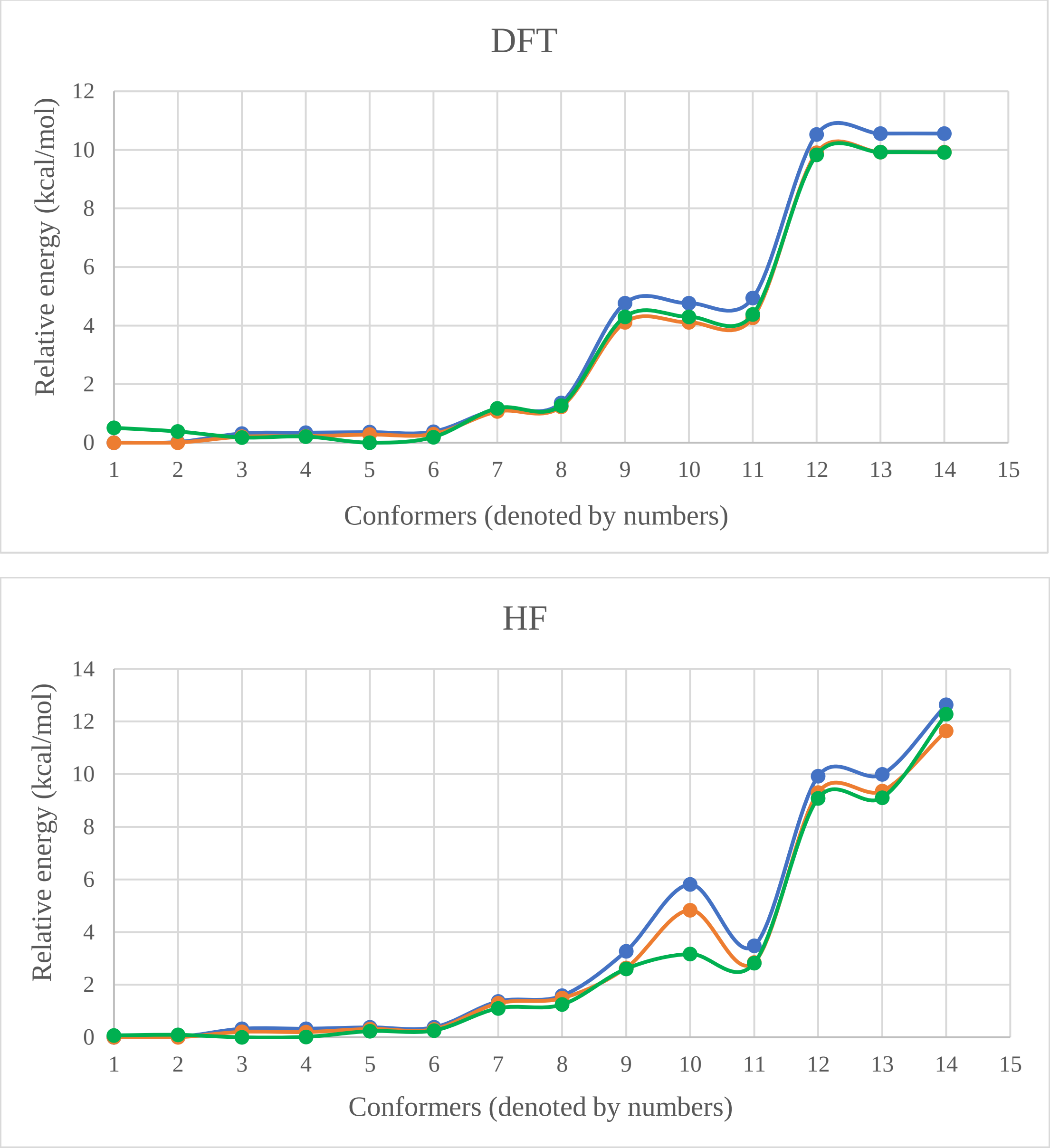
conformer	#	Conformers	#	Conformers	#	Conformers	#
DLQ-p-q	1	DLQ-m-r	4	DLQ-m-q′	7	DLQ-j-r	9
DLQ-k-q	2	DLQ-m-q	5	DLQ-j-q	8	DLQ-j-t	10
DLQ-k-r	3	DLQ-m-r′	6				

Figure 6.133. Diagrams comparing the uncorrected relative energies (—●—), relative energies corrected for ZPE (—●—) and Gibbs free energies (—●—) of the calculated conformers of compound EGP.



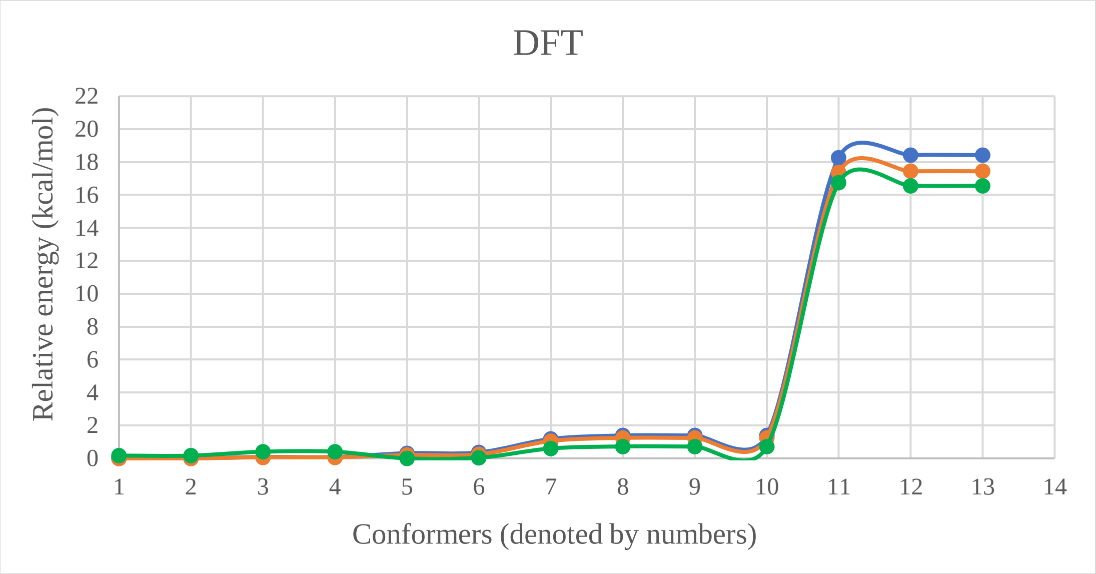
conformer	#	Conformers	#	Conformers	#	Conformers	#
EGP-m-r-x4	1	EGP-p-q-x3	6	EGP-k-q-x1	11	EGP-j-q-x3	15
EGP-m-s-x4	2	EGP-p-s-x3	7	EGP-k-s-x1	12	EGP-j-r-x3	16
EGP-m-q-x4	3	EGP-m-q-x1	8	EGP-g-r-x1	13	EGP-j-s-x3	17
EGP-m-r-x1	4	EGP-k-q-x1	9	EGP-g-q-x1	14		
EGP-m-s-x1	5	EGP-k-r-x2	10				

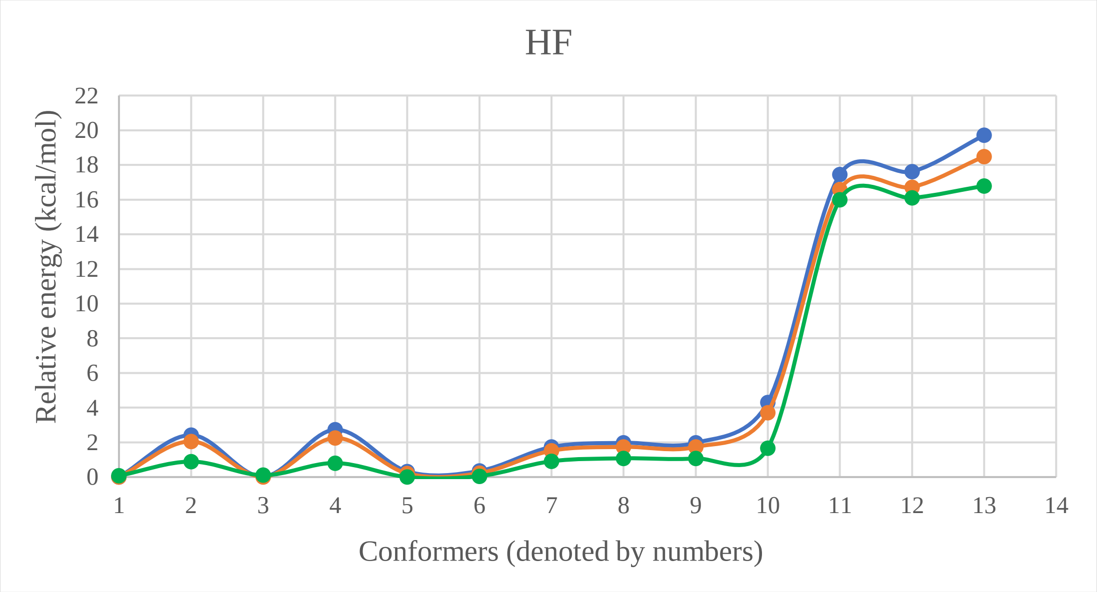
Figure 6.134. Diagrams comparing the uncorrected relative energies (—●—), relative energies corrected for ZPE (—●—) and Gibbs free energies (—●—) of the calculated conformers of compound EGQ.



conformer	#	Conformers	#	Conformers	#	Conformers	#
EGQ-m-r-x4	1	EGQ-p-q-x3	5	EGQ-g-r-x1	9	EGQ-j-q-x3	12
EGQ-m-q-x4	2	EGQ-p-r-x3	6	EGQ-g-t-x1	10	EGQ-j-r-x3	13
EGQ-m-r-x1	3	EGQ-k-q-x4	7	EGQ-g-q-x1	11	EGQ-j-t-x3	14
EGQ-m-q-x1	4	EGQ-k-r-x4	8				

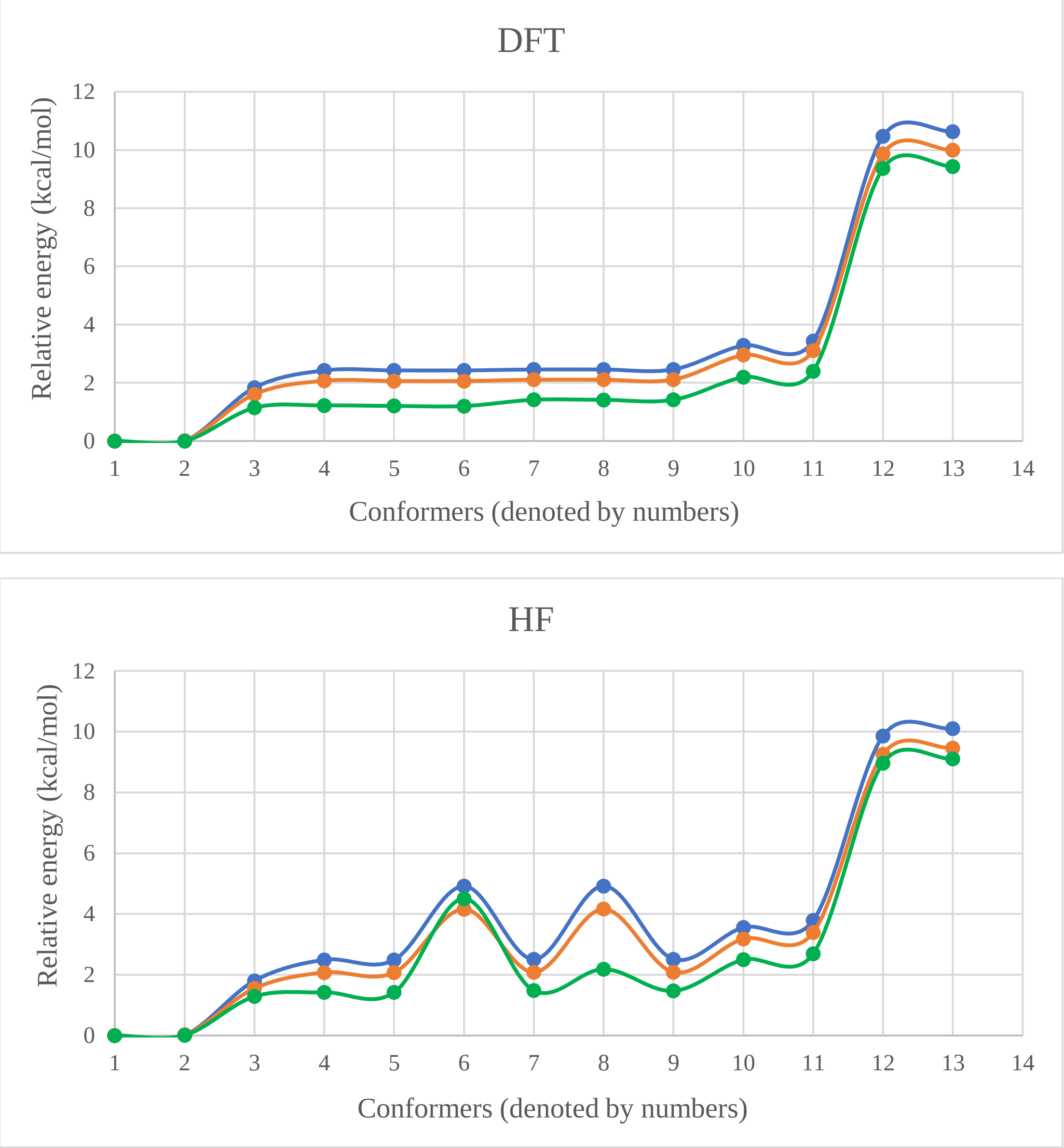
Figure 6.135. Diagrams comparing the uncorrected relative energies (—●—), relative energies corrected for ZPE (—●—) and Gibbs free energies (—●—) of the calculated conformers of compound EJP.





conformer	#	Conformers	#	Conformers	#	Conformers	#
EJP-m-s-x4	1	EJP-p-q-x4	5	EJP-k-r-x1′	9	EJP-j-r-x3	12
EJP-m-r-x4	2	EJP-p-r-x4	6	EJP-k-s-x1	10	EJP-j-s-x3	13
EJP-m-q-x4	3	EJP-k-q-x1	7	EJP-j-q-x3	11		
EJP-p-s-x4	4	EJP-k-r-x1	8				

Figure 6.136. Diagrams comparing the uncorrected relative energies (—●—), relative energies corrected for ZPE (—●—) and Gibbs free energies (—●—) of the calculated conformers of compound EJQ.

