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CORRELATION BETWEEN BAND GAP, REFRACTIVE INDEX, OPTICAL ELECTRONEGATIVITY AND DIELECTRIC CONSTANT OF EPINEPHRINE SUBSTITUTION WITH PHOSPHORUS (P) AND SELENIUM (Se): DFT STUDY

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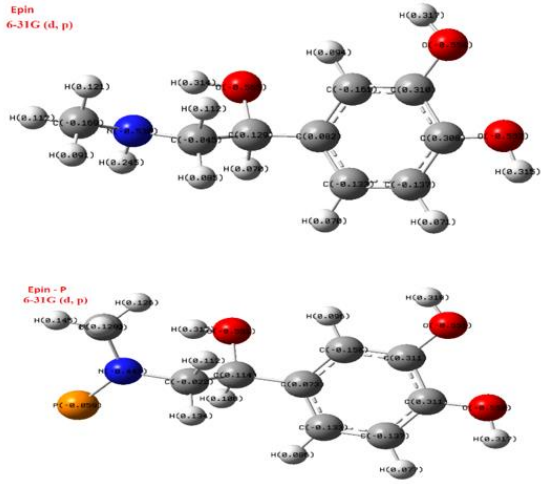
Epinephrine is a neurotransmitter that plays a key role in the connection of two nerve cells. This connection allows for the transmission of a signal, which is a message, to be sent between the nerve cells. Our study has discovered some interesting connections between the HOMO-LUMO energy gap, the refractive index (n), the dielectric constant (ε), and the optical electronegativity (Δχ∗) of three different types of epinephrine with names (Epin, Epin-P, and Epin-Se). The main goal of this study is to find out what changes happen to the epinephrine molecule when phosphorus (P) and selenium (Se) are substituted, looking at its refractive index, dielectric constant, optical negativity, global reactivity, and other factors. Running the Gaussian program with the DFT/6-31G (d, p) and 6-31G+(d, p) basis sets with neutral and protonated structures of the epinephrine compounds produced the best results. According to the results, the refractive index and the HOMO-LUMO energy gap of epinephrine are inversely associated. A narrow refractive index is correlated with a high energy gap. Also, optical electronegativity (Δ χ*) and the HOMO-LUMO energy gap are directly related.



INTRODUCTION

In recent years, there has been significant growth in the use of machine learning techniques to predict the structure and chemical characteristics of a substance. This is contingent upon the atomistic structure and factors that are supplied.[1,2] Epinephrine is a neurotransmitter that plays a significant role in the connection of two nerve cells, enabling the transfer of a message in the form of a signal. The examination of epinephrine's conformational structure has the potential to reveal profound insights into the significant biological actions that it does. Epinephrine is classified as a neurotransmitter, a medicine, and a hormone. Several neurons and adrenal glands are responsible

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for its production in the central nervous system. The degree of pupil dilation and blood sugar are both increased by epinephrine, which plays a crucial part in the fight-or-flight response.[3] The chemical and physical characteristics of epinephrine have been the primary focus of research to explore the activity of the substance and its interaction with biological systems. A better knowledge of the roles and actions of hormones may be gained via the study of the energetic and conformational properties of epinephrine by researchers. Experimental and theoretical research on epinephrine reveals that catecholamine neurotransmitter structure modulates receptor binding and directly impacts metabolism.[4] In both the central noradrenergic and peripheral sympathetic synapses of the brain, the neurotransmitter norepinephrine (NE) plays a role in the process of reuptaking any NE that has been released into the nerve terminals. Hyperregulation of this neurotransmitter has been associated with a wide variety of severe types of psychosis and mental illness.[5] The development of pharmaceutical targets that block the norepinephrine transporter (NET) has great promise for the treatment of several neurological and psychiatric disorders. Researchers have hypothesized for half a century that NE acts as a significant factor in the pathogenesis of the disease. Studies have shown that those suffering from depression, withdrawal symptoms, and other disorders may have elevated amounts of NE, which is essential for proper brain development. In addition, NE is a chemical messenger that carries signals from one nerve cell to another.[6,7,8] Current research suggests that norepinephrine is one of the neurotransmitters associated with depression and that antidepressants that act on this specific neurotransmitter are useful.[9] The DFT method's predicted spectrum intensities are critical for interpreting experimental epinephrine spectra, particularly the unique wavenumbers for each atom.[10,11] Phosphorus or (P), which is ranked 15 in the periodic table, is a non-metallic element that has a density of 1.8 grams per cubic centimeter and an atomic volume of 17 cubic centimeters per mole. One of the most important elements for growing food is phosphorus (P).[12,13] The chemical properties of selenium or (Se) indicate that, within biological systems. In vivo, selenium (Se) compounds often experience a reduction process, while sulfur compounds are typically obtained in a reduced state and usually undergo oxidation. Selenium (Se) seems to be integrated into proteins by post-translational modification of polypeptides.[14]

The fundamental purpose of this study is to evaluate the impacts of phosphorus (P) and Selenium (Se) replacement by Hydrogen atom on the molecule of epinephrine in terms of its refractive index, dielectric constant, optical negativity, global reactivates, and other characteristics. Specifically, the research will explore how these substitutions affect the chemical reactivities and stability of molecules with names: (Epin, Epin -P, and Epin -Se). By using the density functional theory DFT/B3LYP level of theory (method) with the 6-31G (d, p) neutral and 6-31G + (d, p) protonated basis sets.

COMPUTATIONAL METHODOLOGY

The density-functional theory (DFT) is an important method for researching the electrical characteristics of nanoclusters. The DFT technique has been effectively employed in a variety of fields in recent years, including materials science, nanoelectronics, chemical engineering, physics, biology, life sciences, surface sciences, and earth sciences. The quantum software known as Gaussian 0.9 version was used to carry out every one of the calculations on the Epinephrine chemical for this latest investigation. The chemical compounds' initial geometries were estimated using the software program called the Gauss View 5.0 package. In addition, a DFT method was used to calculate outputs using the Gaussian 09W.[15]

The primary objective of this research is to determine the effects of phosphorus (P) and selenium (Se) substitution on the epinephrine molecule in terms of its refractive index, dielectric constant, optical negativity, global reactivates, and other properties.[16] The electronic properties and physical parameters of this compound, such as Highest Occupied Molecular Orbital (E_{HOMO}), Lowest Unoccupied Molecular Orbital (E_{LUMO}), band gap (BG), ionization energy (IE), electron affinity (EA), absolute electronegativity (χ), global hardness (η), and softness (S).[17,18] The optical properties of epinephrine, including its refractive index, dielectric constant, and optical electronegativity, are calculated for the compounds listed with names: (Epin, Epin -P, and Epin -Se). Refractive index parameter and dielectric constant of (Epin, Epin -P, and Epin -Se) are calculated by: Moss *et al.*,[19] Ravindra *et al.*,[20,21] Herve *et al.*,[22,23] Reddy *et al.*,[24] Kumar *et al.*, and Tripathy *et al.*[25]

RESULT AND DISCUSSION

1. Equilibrium Geometry

Running the Gaussian program with the DFT/ 6-31G (d, p), and 6-31G +(d, p) basis sets with neutral to the structure of the Epinephrine compounds produced the best shape, as shown in Fig. 1 left hand. The chemical and biological activity of organic substances is directly linked to the shape and type of their molecular orbitals (MOs), also known as HOMO and LUMO.[26,27] The first step of a geometry optimization technique that can be used for this method is to look at the energy that is linked to a certain starting shape of the molecules. As can be seen from Table 1, the energy ground states are negative. When the energy of a bound system (such as an atom) is negative, it signifies that the system's energy is lower than the energy of its constituent particles. The force that propels electrostatic interactions is the electrical charge density inside the molecule. Figure 1 right-hand shows that the physicochemical characteristics and chemical reactions of the compounds Epin, Epin -P, and Epin -Se are influenced by electron charge density and electrostatic potential (ESP) map. A chemical reactivity index or a measure of weak intermolecular interactions may be found using charge-based descriptors. A great number of quantum chemical descriptors are produced from the partial charge distribution inside a molecule or from the electron density on certain atoms. Under the effect of phosphorus (S) and selenium (Se) components, charge distribution was discovered for all molecules using the neutral and protonated technique.[28,29]