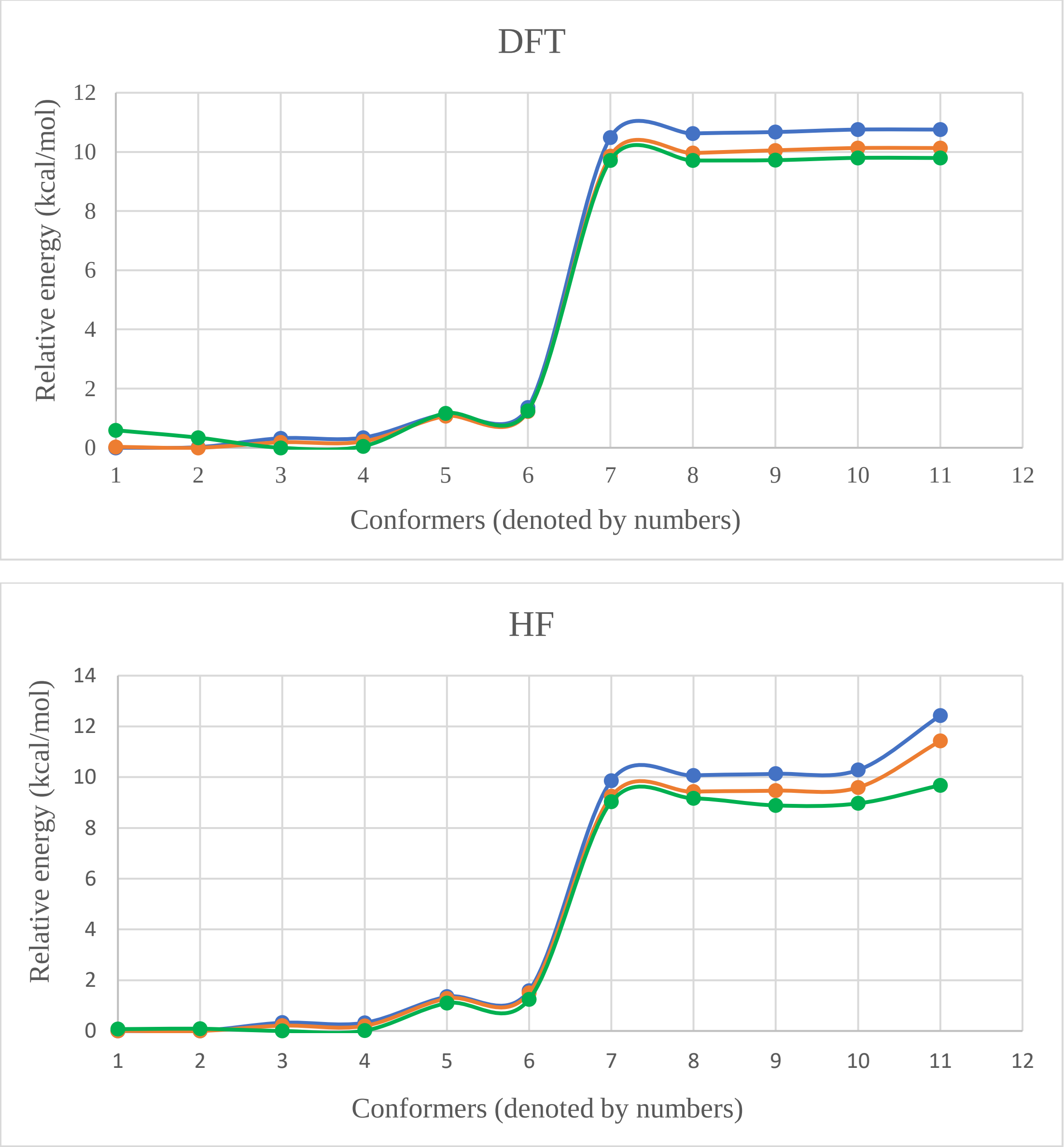


conformer	#	Conformers	#	Conformers	#	Conformers	#
EJQ-m-q-x4	1	EJQ-m-r-x1	5	EJQ-m-q-x1	9	EJQ-j-q-x3	12
EJQ-m-r-x4	2	EJQ-m-s-x1	6	EJQ-k-q-x4	10	EJQ-j-r-x3	13
EJQ-p-q-x4	3	EJQ-p-r-x4	7	EJQ-k-r-x4	11		
EJQ-p-q-x4′	4	EJQ-p-s-x4	8				

Figure 6.137. Diagrams comparing the uncorrected relative energies (—●—), relative energies corrected for ZPE (—●—) and Gibbs free energies (—●—) of the calculated conformers of compound ELP.

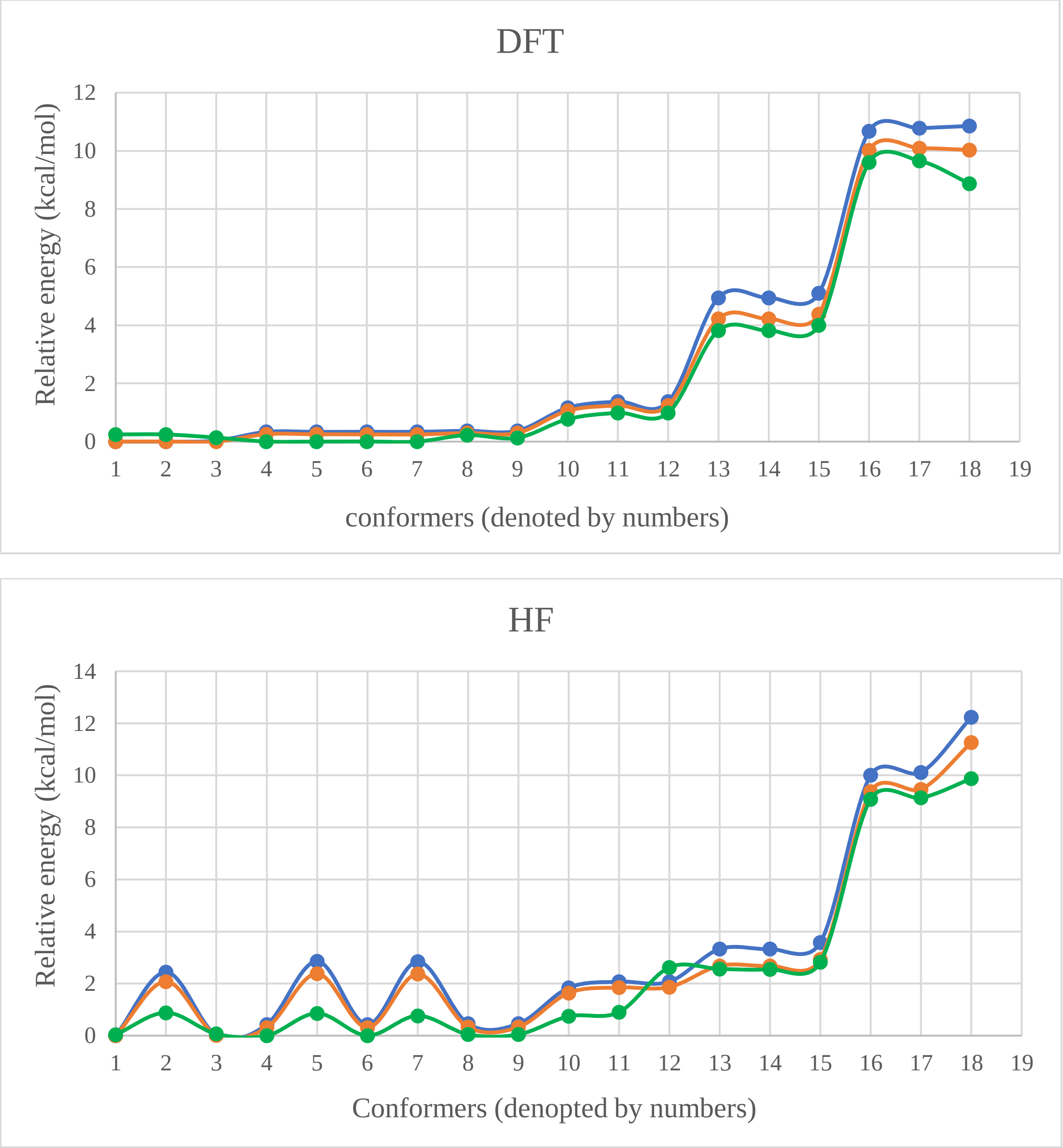
conformer	#	Conformers	#	Conformers	#	Conformers	#
ELP-m-s-x4	1	ELP-p-s-x4	6	ELP-k-s-x1	11	ELP-j-q-x3′	15
ELP-m-q-x4	2	ELP-p-s-x4′	7	ELP-j-q-x3	12	ELP-j-r-x3′	16
ELP-m-q-x4	3	ELP-m-q-x1	8	ELP-j-r-x3	13	ELP-j-s-x3′	17
ELP-m-r-x1	4	ELP-k-q-x1	9	ELP-j-s-x3	14		
ELP-m-s-x1	5	ELP-k-r-x1	10				

Figure 6.138. Diagrams comparing the uncorrected relative energies (—●—), relative energies corrected for ZPE (—●—) and Gibbs free energies (—●—) of the calculated conformers of compound ELQ.



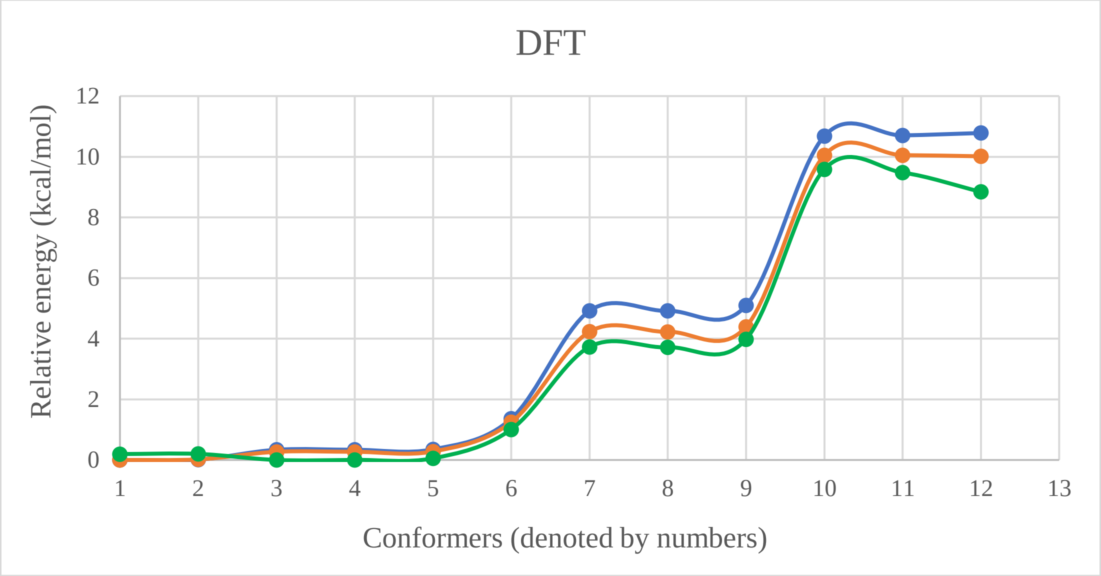
conformer	#	Conformers	#	Conformers	#	Conformers	#
ELQ-m-r-x4	1	ELQ-m-q-x1	4	ELQ-j-q-x3	7	ELQ-j-r-x3′	10
ELQ-m-q-x4	2	ELQ-k-q-x4	5	ELQ-j-r-x3	8	ELQ-j-s-x3	11
ELQ-m-r-x1	3	ELQ-k-r-x4	6	ELQ-j-q-x3′	9		

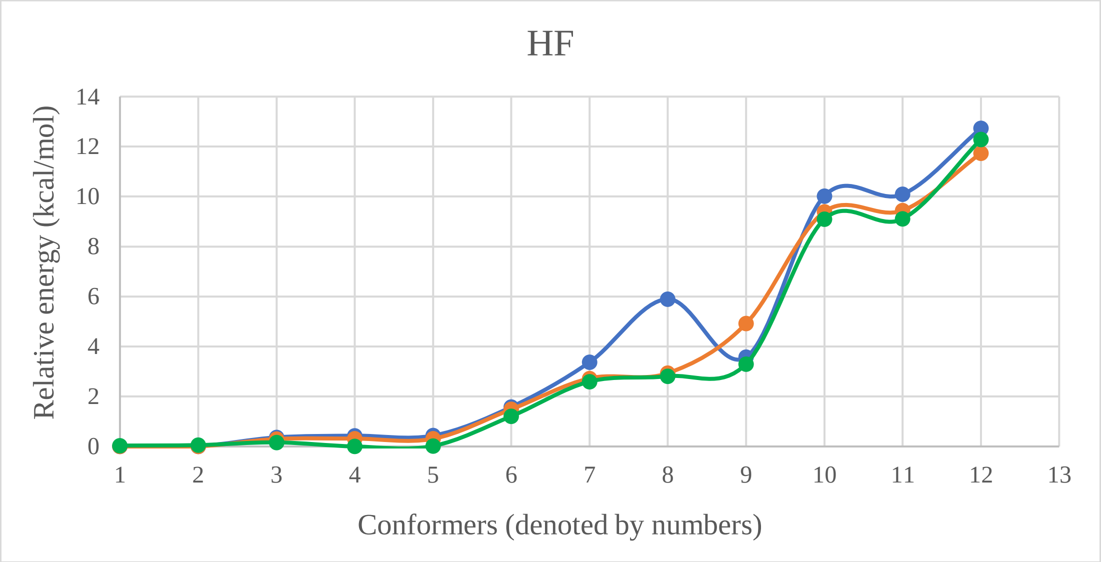
Figure 6.139. Diagrams comparing the uncorrected relative energies (—●—), relative energies corrected for ZPE (—●—) and Gibbs free energies (—●—) of the calculated conformers of compound FGP.



conformer	#	Conformers	#	Conformers	#	Conformers	#
FGP-m-r-x4	1	FGP-p-q-x4	6	FGP-k-r-x1	11	FGP-g-q-x1	15
FGP-m-s-x4	2	FGP-p-s-x4	7	FGP-k-r-x1	12	FGP-j-q-x3	16
FGP-m-q-x4	3	FGP-m-q-x1	8	FGP-g-r-x1	13	FGP-j-r-x3	17
FGP-m-r-x1	4	FGP-p-r-x4	9	FGP-g-r-x1′	14	FGP-j-s-x3	18
FGP-m-s-x1	5	FGP-k-q-x1	10				