Table 1

SCF Done E(RB3LYP) level of theory

Compounds	**Ground State energy (a.u)**	
Compounds Name	**6-31G (d, p)**	**6-31G + (d, p)**
Epin	–631.202	–631.235
Epin -P	–971.895	–971.928
Epin -Se	–3029.953	–3030.016

In comparison to other elements such as carbon (C), nitrogen, hydrogen (H), sulfur (S), and selenium (Se), the oxygen (O) atom of the hydroxyl group (OH^{-1}) was found to be the most negatively charged of all the atoms. The charge density of each element fell from the neutral to the protonated state, as illustrated in Fig. 1, which is related to charge density. By this, the charge density of neutral is greater than the charge density of protonated. According to the results, the N element with Epin -Se has a lower charge density because it has a smaller number of charge nitrogen atoms (N=–0.410, –0.143). This is because the electronegativity of the Se element is higher than that of the H element and the P element or ranking of electronegativity: Se = 2.59 > H = 2.20 > P = 2019. The molecule of epinephrine has a higher propensity for nucleophilic rivalry than electrophilic competition due to its three oxygen atoms and one nitrogen atom. Epinephrine has a higher number of negatively charged atoms compared to positively charged atoms. This is one of the things that makes the substance good at anticorrosion properties.[1] The generation of the ESP around molecules in a place at a point *r* (in atomic units) can be shown quantitatively with Eq. 1:[30]

$$V_{(r)} = \sum_A \frac{Z_A}{\lceil R_A - r \rceil} - \int \frac{\rho(r) d\acute{r}}{\lceil \acute{r} - r \rceil} \quad (1)$$

The ESP is linked to several things, such as partial charges, the dipolar moment, electronegativity, and where the chemical reactions happen in the molecule structure. The MEP can identify molecules with proton affinity, which relates to charge-regulated hard-hard interactions and relative polarity. Red regions have more electrons, a negative charge, and a proton affinity. The negative charge density of C–OH and the red zone was larger than that of other groups, as illustrated in Fig. 1. Blue regions have more positive charge, lower electron density, and weaker proton affinity. Red represents fields with the strongest negative electrostatic potential. This pattern of red < yellow < green < blue results in an increase in potential. The observation that only a small fraction of the epinephrine molecule occupied the positive (blue) region and the majority was in the negative (green) range indicates that the epinephrine molecular structure (Epin, Epin -P, and Epin -Se) is exceptionally reactive with nucleophilic species.[30,31]

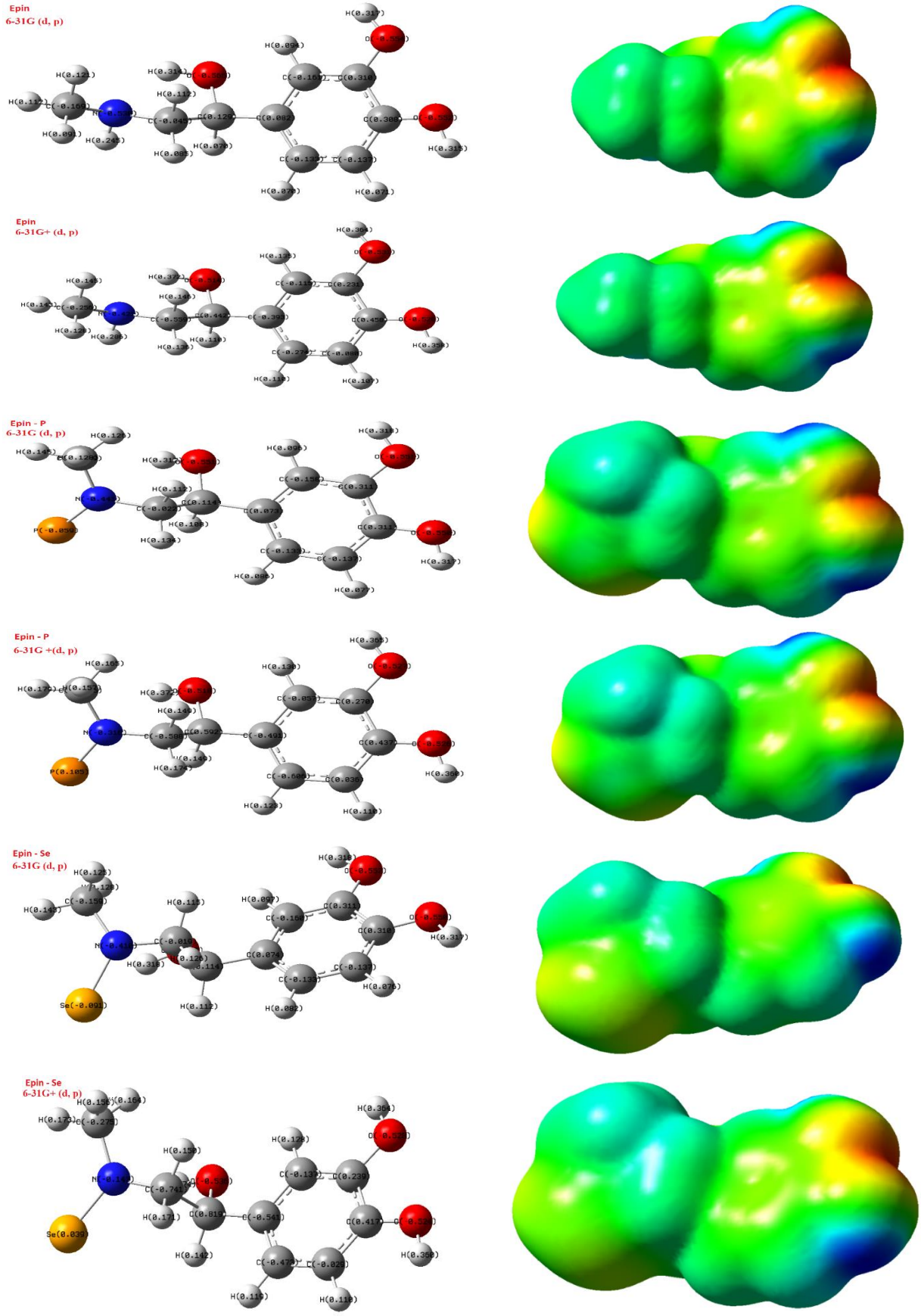

Fig. 1 – Geometry optimization is performed for the left-hand side; right hand side is Electrostatic Potential (ESP) surface approach based on Density Functional Theory (DFT).