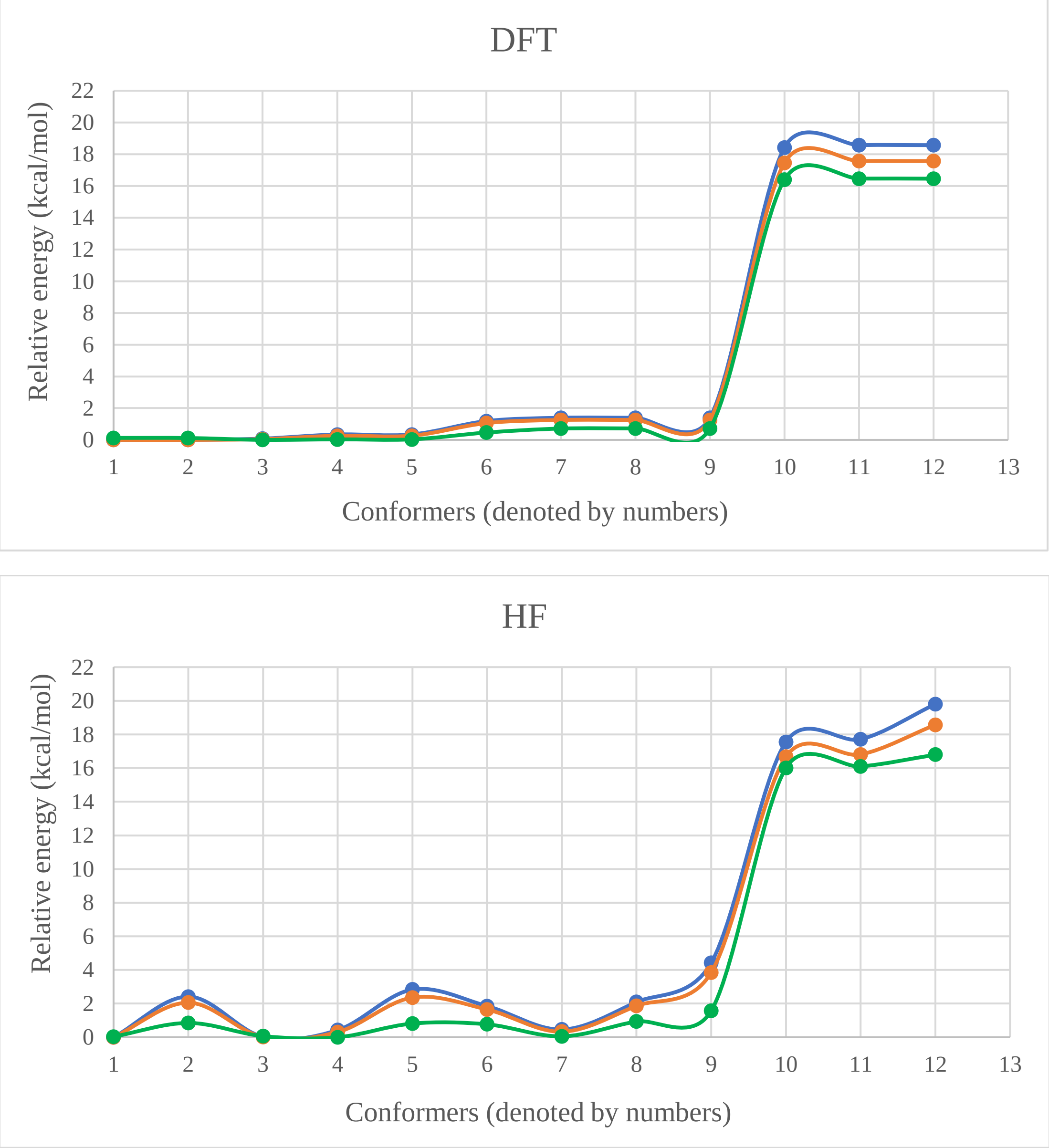
Figure 6.140. Diagrams comparing the uncorrected relative energies (—●—), relative energies corrected for ZPE (—●—) and Gibbs free energies (—●—) of the calculated conformers of compound FGQ.





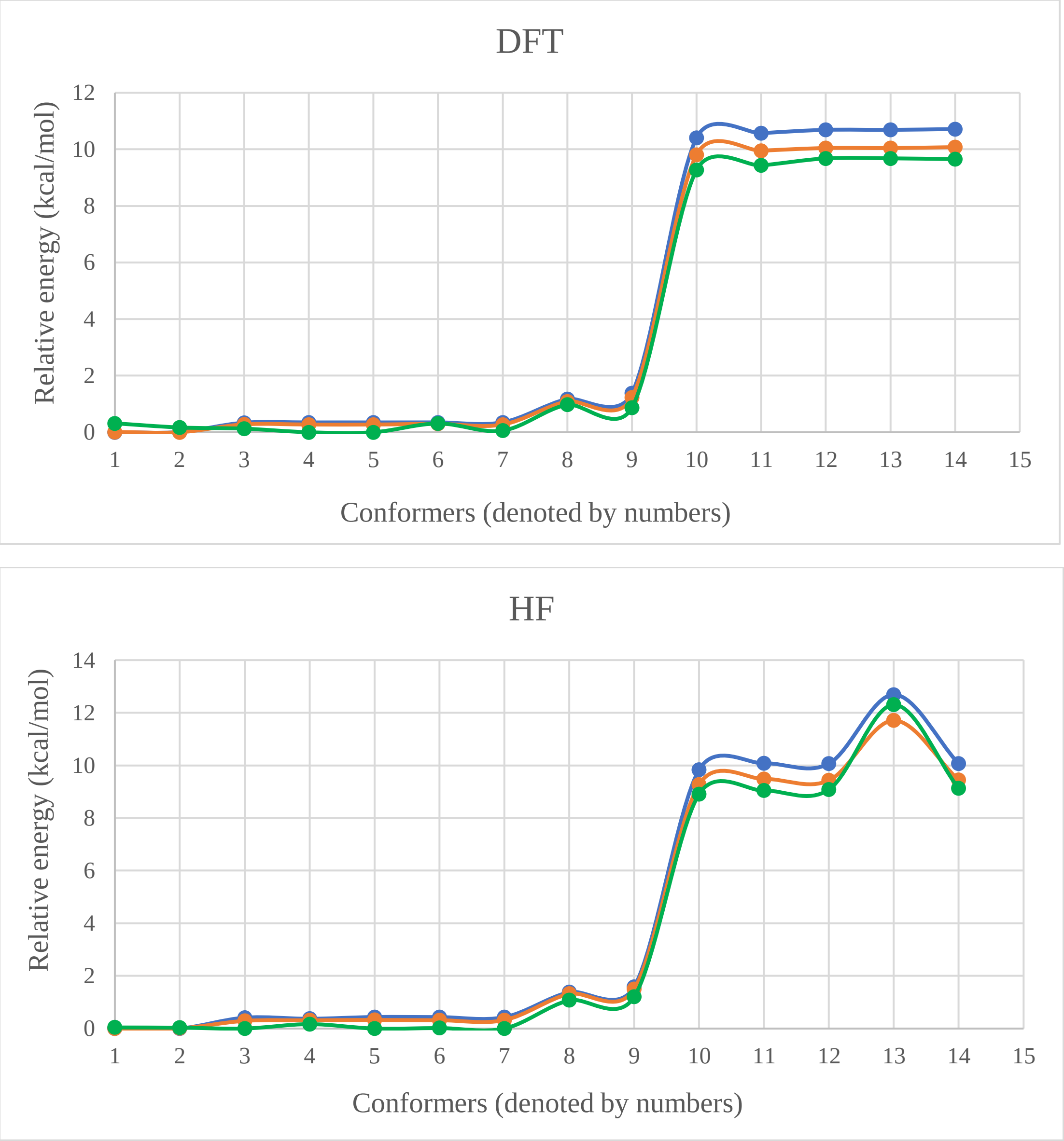
conformer	#	Conformers	#	Conformers	#	Conformers	#
FGQ-m-r-x4	1	FGQ-m-r-x1	4	FGQ-g-r-x1	7	FGQ-j-q-x3	10
FGQ-m-q-x4	2	FGQ-m-q-x1	5	FGQ-g-t-x1	8	FGQ-j-r-x3	11
FGQ-p-q-x4	3	FGQ-k-r-x4	6	FGQ-g-q-x1	9	FGQ-j-t-x3	12

Figure 6.141. Diagrams comparing the uncorrected relative energies (—●—), relative energies corrected for ZPE (—●—) and Gibbs free energies (—●—) of the calculated conformers of compound FJP.



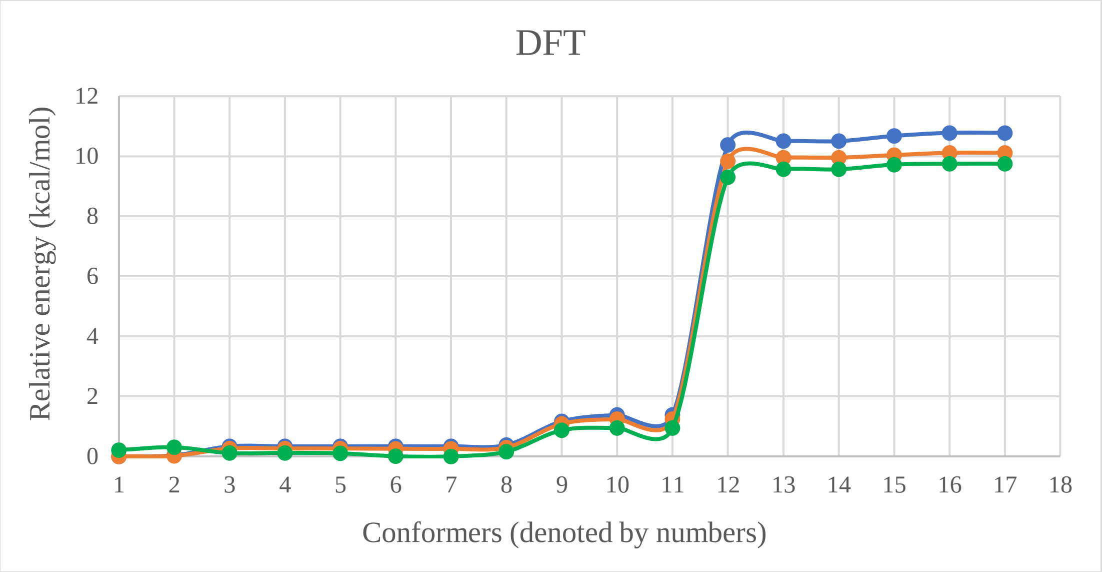
conformer	#	Conformers	#	Conformers	#	Conformers	#
FJP-m-r-x4	1	FJP-p-q-x4	4	FJP-p-r-x1	7	FJP-j-q-x3	10
FJP-m-s-x4	2	FJP-p-s-x4	5	FJP-k-r-x1	8	FJP-j-r-x3	11
FJP-m-q-x4	3	FJP-k-q-x1	6	FJP-k-s-x1	9	FJP-j-s-x3	12

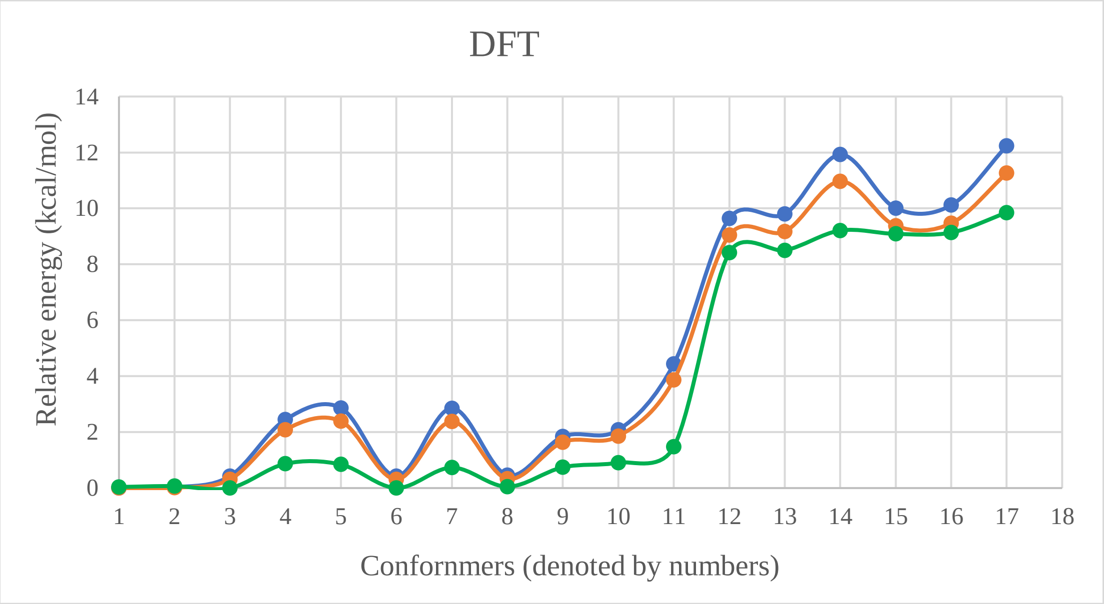
Figure 6.142. Diagrams comparing the uncorrected relative energies (—●—), relative energies corrected for ZPE (—●—) and Gibbs free energies (—●—) of the calculated conformers of compound FJQ.



conformer	#	Conformers	#	Conformers	#	Conformers	#
FJQ-m-q-x4	1	FJQ-p-q-x4′	5	FJQ-k-r-x4	9	FJQ-j-r-x3′	12
FJQ-m-r-x4	2	FJQ-m-q-x1	6	FJQ-j-q-x3	10	FJQ-j-t-x3	13
FJQ-p-r-x4	3	FJQ-m-r-x1	7	FJQ-j-r-x3	11	FJQ-j-q-x3′	14
FJQ-p-q-x4	4	FJQ-k-q-x4	8				

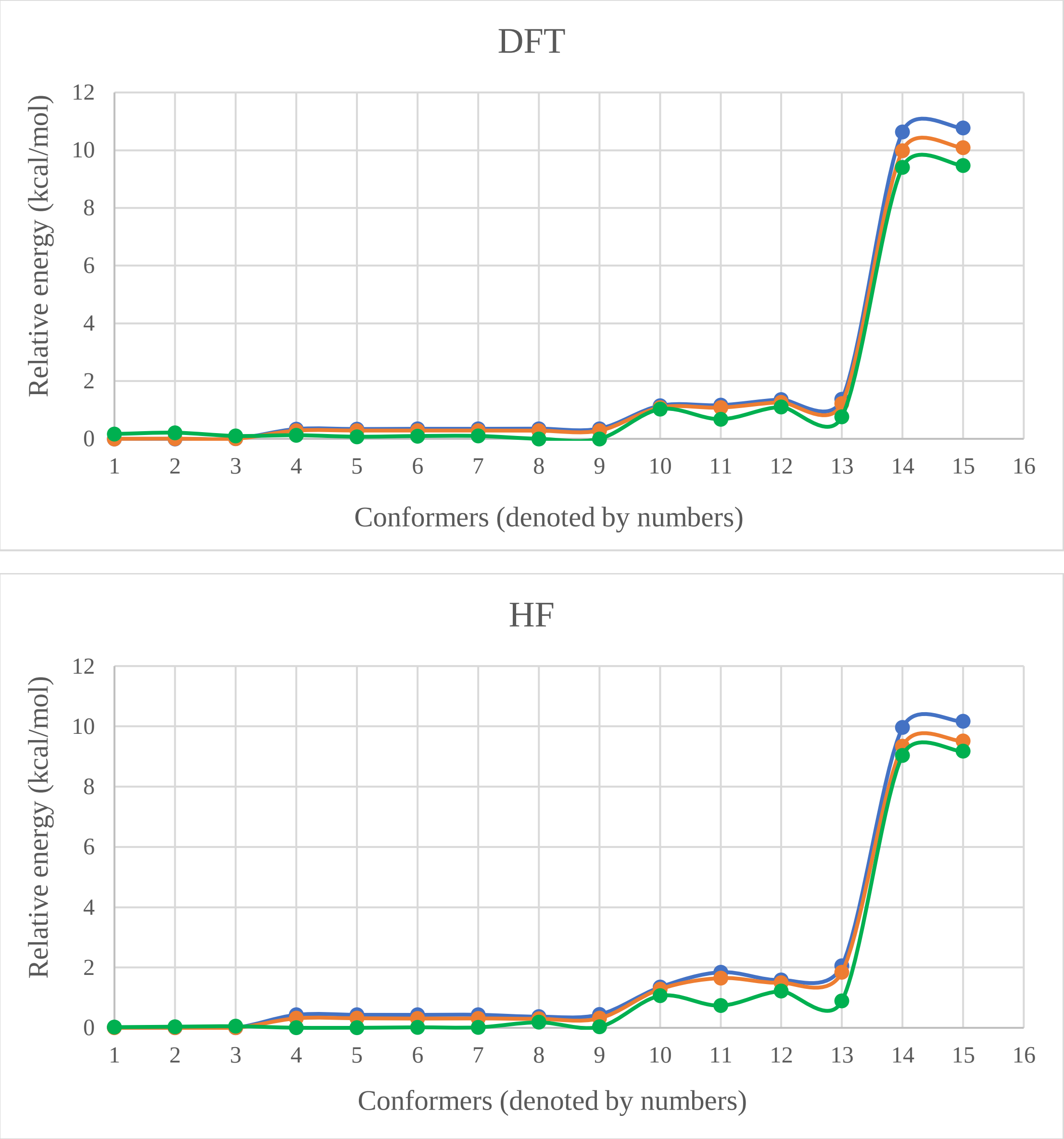
Figure 6.143. Diagrams comparing the uncorrected relative energies (—●—), relative energies corrected for ZPE (—●—) and Gibbs free energies (—●—) of the calculated conformers of compound FLP.





conformer	#	Conformers	#	Conformers	#	Conformers	#
FLP-m-r-x4	1	FLP-p-q-x4	6	FLP-k-s-x1	11	FLP-j-q-x3′	15
FLP-m-q-x4	2	FLP-p-s-x4	7	FLP-j-q-x3	12	FLP-j-r-x3′	16
FLP-m-r-x1	3	FLP-m-q-x1	8	FLP-j-r-x3	13	FLP-j-s-x3	17
FLP-m-s-x4	4	FLP-k-q-x1	9	FLP-j-s-x3′	14		
FLP-m-s-x1	5	FLP-k-r-x1	10				

Figure 6.144. Diagrams comparing the uncorrected relative energies (—●—), relative energies corrected for ZPE (—●—) and Gibbs free energies (—●—) of the calculated conformers of compound FLQ.



conformer	#	Conformers	#	Conformers	#	Conformers	#
FLQ-p-q-x2	1	FLQ-m-r-x1	5	FLQ-p-r-x4′	9	FLQ-k-r-x1	13
FLQ-m-r-x4	2	FLQ-m-q-x1	6	FLQ-k-q-x4	10	FLQ-j-q-x3	14
FLQ-m-q-x4	3	FLQ-m-q-x1′	7	FLQ-k-q-x1	11	FLQ-j-r-x3	15
FLQ-p-q-x4	4	FLQ-p-r-x4	8	FLQ-k-r-x4	12		

References

1. S. Riaz, Diabetes mellitus, *Scientific Research and Essay*, **4 (5),** 367–373, 2009.
2. Global rph online, http://www.globalrph.com/sulphonylureas.htm, accessed on 26/04/2018.
3. J. N. Murrell, The potential energy surface of polyatomic molecules, Structure and Bonding, 32, 146, 1977.
4. M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, *Gaussian 16* (Gaussian, Inc., Wallingford CT, 2016).
5. R. Dennington, T. Keith, J. Millam, Gauss View, Version 4.1.2. Semichem Inc., Shawnee Mission, 2007.
6. C. E Housecroft, A. G. Sharpe, *Inorganic chemistry 3rd ed*., Harlow: Pearson Education, 44–46, 2008.
7. J. E. Del Bene, Basis set and correlation effects on computed hydrogen bond energies of the dimers $(AHn)_2$: $AHn=NH_3$, OH_2, and FH, *Journal of Chemical Physics*, **86 (4)**, 2110–2113, 1987.
8. J. E. McMurry, R. C. Fay, J. K. Robinson, *Chemistry 7th edition*, Pearson, 97, 2014.
9. E. Tajkhorshid, K. J. Jalkanen, S. Suhai, Structure and vibrational spectra of the zwitterion l-alanine in the presence of explicit water molecules: A Density Functional analysis, *Journal of Physical Chemistry*, **102 (30)**, 5899–5913, 1998.
10. P. S. Kalsi, *Spectroscopy of Organic Compounds*, New Age International, 2007.
11. L. D. S. Yadav, *Organic Spectroscopy*, Dordrecht: Springer, 2004.

12. I. Cousins, *Physical-chemical properties and estimated environmental fate of brominated and Iodinated organic compounds: organic bromine and iodine compounds*, Berlin: Springer, 1506, 2003.
13. R. J. Gillespie, P. L. A. Popelier, *Chemical bonding and molecular geometry: from Lewis to electron densities*, oxford university press, 25–43, 2001.
14. R. Notario, Strong Chemical bonds, *Encyclopedia of physical organic chemistry*, **1(6),** 2006.
15. A. Rodger, M. Rodger, Molecular geometry, *Elsevier*, 1-33, 1995.
16. J. R. Reimers, L. K. McKemmish, R. H. McKenzie, N. S. Hush, Bond angle variations in XH_3 [X = N, P, As, Sb, Bi]: the critical role of Rydberg orbitals exposed using a diabatic state model, *journal of Physical Chemistry/ chemical Physics*, **38**, 2015.
17. G. L. Miessler. and D. A. Tarr, *Inorganic Chemistry 2nd ed.*, New jersey: Prentice-Hall, 57–58, 1999.
18. L. K. Ojha, Hybridization and molecular geometry: A number, *African journal of Chemical education*, **7(1)**, 2017.
19. Spark notes online: https://www.sparknotes.com/chemistry/organic1/orbitals/section1/, accessed on 15/11/2019.
20. H. B. Schelegel, Exploring Potential Energy Surfaces for Chemical Reactions: An Overview of Some Practical Methods, *journal of computational chemistry*, **24**, 1515–1527, 2003.
21. Z. K. Papanyan, A. S. Mkhitaryan, L. S. Gabrielyan, Ab Initio Hatree-Fock and density functional theory investigation on the potential energy and vibrational spectra of diethyl sulfone, *Proceedings of the Yerevan State University*, **52 (3)**, 147–154, 2018.
22. D. J. J. Marchand, M. Noori, A. Roberts, G. Rosenberg, B. Woods, U. Yildiz, M. Coons, D. Devore, and P. Margl, A Variable Neighborhood Descent Heuristic for Conformational Search Using a Quantum Annealer, *Scientific Reports*, 2009.
23. J. Espinosa-Garcia, M. Monge-Palacios, J. C. Corchado, Constructing Potential Energy Surfaces for Polyatomic Systems: Recent Progress and New Problems, *Advances in physical chemistry*, 2012.
24. SlideShare online: https://www.slideshare.net/prasanthperceptron/potential-energy-surface-molecular-graphics, accessed on 25/08/2019.
25. S. S. Xantheas, "Potential energy surfaces governing chemical reactions involving carbon, oxygen and hydrogen ", *Retrospective Theses and Dissertations*, 1991.

26. P. Atkins, R. Friedman, *Molecular quantum mechanics 4th edition.*, New York: Oxford university press, 332, 2005.
27. E. Schrödinger, Quantisierung Als Eigenwertproblem, *Zweiter Mitteilung*, **79**, 527, 1926.
28. E. Schrödinger, Quantisierung Als Eigenwertproblem, *Erste Mitteilung*, **79**, 376, 1926.
29. M. Born, R. Oppenheimer, Zur Quantentheorie Der Molekeln, *Annalen der Physik*, **84**, 484, 1927.
30. A. Szabo, N. S. Ostlund, *Modern quantum chemistry, introduction to advanced electronic structure theory*, New York: Dover Publishing, 1996.
31. G. I. Kerley. On corrections to the Born-Oppenheimer approximation, *A Kerley Technical Services Research Report, Consultant*, 2011.
32. F. Jensen, *Introduction to computational chemistry 2nd edition*, London: Wiley & sons, 82–86, 2007.
33. K. Szalewicz, Hydrogen bond, *Encyclopedia of physical science and technology 3rd edition*, **7**, 505, 2003.
34. J. Michl, Organic chemical systems and theory, *Encyclopedia of physical science and technology 3rd edition*, **11**, 435, 2003.
35. J. B. Foresman, A. Frisch, Exploring chemistry with electronic structure methods, *Gaussian*, Inc., Pittsburg, PA (USA), **59**, 1995.
36. K. I. Ramachandran, D. Gopakumar, K. Namboori, *Computational chemistry and molecular modeling: principles and applications*, Berlin: Springer, 155–170, 2008.
37. K. Ohno, K. Ersfarjani, Y. Kawazoe. *Computational material science*, Berling: Springer, 7–197, 2017.
38. P. Atkins, R. Friedman, Molecular quantum mechanics 5th edition, New York: Oxford university press, 296–298, 2012.
39. P. C. Deshmukh, A. Banik, D. Angom, Hartee-Fock Self-Consistent Field Method for Many-Electron Systems, 2008.
40. B. O. Roos. Lecture notes in Quantum chemistry, *European summer school in quantum chemistry*, Springer, **53**, 177–254, 1992.
41. T. Gund, *Guidebook on molecular modeling in drug design,* San diego: Academic press, *55*–99, 1996.

42. R. Eisberg, R. Resnick, *Quantum Physics Of Atoms, Molecules, Solids, Nuclei, And Particles 2nd edition*, Toronto: Wiley and sons, 1985.
43. L. Mammino, Highlighting logical structures in the teaching of theoretical chemistry, *XXIV International Conference of Theoretical Chemists of Latin Expression (QUITEL)*, 20–25, 1998.
44. E. G. Lewars, *Computational chemistry: Introduction to the theory and applications of molecular and quantum mechanics 2nd edition*, New York: Springer, 2011.
45. E. G. Lewars, *Computational chemistry: Introduction to the theory and applications of molecular and quantum mechanics 3rd edition*, New York: Springer, 2016.
46. F. Jensen, Introduction to Computational Chemistry Chapter 4 online: http://www.pitt.edu/~jordan/chem3430/chapter4.pdf, accessed on 22/01/2020.
47. R. E. Davidson, D. Feller, Basis set selection for molecular calculations, *Chemical Reviews*, **86**, 696, 1988.
48. J. B. Adams. Bonding energy models. *Encyclopedia of materials: science and technology*, 763–767, 2001.
49. R. G. T. Rosa. Hatree-Fock method, *Instituto de Fısica de Sao Carlos, Universidade de Sao Paulo*, 2017.
50. I. Levine, *Quantum chemistry 6th edition*, London: Pearson, 2009.
51. M. S. Blinder. Basic concepts of self-consistentfield theory, *American Journal of Physics*, **33(6)**, 431–443, 1965.
52. P. W. Atkins, *Molecular Quantum Mechanics Parts I and II: An Introduction to Quantum chemistry*, Oxford University Press, **1**, 1977.
53. P.A.M. Dirac, *The Principles of Quantum Mechanics 4th edition*, London: Oxford UK, 248, 1958.
54. C. D. Sherrill, An Introduction to Hartree-Fock Molecular Orbital Theory, *Georgia institute of technology*, 2000.
55. V. Magnasco, *Post-Hatree-Fock methods: Elementary molecular quantum mechanics 2nd edition*, Amsterdam: Elsevier, 681–722, 2013.
56. R. Petruzielo, J. Toulouse, J. Umrigar, Basis set construction for molecular electronic structure theory: Natural orbital and Gauss–Slater basis for smooth pseudopotentials, *Journal of chemical physics*, **134 (6)**, 2011.
57. M. Kozlov, I. Tupitsyn, Mixed Basis Sets for Atomic Calculations, *Atoms*, **7 (3)**, 92, 2019.

58. M. Dupuis, M. Nellapu, Maximal orbital analysis of molecular wavefunctions, *Journal of computational chemistry*, **40 (1)**, 39–50, 2018.
59. S. Huzinaga, Basis sets for molecular calculations, *Computer Physics Reports*, **2 (6)**, 281–339, 1985.
60. D. Belkic, H. S. Taylor, "A unified formula for the Fourier transform of Slater-type orbitals". *Physica Scripta*, **39 (2)**, 226–229, 1989.
61. P. E. Hoggan, Four-center Slater-type orbital molecular integrals without orbital translations, *International journal of quantum chemistry*, **110 (1)**, 98–103, 2009.
62. J. K. Lebanowski, Simplified introduction to *ab initio* basis sets: Terms and Notations online http://www.ccl.net/cca/documents/basis-sets/basis.html, accessed 16/10/2019.
63. J. Almlof, T. Helgaker, P. R. Taylor, "Gaussian basis sets for high- quality ab initio calculations," *Journal of Physical chemistry*, **92**, 3029–3033, 1988.
64. R. Ahlrichs, P. R.Taylor, "The choice of gaussian basis sets for molecular electronic structure calculations," *Journal of Physical chemistry*, **78**, 315–324, 1981.
65. T.H. Dunning, P.J. Hay, "Gaussian basis sets for molecular calculations," in: "Modern Theoretical Chemistry," Plenum Press, New York, **3**, 1-28, 1977.
66. R. Ahlrichs, P. R.Taylor, , "The choice of gaussian basis sets for molecular electronic structure calculations," *Journal of .Chemical Physics*, **78**, 315-324, 1981.
67. J. G. Hill, Gaussian basis sets for molecular applications, *International journal of quantum chemistry*, **113 (1)**, 21–34, 2012.
68. M. M. Francl, J. S. Binkley, M. S. Gordon, D. J. De Frees, J. A. Pople, "Self- consistent molecular orbital methods. XXIII. A polarization-type basis set for second-row element," *Journal of chemical physics*, **77**, 3654–3665, 1982.
69. M. Towler, An introductory guide to Gaussian basis sets in solid-state electronic structure calculations, Notes for Summer School "*Ab initio modelling in solid-state chemistry*", Torino, September 2000.
70. C. J. Cramer, *Essentials of Computational Chemistry 2nd edition*, Sussex: John Wiley & Sons, 166, 2004.
71. T. Van Mourik, M. Buhl, M. Gaigeot, Density functional theory across chemistry, physics and biology, *Philosiphical transactions of Royal society*, 372, 1–5, 2014.
72. T. Tsunedo, Density functional theory in quantum chemistry, Japan: Spinger, 101–124, 2014.

73. S. Kurth, M. A. L. Marques, E. K. U. Gross, Electronic Structure: Density Functional Theory, https://www-old.mpi-halle.mpg.de/mpi/publi/br/gross_persoenlich/KMG05.pdf.

74. N. M. Harrison, An Introduction to Density Functional Theory, https://www.imperial.ac.uk/media/imperial-college/research-centres-and-groups/computational-materials-science/teaching/DFT_NATO.pdf

75. R. van Leeuwen. Kohn-Sham potentials in density functional theory, *PHD thesis*, Vrije Universiteit Amsterdam, 1994.

76. P. Samal, Studies in Excited-State Density-Functional Theory, Indian Institute of Technology Kanpur, 2006.

77. W. Kohn, L. J. Sham. “Self-consistent equations including exchange and correlation effects”, *Physical Review*, **140**, A1133–A1138, 1965.

78. K. Capelle, A Bird’s-Eye View of Density-Functional Theory, *Brazilian Journal of Physics*, **36 (4)**, 1318–1340, 2006,

79. L. F. Cabeza. I. Martorell, L. Miro, A. I. Fernandez, C. Barreneche, Introduction to thermal energy storage (TES) systems, *Advances in Thermal Energy storage systems*, **66**, 1–28, 2015.