2. Electronic Properties and DFT

In this section, the energy gap between the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO), as well as the front molecular orbitals (FMOs) of Epin, Epin -P, and Epin -Se compounds, are discussed as shown in bellow Fig. 2. In the context of molecular orbitals, the HOMO-LUMO energy gap refers to the least amount of energy required to move a molecular orbital from its occupied state to its unoccupied state. Both HOMO and LUMO are essential components in gaining knowledge of the electronic structure of the molecular system, as well as the process that determines the transfer of potential energy. In Table 2, the HOMO-LUMO energy gap of all compounds is listed. This gap was calculated using the DFT/B3LYP level of theory (method) using 6-31G (d, p), and 6-31G +(d, p), basis sets.[32,33,34] As a result of the energy gap of Epin and Epin -P, the BG energy has always been decreased. When a material's band gap energy drops, it could become more reactive, less chemically stable, and exhibit different corrosion behavior or cause new problems when trying to limit corrosion. However, with an energy gap of 1.684 eV when neutral and 1.655 eV when protonated, the Epin-P conformer was the most energy efficient. In comparison to the other conformers, this one shows much less stability and more chemical reactivity than Epin, and Epin – Se compounds. When considering structural stability and responsiveness, absolute hardness and softness are two of the most crucial properties to consider. Compared to hard molecules, soft ones are more reactive because they can transfer electrons more easily. Based on the information shown in Table 2, the molecular hardnesses have been ranked from highest to lowest for neutral, and protonated: Epin > Epin -Se > Epin - P, while molecular softness Epin -P > Epin - Se > Epin compounds. The Epin - P molecule has a softness of 0.694 and an energy of 0.604 eV, which indicates that it is very capable of transferring electrons. The conclusion that can be drawn from this is that the energy band gap is directly related to the hardness of the molecule and that a greater molecular hardness is associated with a lower softness (the low molecular softness is a result of a large band gap). The most recent assertions are corroborated by these results, according to the HOMO and LUMO calculation methodologies.[35] Both electronegativity and electrochemical potential are examples of chemical qualities that have a significant relationship with one another. Electronegativity, denoted by the symbol χ, is a measurement that quantifies the capacity of an atom to accept an electron. When the electronegativity of Epin - Se is high (3.372 eV), it indicates that the element attracts electrons more strongly, which results in the formation of polar or ionic bonds. On account of the powerful electrostatic forces. A higher electronegativity value suggests a stronger attraction of 6-31G + (d, p) to protons. Compression HOMO, LUMO, BG, hardness, and softness computations are all depicted in Figs. 3a–c**.**

Table 2

Calculation of global reactivates parameters

Parameters Calculation[30,38–43]	**6-31G (d, p)**			**6-31G + (d, p)**		
	Epin	**Epin -P**	**Epin -Se**	**Epin**	**Epin -P**	**Epin -Se**
HOMO (eV)	–4.38007	–3.65109	–4.47547	–4.72101	–3.90919	–4.76532
LUMO (eV)	0.2712	–1.96725	–2.26911	0.223001	–2.25445	–1.49615
IP (eV)	4.380	3.651	4.475	4.721	3.909	4.765
EA (eV)	–0.271	1.967	2.269	–0.223	2.254	1.496
Band gap energy (E_g) (eV)	4.651	1.684	2.206	4.498	1.655	3.269
Hardness (η) (eV)	2.326	0.842	1.103	2.472	0.827	1.635
Softness (S) (eV)	0.215	0.594	0.453	0.202	0.604	0.306
Electronegativity (χ) (eV)	2.054	2.809	3.372	2.249	3.082	3.131
Chemical potential (μ) (eV)	–2.054	–2.809	–3.372	–2.249	–3.082	–3.131