80. C. C. M. Rindt, S. V. Gaastra-Nedea, Modeling thermochemical reactions in the thermal energy storage system, *Advances in Thermal Energy storage systems*, **66**, 375–415, 2015.

81. D. Bagayoko, Understanding density functional theory (DFT) and completing it in practice online, https://aip.scitation.org/doi/pdf/10.1063/1.4903408, accessed on 16/10/2019.

82. K. J. H. Giesbertz, R. van Leeuwen. U. von Barth, Towards non-local density functionals by explicit modeling of the exchange-correlation hole in inhomogeneous systems, *Physical Review*, **87**, 1–14, 2018.

83. T. J. Giese, D. M. York, Density-functional expansion methods: Evaluation of LDA, GGA, and meta-GGA functionals and different integral approximations, *Journal of Chemical physic*, **133(24)**, 244107-244107, 2010.

84. C. Lee, W. Yang, R. G. Parr, Development of the Colle-Salvetti Correlation-Energy Formula into a Functional of the Electron Density, *Physical Review*, **B 37 (2)**, 785–789 1998.

85. A. D. Becke, A New Mixing of Hartree-Fock and Local Density-Functional Theories, *Journal of Chemical Physics*, **98 (2)**, 1372–1377 (1993).

86. A. D. Becke, Density Functional Thermochemistry III, The role of Exact Exchange, J. *Chemical Physics,* **98(7)**, 5648–5652 (1993).

87. I. Y. Zhang, J. Wu, X. Xu, Extending the reliability and applicability of B3LYP, *Journal of chemical communications*, **46 (18)**, 3057–3070, 2010.
88. K. E. Hermann, F. Qi, R. Zhao, R. Zhang, M. van Hove, Fragment motion in motor molecules: basic concepts and application to intra-molecular rotations, *Journal of physical chemistry/Chemical physics*, **20 (33)**, 21487–21497, 2018
89. M. Walther, P. Plochocka, B. Fischer, H. Helm, P. Uhd Jepsen, "Collective vibrational modes in biological molecules investigated by THz Time-Domain spectroscopy", *Biopolymers* (Biospectroscopy), **67 (4)**, 310–313, 2002.
90. D. A. McQuarrie, *Quantum chemistry 2nd edition*, California: University science books, 275, 2008.
91. M. E. Jacox, Vibrational and Electronic Energy Levels of Polyatomic Transient Molecules, NIST online: https://webbook.nist.gov/chemistry/polyatom/, accessed on 14/01/2020.
92. B. stevens, Some effects of intermolecular vibrational energy in complex fluorescent molecules, *Canadian Journal of chemistry*, **36 (1)**, 96–101, 1958.
93. ResearchGate online: https://www.researchgate.net/figure/Model-of-the-harmonic-and-anharmonic-oscillators_fig9_264496330, accessed on 16/01/2020.
94. K. R. Adhikari, Zero point energy, *The Himalayan Physics*, **1 (1)**, 67–68, 2010.
95. M. Wolfserg, The Calculation of Zero-Point Energies of Molecules by Perturbation Methods, *Journal of Physical sciences,*18 (2), 216–224, 1962.
96. Introduction to Inorganic Chemistry/Molecular online: http://www.physics.utah.edu/~rogachev/5460/Z_Introduction_to_Inorganic_Chemistry_Molecular_Orbital_Theory%20(2).pdf, accessed on 17/01/2020.
97. Y. Huang, C. Rong, R. Zhang, S. Liu, Evaluating frontier orbital energy and HOMO/LUMO gap with descriptors from density functional reactivity theory, *Journal of molecular modeling*, 23 (3), 1–12, 2017.
98. S. B. Gopalakrishna, T. Kalaiarasai, R. Subramanian, Comparative DFT Study of Phytochemical Constituents of the Fruits of *Cucumis trigonus Roxb*. and *Cucumis sativus Linn*, *Journal of computational methods in physics*, **3**, 1–6, 2014.
99. J. Aihara, Reduced HOMO−LUMO Gap as an Index of Kinetic Stability for Polycyclic Aromatic Hydrocarbons, *Journal of Physical chemistry*, **103 (37)**, 7487–7495, 1999.

100. D. C. Ghosh, J. Jana, A study of correlation of the order of chemical reactivity of a sequence of binary compounds of nitrogen and oxygen in terms of frontier orbital theory, *JSTOR.*, **76 (4)**, 570–573, 1999.

101. G. Reecht, C. Lotze, D. Sysosiev, T. Huhn, K. J. Franke, Visualizing the Role of Molecular Orbitals in Charge Transport through Individual Diarylethene Isomers, *ACS nano*, **10 (11)**, 10555–10562, 2016.

102. V. I. Minkin, *Dipole moments in organic chemistry*, New York: Plenum press, 1970.

103. P. Atkins, J de Paula, J. Keeler, *Atkin's physical chemistry 11th edition*, New York: Oxford university press, 2018.

104. Chemistry301 online: https://ch301.cm.utexas.edu/section2.php?target=imfs/vsepr/shape-dipole.html, accessed on 21/01/2020.

105. P. Gilli, G. Gilli, Hydrogen bond models and theories: The dual hydrogen bond model and its consequences, *Journal of Molecular Structure*, **972**, 10, 2010.

106. J. Poater, X. Fradera, M. Sola, M. Duran, S. Simon, On the electron-pair of the hydrogen bond in the framework of the atoms in molecules theory, *Chemical Physics Letters*, **369**, 255, 2003.

107. G. A. Jeffrey, *An introduction to hydrogen bonding*, Oxford: Oxford University Press, Oxford, 1997.

108. J. M. Hermida-Ramon, R. A. Mosquera. Do small carboxylic acids present intramolecular hydrogen bond?. *Chemical Physics*, **323 (2-3)**, 211–217, 2006.

109. G. A. Jeffrey, W. Saenger, *Hydrogen Bonding in Biological Structures*, Berlin: Springer, 1994.

110. A. L McClellan, The significance of hydrogen bonds in biological structures, *Journal of Chemical education*, **44 (9)**, 547, 1967.

111. ResearchGate online: https://www.researchgate.net/figure/Scheme-4-Intramolecular-hydrogen-bonding-in-salicylaldehyde_fig1_325430136, accessed on 22/01/2020.

112. E. S. Feldblum, I. T. Arkin, Strength of a bifurcated H bond, *Journal of biophysics and computational biology*, **111 (11)**, 4085–4090, 2014.

113. R. D. Parra, J. Ohlssen, Cooperativity in Intramolecular Bifurcated Hydrogen Bonds: An Ab Initio Study, *Journal of physical chemistry*, **112 (15)**, 3492–3498, 2008.

114. Y. Yang, W. Zhang, X. Gao, Blue-Shifted and Red-Shifted Hydrogen Bonds: Theoretical Study of the $CH_3CHO\cdots HNO$ Complexes, *International Journal of Quantum Chemistry*, **106**, 1199 –1207, 2006.

115. “World Health Organisation, global report on diabetes, 2016”.

116. X. Zhou, PhD thesis, RMIT University, Melbourne, Australia, March 2014.

117. American Diabetes Association, Diagnosis and classification of diabetes mellitus, *Diabetes Care*, **37**, 81–90, 2014.

118. J. A. Bluestone, K. Herold, and G. Eisenbarth, Genetics, pathogenesis and clinical interventions in type 1 diabetes, *Nature*, **464**, 1293-1300, 2010.

119. I. B. Hirsch, Clinical review: Realistic expectations and practical use of continuous glucose monitoring for the endocrinologist. *Journal of Clinical Endocrinology and Metabolism*, **94**, 2232–2238, 2009.

120. W. T. Cefalu, S. Waldman, and S. Ryder, Pharmacotherapy for the treatment of patients with type 2 diabetes mellitus: rationale and specific agents, *Clinical Pharmacological Therapy*, **81 (5)**, 636–649, 2007.

121. W. Rathmann, and G. Giani, Global prevalence of diabetes: estimates for the year 2000 and projections for 2030, *Diabetes Care*, **27**, 2568–2569, 2004.

122. Definition, Diagnosis and Classification of Diabetes Mellitus and its Complications. Part 1: Diagnosis and Classification of Diabetes Mellitus (WHO/NCD/NCS/99.2), Geneva: World Health Organization, 1999.

123. J. Lindström, P. Ilanne-Parikka, M. Peltonen, S. Aunola, J. G. Eriksson, K. Hemiö, H. Hämäläinen, P. Härkönen, S. Keinänen-Kiukaanniemi, M. Laakso, A. Louheranta, M. Mannelin, M. Paturi, J. Sundvall, T. T. Valle, M. Uusitupa, J. Tuomileht, Finnish Diabetes Prevention Study Group, “Sustained reduction in the incidence of type 2 diabetes by lifestyle intervention: follow-up of the Finnish Diabetes Prevention Study”, *Lancet*, **368**, 1673–1679, 2006.

124. K. L. Whalen, and J. R. Taylor, Gestational diabetes mellitus, *Endocrinology/ neuropathy*, **48 (3)**, 479-493, 2017.

125. A. S. Rahman, M. S. Abbas, A. Jaffri, S. R. Raza, F. A. Sattar. The prevalence of gestational diabetes in patients attending diabetic clinic at Sir Syed Hospital, *Pakistan Journal of Pharmacology*, **24 (1)**, 37–42, 2007.

126. L. Hartling, D. M. Dryden, A. Guthrie, M. Muise, B Van der Meer, and L. Donovan, Benefits and harms of treating gestational diabetes mellitus: A systematic review and meta-analysis for the U.S. Preventive Services Task Force and The National Institutes of Health Office of Medical Applications of research, *Annals of Internal Medicine*, **159 (2)**, 123–129, 2013.

127. Health E-news online, https://www.health-e.org.za/2017/03/01/big-increasediabetes-deaths/, accessed on 19/04/2018.

128. CDE online, https://www.cdediabetes.co.za/uploads/images/files/Diabetes%20in%20South%20Africa.pdf, accessed on 19/04/2018.

129. International Diabetes Federation, IDF diabetes atlas 4th Edition. Brussels, IDF, 2009.

130. EWN online, http://ewn.co.za/2018/03/27/stats-sa-tb-diabetes-top-2-killersin-sa, accessed on 19/04/2018.

131. International Diabetes Federation, IDF Diabetes Atlas Sixth edition, Brussels, IDF, 2013.

132. International Diabetes Federation, IDF Diabetes Atlas Seventh Edition, Brussels, IDF, 2015.

133. Medical brief online, https://www.medicalbrief.co.za/archives/statistics-saswings-roundabouts-die/, accessed on 22/04/2018.

134. Healthline online: https://www.healthline.com/health/diabetes-symptoms, accessed on 15/08/2019.

135. Mayo clinic online: https://www.mayoclinic.org/diseases-conditions/diabetes/symptoms-causes/syc-20371444, accessed on 15/08/2019.

136. Active beat online: https://www.activebeat.com/your-health/10-common-symptoms-of-diabetes/, 15/08/2019.

137. WebMD online: https://www.webmd.com/diabetes/type-2-diabetes-symptoms, accessed on 15/08/2019.

138. Centre for disease control and prevention online: https://www.cdc.gov/diabetes/basics/symptoms.html, accessed on 16/08/2019.

139. Diabetes.co.uk online, https://www.diabetes.co.uk/diabetescomplications/diabetes-and-blindness.html, accessed on 5/05/2018.

140. Healthline online: https://www.healthline.com/health/diabetes/diabetesamputation, accessed on 26/03/2018.

141. Health online: http://www.health.com/health/conditionarticle/0,,20189334,00.html, accessed on 26/03/2018.

142. Medical news today online: https://www.medicalnewstoday.com/articles/319686, accessed on 17/08/2019.

143. UNC kidney center online: https://unckidneycenter.org/kidneyhealthlibrary/glomerular-disease/diabetes/, accessed on 17/08/2019.

144. Diabetes.co.uk online: https://www.diabetes.co.uk/body/blood-vessels.html, accessed on 17/08/2019.

145. NIDDK online: https://www.niddk.nih.gov/health-information/diabetes/overview/preventing-problems/diabetic-kidney-disease, accessed on 17/08/2019.

146. Mayo clinic online: https://www.mayoclinic.org/diseases-conditions/diabetic-nephropathy/symptoms-causes/syc-20354556, accessed on 17/08/2019.

147. American diabetes association online: https://www.diabetes.org/diabetes/complications/kidney-disease-nephropathy, accessed on 17/08/2019.

148. S. B. Ghaderian, F. Hayati, S. Shayanpour, S. S. B. Mousavi, Diabetes and end-stage renal disease; a review article on new concepts, *Journal of renal and injury prevention*, **4 (2)**, 28–33, 2015.

149. G. Jia, M. A. Hill, R. Sowers, Diabetic Cardiomyopathy: An update of mechanisms contributing to this clinical entity, **122**, 624-638, 2018.

150. Patient online: https://patient.info/news-and-features/diabetes-increases-heart-failure-risk-particularly-in-women, accessed on 18/08/2019.

151. Yahoo news online: https://news.yahoo.com/type-2-diabetics-are-50-more-likely-to-die-prematurely-000152149.html, accessed on 10/03/2020.

152. G. Jia, A. Whaley-Connell, J. M. Sowers, Diabetic cardiomyopathy: A hyperglycemia and insulin-induced heart disease, **61 (1)**, 21–28, 2018.

153. G. Jia, V. G. DeMarco, J. R. Sowers, Insulin resistance and hyperinsulinemia in diabetic cardiomyopathy, *National Rev Endocrinology*, **12 (3)**, 144–153, 2016.

154. Acuity eye group online: https://www.acuityeyegroup.com/patient-info/eye-conditions/diabetic-eye-disease, accessed on 18/08/2019.

155. Strathfield retina clinic online: https://www.strathfieldretina.com.au/eye-conditions/, accessed on 18/08/2019.

156. Mayo clinic online: https://www.mayoclinic.org/diseases-conditions/diabetic-retinopathy/symptoms-causes/syc-20371611, accessed on 18/08/2019.

157. WebMD online: https://www.webmd.com/diabetes/diabetic-retinopathy, accessed on 18/08/2019.

158. Sonas home health care online: https://www.sonashomehealth.com/diabetic-retinopathy/, accessed on 18/08/2019.

159. American academy of ophthalmology online: https://www.aao.org/eye-health/diseases/what-is-diabetic-retinopathy, accessed on 18/08/2019.

160. Medical news today online: https://www.medicalnewstoday.com/articles/183417#symptoms, accessed on 18/08/2019.

161. Health engine online: https://healthengine.com.au/info/diabetic-eye-disease-non-proliferative-diabetic-retinopathy, accessed on 18/08/2019.

162. Manna health products online: https://www.mannaplus.co.za/how-diabetes-damages-the-eyes/, accessed on 18/08/2019.

163. IFL science online: https://www.iflscience.com/health-and-medicine/no-doctor-needed-us-health-regulators-approve-ai-device-to-detect-eye-diseases/, accessed on 18/08/2019.

164. National health institute online: https://www.nei.nih.gov/learn-about-eye-health/eye-conditions-and-diseases/macular-edema, accessed on 18/08/2019.

165. Eye7 eye hospitals online: https://www.eye7.in/retina/diabetic-retinopathy/, accessed on 18/08/2019.

166. Medicine Net online: https://www.medicinenet.com/glaucoma/article.htm, accessed on 19/08/2019.

167. Ontrack diabetes online: https://www.ontrackdiabetes.com/related-conditions/vision/diabetic-eye-disease-cataracts-glaucoma, accessed on 18/08/2019.

168. Nvision online: https://www.ontrackdiabetes.com/related-conditions/vision/diabetic-eye-disease-cataracts-glaucoma, accessed on 19/08/2019.

169. Diabetes UK online: https://www.diabetes.org.uk/Guide-to-diabetes/complications/Nerves_Neuropathy, accessed on 20/08/2019.

170. Mayo clinic online: https://www.mayoclinic.org/diseases-conditions/diabetic-neuropathy/symptoms-causes/syc-20371580, accessed on 20/08/2019.

171. Endocrine web online: https://www.endocrineweb.com/guides/diabetic-neuropathy/types-diabetic-neuropathy, accessed on 20/08/2019.

172. Diabetes: facts and stats, March 2014.

173. I. M. Stratton, A. L. Adler, H. A. W. Neil, Association of glycaemia with macrovascular and microvascular complications of Type 2 diabetes (UKPDS 35): prospective observational study, *British medical journal*, **321**; 405– 412, 2000.

174. Amputee Statistical Database for the United Kingdom, Lower limb amputations, 2007.

175. HSCIC (2013) National Diabetes Audit 2011/12: The Information Centre for Health and Social Care Hospital Episode Statistics 2007/8–2011/12.

176. American diabetes association online, http://www.diabetes.org/living-withdiabetes/complications/heart-disease/peripheral-arterial-disease.html, accessed on 20/04/2018.

177. Diabetes self-management online, https://www.diabetesselfmanagement.com/managing-diabetes/complicationsprevention/diabetic-leg-pain-and-peripheral-arterial-disease/, accessed on 20/04/2018.

178. M. P. Khanolkar, The Diabetic Foot. QJM, *An international journal of medicine*, **101**, 685–695, 2008.

179. Mayo clinic online: https://www.mayoclinic.org/diseases-conditions/diabetes/in-depth/diabetes/art-20049314, accessed on 21/08/2019.

180. The medical biochemistry online, https://themedicalbiochemistrypage.org/insulin.php, accessed on 26/04/2018.

181. Mcb online, https://mcb.berkeley.edu/courses/mcb135e/pancreas.html, accessed on 16/04/2018.

182. Q. Sun, M. C. Cornelis, J. E. Manson, F. B. Hu, Plasma levels of fetuin-A and hepatic enzymes and risk of type 2 diabetes in women in the U.S, 2013. Diabetes. Biochemistry, **62**, 49–55, 2013.

183. APPG for diabetes online: https://diabetesappg.wordpress.com/2016/05/10/the-technology-jigsaw-for-the-artificial-pancreas/, accessed on 20/08/2019.

184. V. T. Samuel, G. I. Shulman, Mechanisms for insulin resistance: common threads and missing links, *Cell metabolism*, **148**, 852–871, 2012.

185. LIWLI online: http://liwli.com/insulin-resistance/, accessed on 18/02/2020.

186. C. Ruchalski, frequently prescribed medications: drugs you need to know, *anti-diabetic drugs*, 2012.

187. L. H. Bösenberg, D. G. van Zyl, The mechanism of action of oral antidiabetic drugs: A review of recent literature, *Journal of Endocrinology, Metabolism and Diabetes of South Africa*, **13 (3)**, 80-87, 2008.

188. Drugs.com online, https://www.drugs.com/drug-class/antidiabetic-agents.html, accessed on 26/04/2018.

189. L. J. Patel PhD thesis Ganpat University, January 2012.

190. S. Sen, Ruchika, D. Kumar, T. S. Easwari, S. Gohri, Therapeutic Aspects of Sulphonylureas: A Brief Review, *Journal of Chemical and Pharmaceutical Research*, **8 (12)**, 121–130, 2016.

191. D. Sola, L. Rossi, G. P. C. Schianca, P. Maffioli, M. Bigliocca, R. Mella, F. Corlianò, G. P. Fra, E. Bartoli, G. Derosa, Sulphonylureas and their use in clinical practice, *Archives of medical science*, **11 (4)**, 2015

192. B. L. Furman, xPharm: The Comprehensive Pharmacology Reference, 2007.

193. S. Seino, "Cell signaling in insulin secretion: the molecular targets of ATP, cAMP and sulphonylurea", *Diabetologia*, **55**, 2096–2108, 2012.

194. P. Proks, F. Reimann, N. Green, F. Gribble, F. Ashcroft. Sulphonylureas stimulation of insulin secretion, *Diabetes*, **51 (3)**, S368–S376, 2002.

195. H. C. Gerstein, M. E. Miller, R. P. Byington, D. C. Goff, J. T. Bigger, J. B. Buse, W. C. Cushman, S. Genuth, F. Ismail-Beigi, R. H. Grimm, J. L. Probstfield, D. G. Simons-Morton, W. T. Friedewald, Effects of intensive glucose lowering in type 2 diabetes, *The New England Journal of Medicine*, **358**, 2545–2559, 2008.

196. W. Rathmann, K. Kostev, J. B. Gruenberger, M. Dworak, G. Bader, G. Giani, Treatment persistence, hypoglycaemia and clinical outcomes in type 2 diabetes patients with dipeptidyl

peptidase-4 inhibitors and sulphonylureas: a primary care database analysis, *Diabetes Obesity Metabolism*, **15**, 55–61, 2013.

197. R. Parker, The role of adipose tissue in fatty liver diseases, *Liver Research*, **2 (1)**, 35–42, 2018.

198. L. Mammino, Bowl-shaped structures from acylphloroglucinols: an *ab initio* and DFT study, *journal of Molecular Physics*, 1–13, 2017.

199. L. Mammino, M. M. Kabanda, "Considering the Medium when Studying Biologically Active Molecules: Motivation, Options and Challenges", In Zaheerul-Haq and J. D. Madura (Eds), Frontiers in Computational Chemistry, Bentham Science Publishers, 197–256, 2014.

200. J. P. Merrick, D. Moran, L. Radom, An Evaluation of Harmonic Vibrational Frequency Scale Factors. *Journal of physical chemistry*, **111**, 11683–11700, 2007.

201. A.J. Barnes, Blue-shifting hydrogen bonds—are they improper or proper. *Journal of Molecular Structure*, **704**, 3–9, 2004.

202. S. Pinchas, Infrared Absorption of the Aldehydic C-H Group. *Analytical Chemistry*, **27**, 2–61, 955.

203. P. Hobza, V. Spirko, Z. Havlas, K. Buchhold, B. Reinmann, H. Barth, B. Brutschy, Anti-hydrogen bond between chloroform and fluorobenzene, *Chemical physics letters*, **299**,180–186, 1999.

204. B. G. Olivera, Blue-shifted hydrogen bonds and secondary interactions in the C3 H6 ···HCF3, C2 H4 O···HCF3 AND C2 H4 S···HCF3 cyclic complexes. *Journal of Chilean chemical society*, **56 (1)**, 601–605, 2011.

205. P. Hobza, Z. Havlas, The fluoroform··· ethylene oxide complex exhibits a C–H···O anti-hydrogen bond. *Chemical physics letters*, **303**, 447–452, 1999.

206. E. Nir, C. Janzen, P. Imhof, K. Kleinermanns, M. S. de Vries, Pairing of the nucleobase guanine studied by IR–UV double-resonance spectroscopy and ab initio calculations, *Physical chemistry chemical physics*, **4**, 740, 2002.

207. P. Hobza, V. Sˇpirko, Why is the N1–H stretch vibration frequency of guanine shifted upon dimerization to the red and the amino N–H stretch vibration frequency to the blue?, *Physical chemistry chemical physics*, **6**, 2003.

Appendix A

This section presents additional tables which may be useful in the analysis of results. In the tables for inputs and output geometries, m1 and m2 indicates different geometries considered in the preparation of inputs.

Table A1. Input geometries and resulting optimized conformers for compound AGP.

Inputs	Outputs
AGP-m1-r	AGP-m-r-u1
AGP-m1-t	
AGP-m1-s	AGP-m-s-u1
AGP-p-s	AGP-p-t-u3
AGP-m1-q	AGP-m-q-u1
AGP-p-q	AGP-p-r-u3
AGP-k-r	AGP-k-q-u1
AGP-k-q	AGP-k-r-u1
AGP-k-s	
AGP-m2-q	AGP-m-r-u2
AGP-m2-t	
AGP-m2-s	
AGP-g-q	AGP-g-r-u3
AGP-g-t	
AGP-g-s	
AGP-g-r	AGP-g-q-u3
AGP-j-r	AGP-j-q-u3
AGP-j-q	AGP-j-r-u3
AGP-j-s	
AGP-j-t	AGP-j-s-u3

Table A2. Input geometries and resulting optimized conformers for compound AGQ.

Inputs	Outputs
AGQ-m1-s	AGQ-m-r-u1
AGQ-m1-r	
AGQ-p-s	
AGQ-p-r	
AGQ-m1-q	AGQ-m-q-u1
AGQ-p-q	
AGQ-p-t	
AGQ-m1-t	
AGQ-k-s	AGQ-k-q-u1

AGQ-k-r	
AGQ-k-q	AGQ-k-r-u1
AGQ-k-t	
AGQ-m2-q	AGQ-m-r-u2
AGQ-m2-t	
AGQ-m2-s	AGQ-m-q-u2
AGQ-m2-r	
AGQ-g-q	AGQ-g-r-u3
AGQ-g-t	
AGQ-g-s	AGQ-g-t-u3
AGQ-g-r	AGQ-g-q-u3
AGQ-j-r	AGQ-j-q-u3
AGQ-j-q	AGQ-j-r-u3
AGQ-j-t	
AGQ-j-s	AGQ-j-t-u3

Table A3. Input geometries and resulting optimized conformers for compound AJP.

Inputs	Outputs
AJP-m1-s	AJP-m-r-u1
AJP-m1-r	
AJP-p-s	
AJQ-p-r	
AJP-m1-t	AJP-m-s-u1
AJP-p-t	
AJP-m1-q	AJP-m-q-u1
AJP-p-q	
AJP-g-r	AJP-k-q-u1
AJP-k-r	
AJP-g-q	AJP-k-r-u1
AJP-g-s	
AJP-k-q	
AJP-k-s	
AJP-g-t	AJP-k-s-u1
AJP-k-t	
AJP-m2-q	AJP-m-r-u2
AJP-m2-s	
AJP-m2-t	AJP-m-s-u2
AJP-m2-r	AJP-m-q-u2
AJP-j-r	AJP-j-q-u3
AJP-j-q	AJP-j-r-u3
AJP-j-s	
AJP-j-a	AJP-j-s-u3

Table A4. Input geometries and resulting optimized conformers for compound AJQ.

Inputs	Outputs
AJQ-g-s	AJQ-p-q-u5
AJQ-m1-s	AJQ-m-q-u1
AJQ-m2-s	AJQ-m-q-u2
AJQ-m2-r	
AJQ-m2-q	AJQ-m-r-u2
AJQ-m2-t	
AJQ-p-s	AJQ-p-q-u3
AJQ-m1-r	AJQ-m-r-u1
AJQ-g-r	AJQ-p-q-u5
AJQ-m1-t	AJQ-m-s-u1
AJQ-p-q	AJQ-p-r-u3
AJQ-p-a	AJQ-p-s-u3
AJQ-m1-q	AJQ-m-q-u1
AJQ-k-s	AJQ-k-q-u1
AJQ-k-r	AJQ-k-q-u1
AJQ-k-q	AJQ-k-r-u1
AJQ-k-t	
AJQ-j-t	AJQ-j-q-u1
AJQ-j-r	
AJQ-j-q	AJQ-j-r-u1
AJQ-j-s	

Table A5. Input geometries and resulting optimized conformers for compound ALP.

Inputs	Outputs
ALP-m1-s	ALP-m-r-u1
ALP-m1-r	
ALP-p-s	
ALP-p-r	
ALP-m1-t	ALP-m-s-u1
ALP-p-t	
ALP-m1-q	ALP-m-q-u1
ALP-p-q	
ALP-k-r	ALP-k-q-u1
ALP-k-q	ALP-k-r-u1
ALP-k-s	
ALP-g-r	ALP-k-q-u1
ALP-g-q	ALP-k-r-u1′
ALP-g-t	ALP-k-s-u1
ALP-g-s	ALP-k-r-u3
ALP-m2-q	ALP-m-r-u2
ALP-m2-s	
ALP-m2-t	ALP-m-s-u2
ALP-m2-r	ALP-m-q-u2

ALP-j-r	ALP-j-q-u3
ALP-j-q	ALP-j-r-u3
ALP-j-s	
ALP-j-t	ALP-j-s-u3

Table A6. Input geometries and resulting optimized conformers for compound ALQ.

Inputs	Outputs
ALQ-m1-s	ALQ-m-r-u1
ALQ-m1-r	
ALQ-p-s	
ALQ-p-r	
ALQ-m1-q	ALQ-m-q-u1
ALQ-p-q	
ALQ-m1-t	
ALQ-p-t	
ALQ-k-s	ALQ-k-q-u1
ALQ-k-r	
ALQ-k-q	ALQ-k-r-u1
ALQ-k-t	
ALQ-m2-q	ALQ-m-r-u2
ALQ-m2-t	
ALQ-m2-s	ALQ-m-q-u2
ALQ-m2-r	
ALQ-g-r	ALQ-j-q-u3
ALQ-g-q	ALQ-j-r-u3
ALQ-g-t	
ALQ-j-r	ALQ-j-q-u3
ALQ-j-q	ALQ-j-r-u3
ALQ-j-a	
ALQ-j-s	

Table A7. Input geometries and resulting optimized conformers for compound BGP.

Inputs	Outputs
BGP-p-t	BGP-p-s-v3
BGP-p-s	BGP-p-t-v3
BGP-m1-s	BGP-m-r-v1
BGP-m1-r	
BGP-p-r	
BGP-m1-t	BGP-m-s-v1
BGP-m1-q	BGP-m-q-v1
BGP-p-q	
BGP-k-r	BGP-k-q-v3
BGP-k-q	BGP-k-r-v3
BGP-k-s	
BGP-k-t	BGP-k-s-v3
BGP-m2-q	BGP-m-r-v2
BGP-m2-s	
BGP-m2-t	BGP-m-s-v2
BGP-m2-r	BGP-m-q-v2
BGP-g-q	BGP-g-r-v1
BGP-g-t	
BGP-g-s	
BGP-g-r	BGP-g-q-v1
BGP-j-r	BGP-j-q-v5
BGP-j-q	BGP-j-r-v5
BGP-j-s	
BGP-	BGP-j-s-v5

Table A8. Input geometries and resulting optimized conformers for compound BGQ.

Inputs	Outputs
BGQ-m1-s	BGQ-m-r-v1
BGQ-m1-r	
BGQ-p-s	
BGQ-p-r	
BGQ-m1-q	BGQ-m-q-v1
BGQ-m1-t	
BGQ-p-q	
BGQ-p-t	
BGQ-k-s	BGQ-k-q-v1
BGQ-k-r	
BGQ-g-q	BGQ-k-r-v1
BGQ-g-t	
BGQ-m2-q	BGQ-m-r-v2
BGQ-m2-t	
BGQ-m2-s	BGQ-m-q-v2
BGQ-m2-r	

BGQ-j-r	BGQ-j-q-v3
BGQ-j-q	BGQ-j-r-v3
BGQ-j-t	
BGQ-j-s	BGQ-j-t-v3

Table A9. Input geometries and resulting optimized conformers for compound BJP.