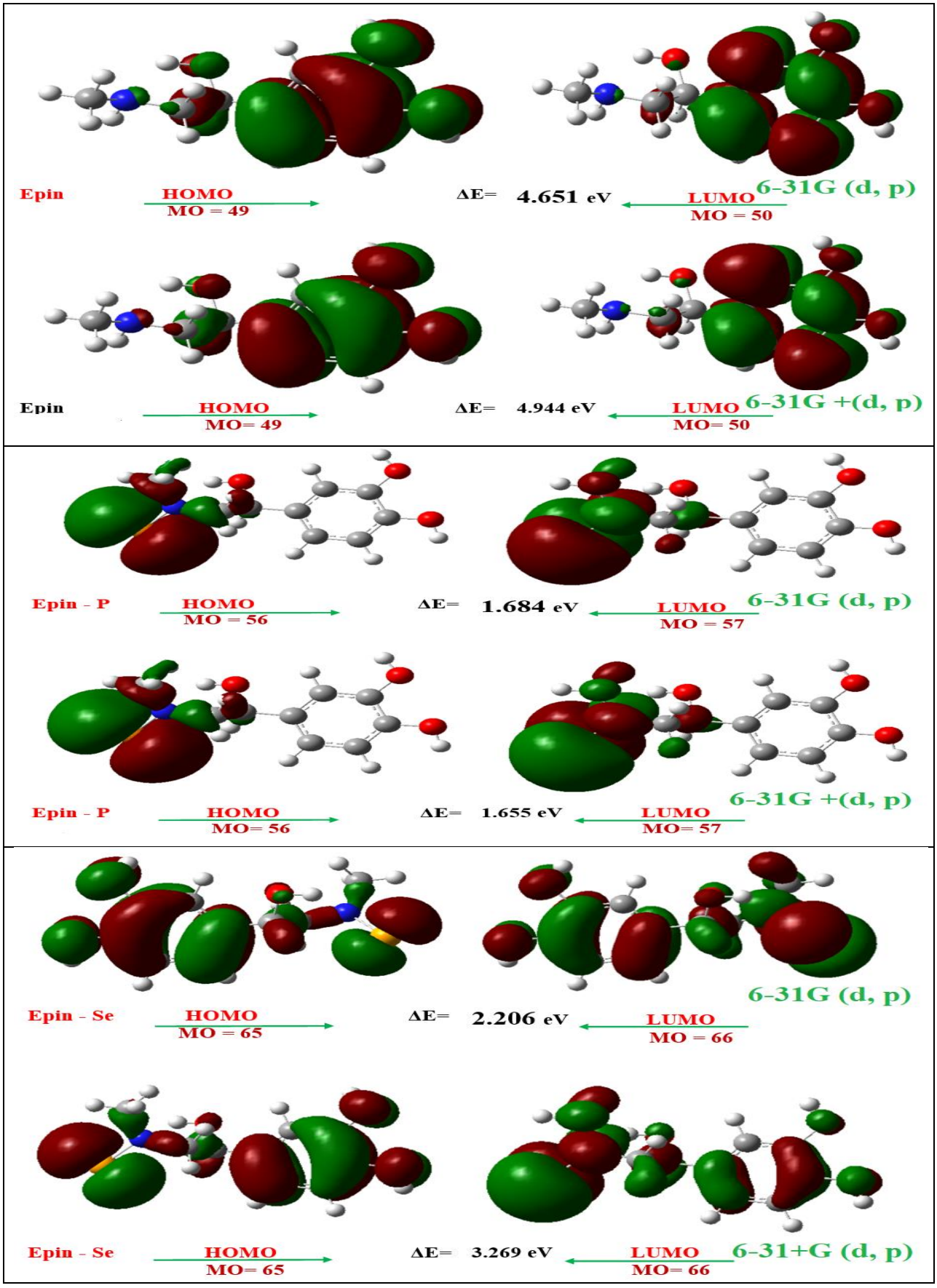

Fig. 2 – The Front molecular orbitals (FMOs) diagram according to HOMO-LUMO.

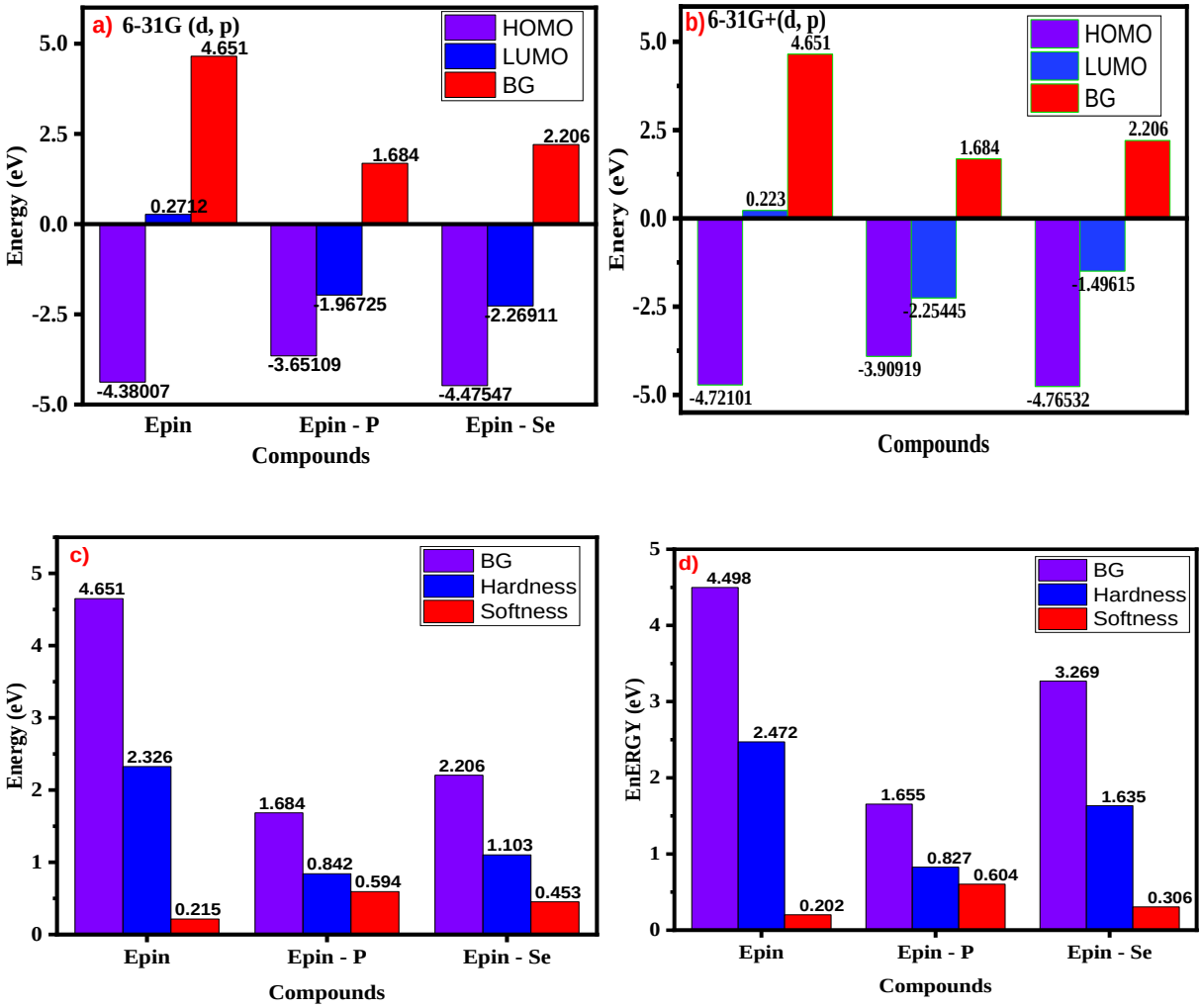

Fig. 3 – Compression HOMO, LUMO, BG, hardness, and softness computations.