Inputs	Outputs
BJP-g-s	BJP-p-q-v3
BJP-g-r	
BJP-m1-t	
BJP-m1-s	
BJP-m1-r	
BJP-p-s	
BJP-p-r	
BJP-p-t	BJP-p-s-v3
BJP-g-q	BJP-p-r-v3
BJP-g-t	
BJP-m1-q	
BJP-p-q	
BJP-k-r	BJP-k-q-v1
BJP-k-q	BJP-k-r-v1
BJP-k-t	BJP-k-s-v1
BJP-m2-q	BJP-m-r-v2
BJP-m2-s	
BJP-m2-t	BJP-m-s-v2
BJP-m2-r	BJP-m-q-v2
BJP-j-r	BJP-j-r-v3
BJP-j-q	BJP-j-s-v3
BJP-j-s	
BJP-j-t	BJP-j-q-v3

Table A10. Input geometries and resulting optimized conformers for compound BJQ.

Inputs	Outputs
BJQ-g-s	BJQ-p-r-v3
BJQ-g-q	
BJQ-k-q	
BJQ-k-s	
BJQ-g-t	
BJQ-k-t	
BJQ-g-r	
BJQ-k-r	
BJQ-m1-t	BJQ-m-s-v1
BJQ-m1-s	BJQ-m-t-v1
BJQ-m2-t	BJQ-m-q-v2
BJQ-m2-r	
BJQ-m2-s	BJQ-m-r-v2
BJQ-m2-q	
BJQ-m1-r	BJQ-m-q-v1
BJQ-m1-q	
BJQ-p-s	BJQ-p-q-v3
BJQ-p-r	BJQ-p-q-v3′
BJQ-p-q	BJQ-p-r-v3
BJQ-p-t	BJQ-p-s-v3
BJQ-j-t	BJQ-j-q-v3
BJQ-j-r	
BJQ-j-q	BJQ-j-q-v3
BJQ-j-s	

Table A11. Input geometries and resulting optimized conformers for compound BLP.

Inputs	Outputs
BLP-k-r	BLP-k-q-v1
BLP-p-t	BLP-p-s-v3
BLP-p-s	BLP-p-t-v3
BLP-m1-s	BLP-m-r-v1
BLP-m1-r	
BLP-p-r	
BLP-m1-t	BLP-m-s-v1
BLP-m1-q	BLP-m-r-v1′
BLP-p-q	
BLP-k-q	BLP-k-r-v1
BLP-k-s	
BLP-k-t	BLP-k-s-v1
BLP-m2-r	BLP-p-q-v4
BLP-m2-t	BLP-p-s-v4
BLP-m2-s	BLP-p-t-v4
BLP-m2-q	BLP-p-r-v4

BLP-g-r	BLP-j-q-v5
BLP-j-r	
BLP-g-q	BLP-j-r-v5
BLP-g-s	
BLP-j-q	
BLP-j-s	
BLP-g-t	BLP-j-s-v5
BLP-j-t	

Table A12. Input geometries and resulting optimized conformers for compound BLQ.

Inputs	Outputs
BLQ-p-s	BLQ-p-q-v3
BLQ-p-r	
BLQ-p-q	BLQ-p-r-v3
BLQ-p-t	
BLQ-k-s	BLQ-p-r-v3
BLQ-k-t	BLQ-k-q-v1
BLQ-k-r	
BLQ-k-q	BLQ-k-r-v1
BLQ-m1-s	BLQ-m-r-v1
BLQ-m1-r	
BLQ-m1-q	BLQ-m-q-v1
BLQ-m1-t	BLQ-m-s-v1
BLQ-m2-s	BLQ-p-q-v4
BLQ-m2-r	
BLQ-m2-t	BLQ-p-r-v4
BLQ-m2-q	
BLQ-j-r	BLQ-j-q-v3
BLQ-g-r	BLQ-j-q-v5
BLQ-j-q	BLQ-j-r-v3
BLQ-j-t	
BLQ-g-q	BLQ-j-r-v5
BLQ-g-t	
BLQ-j-s	BLQ-j-t-v3
BLQ-g-s	BLQ-j-t-v5

Table A13. Input geometries and resulting optimized conformers for compound CGP.

Inputs	Outputs
CGP-k-t	CGP-p-s-w5
CGP-k-s	
CGP-p-t	
CGP-k-r	CGP-p-q-w5
CGP-p-s	
CGP-p-r	
CGP-k-q	CGP-p-r-w5
CGP-m1-s	CGP-m-r-w1
CGP-m1-r	
CGP-p-q	
CGP-m1-t	CGP-m-s-w1
CGP-m1-q	CGP-m-q-w1
CGP-m2-q	CGP-m-r-w2
CGP-m2-s	
CGP-m2-t	CGP-m-s-w2
CGP-m2-r	CGP-m-q-w2
CGP-g-r	CGP-g-r-w5
CGP-g-q	
CGP-g-t	
CGP-g-r	CGP-g-q-w5
CGP-j-r	CGP-j-q-w5
CGP-j-s	CGP-j-r-w5
CGP-j-q	
CGP-j-t	CGP-j-s-w5

Table A14. Input geometries and resulting optimized conformers for compound CGQ.

Inputs	Outputs
CGQ-k-s	CGQ-p-q-w5
CGQ-g-s	
CGQ-g-r	
CGQ-k-r	
CGQ-p-r	
CGQ-m2-s	
CGQ-m2-r	
CGQ-p-s	
CGQ-m2-q	CGQ-m-q-w3
CGQ-m2-t	
CGQ-k-q	CGQ-p-r-w5
CGQ-g-q	
CGQ-g-t	
CGQ-k-t	
CGQ-p-q	
CGQ-p-t	

CGQ-m1-s	CGQ-m-r-w1
CGQ-m1-r	
CGQ-m1-q	CGQ-m-q-w1
CGQ-m1-t	
CGQ-j-r	CGQ-j-q-w5
CGQ-j-s	CGQ-j-t-w5
CGQ-j-q	CGQ-j-r-w5
CGQ-j-t	

Table A15. Input geometries and resulting optimized conformers for compound CJP.

Inputs	Outputs
CJP-k-s	CJP-p-q-w3
CJP-k-r	
CJP-p-s	
CJP-p-r	
CJP-g-s	
CJP-g-r	
CJP-g-t	CJP-p-s-w3
CJP-k-t	
CJP-p-t	
CJP-g-q	CJP-p- r-w3
CJP-k-q	
CJP-p-q	
CJP-m1-t	CJP-m-r-w1
CJP-m1-s	
CJP-m1-r	
CJP-m1-q	
CJP-m2-q	CJP-m-r-w2
CJP-m2-t	CJP-m-s-w2
CJP-m2-s	CJP-m-t-w2
CJP-m2-r	CJP-m-q-w2
CJP-j-r	CJP-j-q-w1
CJP-j-s	CJP-j-r-w1
CJP-j-q	
CJP-j-t	CJP-j-s-w1

Table A16. Input geometries and resulting optimized conformers for compound CJQ.

Inputs	Outputs
CJQ-m2-t	CJQ-m-q-w6
CJQ-m2-r	
CJQ-m2-s	CJQ-m-r-w6
CJQ-m2-q	
CJQ-k-s	CJQ-p-q-w5
CJQ-m1-s	CJQ-m-q-w1
CJQ-g-s	CJQ-p-q-w5
CJQ-p-s	
CJQ-g-r	CJQ-p-q-w5′
CJQ-k-r	
CJQ-k-q	
CJQ-g-q	
CJQ-p-q	
CJQ-p-r	
CJQ-g-t	CJQ-p-s-w5
CJQ-k-t	
CJQ-p-t	
CJQ-m1-r	CJQ-m-r-w1
CJQ-m1-t	CJQ-m-s-w1
CJQ-m1-q	CJQ-m-q-w1′
CJQ-j-t	CJQ-j-q-w5
CJQ-j-r	
CJQ-j-q	CJQ-j-r-w5
CJQ-j-s	

Table A17. Input geometries and resulting optimized conformers for compound CLP.

Inputs	Outputs
CLP-k-s	CLP-p-q-w5
CLP-k-r	
CLP-p-s	
CLP-p-r	
CLP-k-t	CLP-p-s-w5
CLP-p-t	
CLP-p-q	CLP-p-r-w5
CLP-k-q	CLP-p-r-w5′
CLP-m1-s	CLP-m-r-w1
CLP-m1-t	CLP-m-s-w1
CLP-m1-q	CLP-m-q-w1
CLP-m1-r	
CLP-m2-q	CLP-m-q-w2
CLP-m2-s	
CLP-m2-t	CLP-m-s-w2
CLP-m2-r	CLP-m-q-w2

CLP-j-r	CLP-j-q-w5
CLP-j-q	CLP-j-r-w5
CLP-j-s	
CLP-j-t	CLP-j-s-w5
CLP-g-r	CLP-j-q-w6
CLP-g-q	CLP-j-r-w6
CLP-g-s	
CLP-g-t	CLP-j-s-w6

Table A18. Input geometries and resulting optimized conformers for compound CLQ.

Inputs	Outputs
CLQ-k-s	CLQ-p-q-w5
CLQ-k-r	
CLQ-m2-q	
CLQ-m2-t	
CLQ-m2-s	
CLQ-p-s	
CLQ-p-r	
CLQ-k-t	CLQ-p-s-w5
CLQ-p-t	
CLQ-m2-r	CLQ-m-q-w1
CLQ-k-q	
CLQ-p-q	
CLQ-m1-r	CLQ-m-r-w1′
CLQ-m1-s	CLQ-m-r-w1
CLQ-m1-t	CLQ-m-s-w1
CLQ-m1-q	CLQ-m-q-w1′
CLQ-g-r	CLQ-j-q-w5
CLQ-j-r	
CLQ-g-q	CLQ-j-r-w5
CLQ-g-s	
CLQ-j-q	
CLQ-j-s	
CLQ-g-t	CLQ-j-s-w6
CLQ-j-t	

Table A19. Input geometries and resulting optimized conformers for compound DGP.

Inputs	Outputs
DGP-m2-r	DGP-m-r
DGP-m2-s	
DGP-m1-s	
DGP-m1-r	
DGP-m2-t	DGP-m-s
DGP-m1-t	
DGP-p-r	DGP-p-q
DGP-p-t	DGP-p-s
DGP-p-s	DGP-p-t
DGP-m1-q	DGP-m-q
DGP-m2-q	
DGP-p-q	
DGP-k-r	DGP-k-q
DGP-k-q	DGP-k-r
DGP-k-s	
DGP-k-t	DGP-k-s
DGP-g-q	DGP-g-r
DGP-g-s	
DGP-g-t	
DGP-g-r	DGP-g-q
DGP-j-r	DGP-j-q
DGP-j-q	DGP-j-r
DGP-j-s	
DGP-j-t	DGP-j-s

Table A20. Input geometries and resulting optimized conformers for compound DGQ.

Inputs	Outputs
DGQ-m2-q	DGQ-m-r
DGQ-m2-t	
DGQ-k-s	DGQ-p-q
DGQ-m1-s	
DGQ-m1-r	
DGQ-p-s	
DGQ-p-r	
DGQ-m1-q	DGQ-m-q
DGQ-m1-t	
DGQ-p-q	
DGQ-p-t	
DGQ-m2-s	DGQ-m-q′
DGQ-m2-r	
DGQ-k-r	DGQ-k-q
DGQ-k-q	DGQ-k-r
DGQ-k-t	

DGQ-g-s	DGQ-g-t
DGQ-g-q	DGQ-g-r
DGQ-g-t	
DGQ-g-r	DGQ-g-q
DGQ-j-r	DGQ-j-q
DGQ-j-q	DGQ-j-r
DGQ-j-t	
DGQ-j-s	DGQ-j-t

Table A21. Input geometries and resulting optimized conformers for compound DJP.

Inputs	Outputs
DJP-m2-s	DJP-m-r
DJP-g-t	DJP-p-s
DJP-m2-t	
DJP-m1-t	
DJP-p-t	
DJP-g-s	DJP-p-q
DJP-g-r	
DJP-m2-q	
DJP-m1-s	
DJP-m1-r	
DJP-p-s	
DJP-p-r	
DJP-m2-r	DJP-m-q
DJP-m1-q	
DJP-p-r	
DJP-g-q	DJP-p-r
DJP-k-r	DJP-k-q
DJP-k-s	DJP-k-r
DJP-k-q	DJP-k-r′
DJP-k-t	DJP-k-s
DJP-j-r	DJP-j-q
DJP-j-t	DJP-j-s
DJP-j-q	DJP-j-r
DJP-j-s	

Table A22. Input geometries and resulting optimized conformers for compound DJQ.

Inputs	Outputs
DJQ-k-t	DJQ-m-q
DJQ-k-r	DJQ-k-q
DJQ-k-s	DJQ-k-r
DJQ-k-q	
DJQ-m2-q	DJQ-m-r
DJQ-m2-t	DJQ-m-s
DJQ-m2-s	DJQ-m-t
DJQ-m1-t	DJQ-m-s′
DJQ-m2-r	DJQ-m-q
DJQ-g-s	DJQ-p-q
DJQ-p-s	
DJQ-m1-r	DJQ-m-r′
DJQ-g-r	DJQ-p-q′
DJQ-p-r	
DJQ-g-q	DJQ-p-r
DJQ-p-q	
DJQ-m1-s	DJQ-m-q
DJQ-m1-q	
DJQ-j-t	DJQ-j-q
DJQ-j-r	
DJQ-j-q	DJQ-j-r
DJQ-j-s	

Table A23. Input geometries and resulting optimized conformers for compound DLP.

Inputs	Outputs
DLP-m2-q	DLP-m-r
DLP-m2-s	
DLP-m1-s	
DLP-m1-r	
DLP-m2-t	DLP-m-s
DLP-m1-t	
DLP-p-r	DLP-p-q
DLP-p-t	DLP-p-s
DLP-p-s	CLP-p-t
DLP-m2-r	DLP-m-q
DLP-m1-q	
DLP-p-q	DLP-p-r
DLP-k-r	DLP-k-q
DLP-k-q	DLP-k-r
DLP-k-s	
DLP-k-t	DLP-k-s
DLP-j-r	DLP-j-q
DLP-g-r	

DLP-g-t	DLP-j-s
DLP-j-t	
DLP-g-q	DLP-j-r
DLP-g-s	
DLP-j-q	
DLP-j-s	

Table A24. Input geometries and resulting optimized conformers for compound DLQ.

Inputs	Outputs
DLQ-k-s	DLQ-p-q
DLQ-k-r	DLQ-k-q
DLQ-k-q	DLQ-k-r
DLQ-k-t	
DLQ-m2-t	DLQ-m-r
DLQ-m1-q	DLQ-m-q
DLQ-m1-t	
DLQ-m1-s	
DLQ-m1-r	
DLQ-p-q	
DLQ-p-t	
DLQ-p-s	
DLQ-p-r	
DLQ-m2-s	DLQ-m-r′
DLQ-m2-r	DLQ-m-q′
DLQ-g-r	DLQ-j-q
DLQ-j-r	
DLQ-g-q	DLQ-j-r
DLQ-g-t	
DLQ-j-q	
DLQ-j-t	
DLQ-g-s	DLQ-j-t
DLQ-j-s	

Table A25. Input geometries and resulting optimized conformers for compound EGP.

Inputs	Outputs
EGP-m2-q	EGP-m-r-x4
EGP-m2-s	
EGP-m2-t	EGP-m-s-x4
EGP-m2-r	EGP-m-q-x4
EGP-m1-s	EGP-m-r-x1
EGP-m1-r	
EGP-m1-t	EGP-m-s-x1
EGP-p-s	EGP-p-q-x3
EGP-p-r	
EGP-p-t	EGP-p-s-x3
EGP-m1-q	EGP-m-q-x1
EGP-p-q	
EGP-k-r	EGP-k-q-x1
EGP-k-s	EGP-k-r-x2
EGP-k-q	EGP-k-q-x1
EGP-k-t	EGP-k-s-x1
EGP-g-q	EGP-g-r-x1
EGP-g-t	
EGP-g-s	
EGP-g-r	EGP-g-q-x1
EGP-j-r	EGP-j-q-x3
EGP-j-s	EGP-j-r-x3
EGP-j-q	
EGP-j-t	EGP-j-s-x3

Table A26. Input geometries and resulting optimized conformers for compound EGQ.

Inputs	Outputs
EGQ-m2-q	EGQ-m-r-x4
EGQ-m2-t	
EGQ-m2-s	EGQ-m-q-x4
EGQ-m2-r	
EGQ-m1-s	EGQ-m-r-x1
EGQ-m1-r	
EGQ-p-r	
EGQ-m1-q	EGQ-m-q-x1
EGQ-m1-t	
EGQ-p-q	
EGQ-p-t	
EGQ-k-s	EGQ-p-q-x3
EGQ-k-t	EGQ-p-r-x3
EGQ-k-r	EGQ-k-q-x4
EGQ-k-q	EGQ-k-r-x4
EGQ-g-q	EGQ-g-r-x1

EGQ-g-t	
EGQ-g-s	EGQ-g-t-x1
EGQ-g-r	EGQ-g-q-x1
EGQ-j-r	EGQ-j-q-x3
EGQ-j-q	EGQ-j-r-x3
EGQ-j-t	
EGQ-j-s	EGQ-j-t-x3

Table A27. Input geometries and resulting optimized conformers for compound EJP.

Inputs	Outputs
EJP-m2-s	EJP-m-s-x4
EJP-m2-q	
EJP-m-2t	EJP-m-r-x4
EJP-m2-r	EJP-m-q-x4
EJP-g-t	EJP-p-s-x4
EJP-m-t	
EJP-p-t	
EJP-g-s	EJP-p-q-x4
EJP-g-r	
EJP-m1-s	
EJP-m1-r	
EJP-p-s	
EJP-p-r	
EJP-g-q	EJP-p-r-x4
EJP-m1-q	
EJP-p-q	
EJP-k-r	EJP-k-q-x1
EJP-k-s	EJP-k-r-x1
EJP-k-q	EJP-k-r-x1′
EJP-k-t	EJP-k-s-x1
EJP-j-r	EJP-j-q-x3
EJP-j-q	EJP-j-r-x3
EJP-j-s	
EJP-j-t	EJP-j-s-x3

Table A28. Input geometries and resulting optimized conformers for compound EJQ.

Inputs	Outputs
EJQ-m2-t	EJQ-m-q-x4
EJQ-m2-r	
EJQ-m2-s	EJQ-m-r-x4
EJQ-m2-q	
EJQ-g-s	EJQ-p-q-x4
EJQ-p-s	
EJQ-p-r	EJQ-p-q-x4′
EJQ-m1-r	EJQ-m-r-x1
EJQ-m1-t	EJQ-m-s-x1
EJQ-g-q	EJQ-p-r-x4
EJQ-p-q	
EJQ-g-t	EJQ-p-s-x4
EJQ-g-r	
EJQ-p-t	
EJQ-m1-s	EJQ-m-q-x1
EJQ-m1-q	
EJQ-k-s	EJQ-k-q-x4
EJQ-k-r	
EJQ-k-q	EJQ-k-r-x4
EJQ-k-t	
EJQ-j-t	EJQ-j-q-x3
EJQ-j-r	
EJQ-j-q	EJQ-j-r-x3
EJQ-j-s	

Table A29. Input geometries and resulting optimized conformers for compound ELP.

Inputs	Outputs
ELP-m2-s	ELP-m-s-x4
ELP-m2-q	
ELP-m2-t	ELP-m-q-x4
ELP-m2-r	ELP-m-q-x4
ELP-m1-s	ELP-m-r-x1
ELP-m1-r	
ELP-m1-t	ELP-m-s-x1
ELP-p-s	ELP-p-s-x4
ELP-p-r	
ELP-p-t	ELP-p-s-x4′
ELP-m-q	ELP-m-q-x1
ELP-p-q	
ELP-k-r	ELP-k-q-x1
ELP-k-s	ELP-k-r-x1
ELP-k-q	
ELP-k-t	ELP-k-s-x1

ELP-j-r	ELP-j-q-x3
ELP-j-q	ELP-j-r-x3
ELP-j-s	
ELP-j-t	ELP-j-s-x3
ELP-g-r	ELP-j-q-x3′
ELP-g-s	ELP-j-r-x3′
ELP-g-q	
ELP-g-t	ELP-j-s-x3′

Table A30. Input geometries and resulting optimized conformers for compound ELQ.

Inputs	Outputs
ELQ-m2-t	ELQ-m-r-x4
ELQ-m2-q	
ELQ-m2-s	ELQ-m-q-x4
ELQ-m2-r	
ELQ-m1-s	ELQ-m-r-x1
ELQ-m1-r	
ELQ-p-s	
ELQ-p-r	
ELQ-m1-q	ELQ-m-q-x1
ELQ-m1-t	
ELQ-12	
ELQ-p-t	
ELQ-k-t	ELQ-k-q-x4
ELQ-k-r	
ELQ-k-s	ELQ-k-r-x4
ELQ-k-q	
ELQ-g-t	ELQ-j-q-x3
ELQ-g-r	
ELQ-g-s	ELQ-j-r-x3
ELQ-g-q	
ELQ-j-r	ELQ-j-q-x3′
ELQ-j-s	ELQ-j-r-x3′
ELQ-j-q	
ELQ-j-t	ELQ-j-s-x3

Table A31. Input geometries and resulting optimized conformers for compound FGP.

Inputs	Outputs
FGP-m2-s	FGP-m-r-x4
FGP-m2-q	
FGP-m2-t	FGP-m-s-x4
FGP-m2-r	FGP-m-q-x4
FGP-m1-s	FGP-m-r-x1
FGP-m1-r	
FGP-m1-t	FGP-m-s-x1
FGP-p-s	FGP-p-q-x4
FGP-p-r	
FGP-p-t	FGP-p-s-x4
FGP-m1-q	FGP-m-q-x1
FGP-p-q	FGP-p-r-x4
FGP-k-r	FGP-k-q-x1
FGP-k-q	FGP-k-r-x1
FGP-k-s	FGP-k-r-x1
FGP-g-q	FGP-g-r-x1
FGP-g-t	FGP-g-r-x1′
FGP-g-s	
FGP-g-r	FGP-g-q-x1
FGP-j-r	FGP-j-q-x3
FGP-j-q	FGP-j-r-x3
FGP-j-s	
FGP-j-t	FGP-j-s-x3

Table A32. Input geometries and resulting optimized conformers for compound GQ.

Inputs	Outputs
FGQ-m2-q	FGQ-m-r-x4
FGQ-m2-t	
FGQ-m2-s	FGQ-m-q-x4
FGQ-m2-r	
FGQ-k-s	FGQ-p-q-x4
FGQ-m1-s	FGQ-m-r-x1
FGQ-m1-r	
FGQ-p-s	
FGQ-p-r	
FGQ-m1-t	FGQ-m-q-x1
FGQ-m1-q	
FGQ-p-q	
FGQ-p-t	
FGQ-k-q	FGQ-k-r-x4
FGQ-k-t	

FGQ-g-q	FGQ-g-r-x1
FGQ-g-t	
FGQ-g-r	FGQ-g-q-x1
FGQ-g-s	FGQ-g-t-x1
FGQ-j-r	FGQ-j-q-x3
FGQ-j-q	FGQ-j-r-x3
FGQ-j-t	
FGQ-j-s	FGQ-j-t-x3

Table A33. Input geometries and resulting optimized conformers for compound FJP.

Inputs	Outputs
FJP-m1-s	FJP-m-r-x4
FJP-m1-q	
FJP-m1-t	FJP-m-s-x4
FJP-m1-r	FJP-m-q-x4
FJP-g-s	FJP-p-q-x4
FJP-g-r	
FJP-m1-s	
FJP-m1-r	
FJP-p-s	
FJP-p-r	
FJP-g-t	FJP-p-s-x4
FJP-m1-t	
FJP-p-t	
FJP-k-r	FJP-k-q-x1
FJP-g-q	FJP-p-r-x1
FJP-m1-q	
FJP-p-q	
FJP-k-q	FJP-k-r-x1
FJP-k-s	
FJP-k-t	FJP-k-s-x1
FJP-j-r	FJP-j-q-x3
FJP-j-q	FJP-j-r-x3
FJP-j-s	
FJP-j-t	FJP-j-s-x3

Table A34. Input geometries and resulting optimized conformers for compound FJQ.

Inputs	Outputs
FJQ-m2-s	FJQ-m-q-x4
FJQ-m2-r	
FJQ-m2-t	FJQ-m-r-x4
FJQ-m2-q	
FJQ-p-q	FJQ-p-r-x4
FJQ-p-t	
FJQ-k-s	FJQ-p-q-x4
FJQ-p-s	FJQ-p-q-x4′
FJQ-p-r	
FJQ-m1-q	FJQ-m-q-x1
FJQ-m1-s	
FJQ-m1-t	FJQ-m-r-x1
FJQ-m1-r	
FJQ-k-r	FJQ-k-q-x4
FJQ-k-q	FJQ-k-r-x4
FJQ-k-t	
FJQ-j-t	FJQ-j-q-x3
FJQ-j-r	
FJQ-j-q	FJQ-j-r-x3
FJQ-j-s	
FJQ-g-t	FJQ-j-r-x3′
FJQ-g-q	
FJQ-g-s	FJQ-j-t-x3
FJQ-g-r	FJQ-j-q-x3′

Table A35. Input geometries and resulting optimized conformers for compound FLP.

Inputs	Outputs
FLP-m2-s	FLP-m-r-x4
FLP-m2-q	
FLP-m2-r	FLP-m-q-x4
FLP-m1-s	FLP-m-r-x1
FLP-m1-r	
FLP-m2-t	FLP-m-s-x4
FLP-m1-t	FLP-m-s-x1
FLP-p-s	FLP-p-q-x4
FLP-p-r	
FLP-p-t	FLP-p-s-x4
FLP-m1-q	FLP-m-q-x1
FLP-p-q	
FLP-k-r	FLP-k-q-x1
FLP-k-s	FLP-k-r-x1

FLP-k-q	
FLP-k-t	FLP-k-s-x1
FLP-j-r	FLP-j-q-x3
FLP-j-q	FLP-j-r-x3
FLP-j-s	
FLP-j-t	FLP-j-s-x3′
FLP-g-r	FLP-j-q-x3′
FLP-g-q	FLP-j-r-x3′
FLP-g-s	
FLP-g-t	FLP-j-s-x3

Table A36. Input geometries and resulting optimized conformers for compound FLQ.

Inputs	Outputs
FLQ-g-s	FLQ-p-q-x2
FLQ-m2-t	FLQ-m-r-x4
FLQ-m2-q	
FLQ-m2-s	FLQ-m-q-x4
FLQ-m2-r	
FLQ-p-t	FLQ-p-q-x4
FLQ-p-r	
FLQ-m1-s	FLQ-m-r-x1
FLQ-m1-r	
FLQ-m1-q	FLQ-m-q-x1
FLQ-m1-t	FLQ-m-q-x1′
FLQ-k-s	FLQ-p-r-x4
FLQ-p-q	FLQ-p-r-x4′
FLQ-p-s	
FLQ-k-t	FLQ-k-q-x4
FLQ-k-r	
FLQ-g-r	FLQ-k-q-x1
FLQ-k-q	FLQ-k-r-x4
FLQ-g-q	FLQ-k-r-x1
FLQ-g-t	
FLQ-j-t	FLQ-j-q-x3
FLQ-j-r	
FLQ-j-s	FLQ-j-r-x3
FLQ-j-q	

Table A37. Compounds with R′= pyrrolidine and types of conformers possible and what they optimize to.

Compounds	Type of conformers possible				
	m	p	k	g	j
AGP	Possible	possible	Possible	Possible	Possible
AGQ	Possible	Optimized to m	Possible	Possible	Possible
BGP	Possible	Possible	Possible	Possible	Possible
BGQ	Possible	Optimized to m	Possible	Optimized to k	Possible
CGP	Possible	Possible	Optimized to p	Possible	Possible
CGQ	Possible	Possible	Optimized to p	Optimized to p	Possible
DGP	Possible	Possible	Possible	Possible	Possible
DGQ	Possible	Possible	Possible	Possible	Possible
EGP	Possible	Possible	Possible	Possible	Possible
EGQ	Possible	Possible	Possible	Possible	Possible
FGP	Possible	Possible	Possible	Possible	Possible
FGQ	Possible	optimized to m	Possible	Possible	Possible

Table A38. Compounds with R′= morpholine and types of conformers possible and what they optimize to.

Compounds	Type of conformers possible				
	m	p	k	g	j
AJP	Possible	optimized to m	Possible	Optimized to k	Possible
AJQ	Possible	Possible	Possible	Optimized to p	Possible
BJP	Possible	Possible	Possible	Optimized to p	Possible
BJQ	Possible	Possible	optimized to p	Optimized to p	Possible
CJP	Possible	Possible	Optimized to p	Optimized to p	Possible
CJQ	Possible	Possible	Optimized to p	Optimized to p	Possible
DJP	Possible	Possible	Possible	Optimized to p	Possible
DJQ	Possible	Possible	Possible	Optimized to p	Possible
EJP	Possible	Possible	Possible	Optimized to p	Possible
EJQ	Possible	Possible	Possible	Optimized to p	Possible
FJP	Possible	Possible	Possible	Optimized to p	Possible
FJQ	Possible	Possible	Possible	Optimized to j	Possible

Table A38. Compounds with R′= Diethylamine and types of conformers possible and what they optimize to.

Compounds	Type of conformers possible				
	m	p	k	g	j
ALP	Possible	Optimized to m	Possible	Optimized to k	Possible
ALQ	Possible	Optimized to m	Possible	Optimized to j	Possible
BLP	Possible	Possible	Possible	Optimized to j	Possible
BLQ	Possible	Possible	Possible	Optimized to j	Possible
CLP	Possible	Possible	Optimized to p	Optimized to j	Possible
CLQ	Possible	Possible	Optimized to p	Optimized to j	Possible
DLP	Possible	Possible	Possible	Optimized to j	Possible
DLQ	Possible	Possible	Possible	Optimized to j	Possible
ELP	Possible	Possible	Possible	Optimized to j	Possible
ELQ	Possible	Optimized to m	Possible	Optimized to j	Possible
FLP	Possible	Possible	Possible	Optimized to j	Possible
FLQ	Possible	Possible	Possible	Optimized to k	Possible