3. Optical Properties

In this part, we examine the optical properties of epinephrine, namely the refractive index (n), the dielectric constant (ε), and the optical electronegativity (Δχ∗). Refractive index of the (Epin, Epin -P, and Epin -Se) are calculated by Herve *et al*.[23] It is seen, following the information collected in Table 3, that the magnitudes of the refractive index computed by applying the Moss, Herve, Tripathy, Kumar, and Herve equations have values that are near to one another. The refractive index computed from all these relations show the following pattern: Epin -P > Epin -Se > Epin. The data from Tables 2, and 3 demonstrate that epinephrine's refractive index and HOMO-LUMO energy gap are inversely related. The large energy gap is associated with a small refractive index. One of the important aspects to consider while studying the optical properties of epinephrine is its dielectric constant. The dielectric constant of the Epin, Epin -P, and Epin -Se may be seen to rise as the optical refractive index values for these elements are increased, as can be shown in Tables 3 and 4. It is possible to determine the type of bonding in the materials by determining the magnitude of the optical electronegativity. As seen in Tables 4 and 5, it is possible to detect that the refractive index of the Epin, Epin -P, and Epin -Se increases when the optical electronegativity (Δ χ*) values for these elements decrease. Due to the comparatively high refractive index and the relatively modest magnitude of the optical electronegativity (Δ χ*).[36,37] The data from Tables 2, and 5 demonstrate that epinephrine's optical electronegativity (Δ χ*), and HOMO-LUMO energy gap are directly related.

Table 3

Refractive indexes of compounds

Species	6-31G (d, p)			6-31G + (d, p)		
	Epin	**Epin -P**	**Epin -Se**	**Epin**	**Epin -P**	**Epin -Se**
Moss Relation[19–21]	2.12590727	2.740598	2.561707	2.09368473	2.752526	2.321813
Ravind Revelation[22,23]	1.20024799	3.039678	2.716057	1.01859888	3.057657	2.057037
Herve Relation[24,25]	1.9505183	2.821858	2.596358	1.9006839	2.835825	2.252275
Reddy relation[26]	2.44831413	3.287146	3.024243	2.40817209	3.305466	2.698553
Kumar Relation[27]	2.05135314	2.846153	2.608913	2.01135193	2.862134	2.298269
Tripathy Relation[27]	1.99820079	3.057362	2.731837	1.9590199	3.078273	2.294892

Table 4

Dielectric constants of computed clusters

Species	6-31G (d, p)			6-31G + (d, p)		
	Epin	**Epin -P**	**Epin -Se**	**Epin**	**Epin -P**	**Epin -Se**
Moss Relation	4.519482	7.510879	6.5623	4.383516	7.576398	5.3908
Ravind Revelation	1.440595	9.23964	7.377	1.037544	9.349264	4.2314
Herve Relation	3.804522	7.962881	6.7411	3.612599	8.041904	5.0727
Reddy relation	5.994242	10.80533	9.146	5.799293	10.92611	7.2822
Kumar Relation	4.20805	8.100586	6.8064	4.045537	8.191811	5.282
Tripathy Relation	3.992806	9.347463	7.4629	3.837759	9.475766	5.2665

Table 5

Optical electronegativity ($\Delta\chi^*$)

Compounds Name	6-31G (d, p)	6-31G+ (d, p)
Epi	1.246468	1.324992
Epi -P	0.451312	0.44354
Epi -Se	0.591208	0.876092

4. Density of State (DOS)

One way to characterize the amount and composition of energy in a given unit of increase is by looking at the density of states (DOS). In Figure 4, the DOS according HOMO-LUMO energy gap of all compounds is listed. This gap was calculated using the DFT/B3LYP level of theory (method) using 6-31G (d, p) neutral, and 6-31G + (d, p) basis sets. The DOS may be calculated as a function of energy levels by using Equation 2, which can be found here. In this equation, the symbol E is the total energy of the electrons, the symbol 'g' represents a Gaussian function with a fixed Full Width at Half Maximum (FWHM) of 0.3, and the symbol ε_i indicates the energy that corresponds with the i^{th} orbitals:[38]

$$OS(E) = \Sigma\, g(E - \varepsilon_i) \quad (2)$$

The HOMO-LUMO gap,[39,40] which is approximately comparable to the band gap, may be shown to have some very slight changes in the DOS plots. These shifts can be seen in the DOS plots. The substitution of phosphorus (P) and selenium (Se) in the molecule of epinephrine may result in changes to the density of states (DOS) of the molecule as well as peak shifts in its electronic spectra. This is due to several causes, such as the following: changes in the energy levels of electronic states and molecular orbitals.

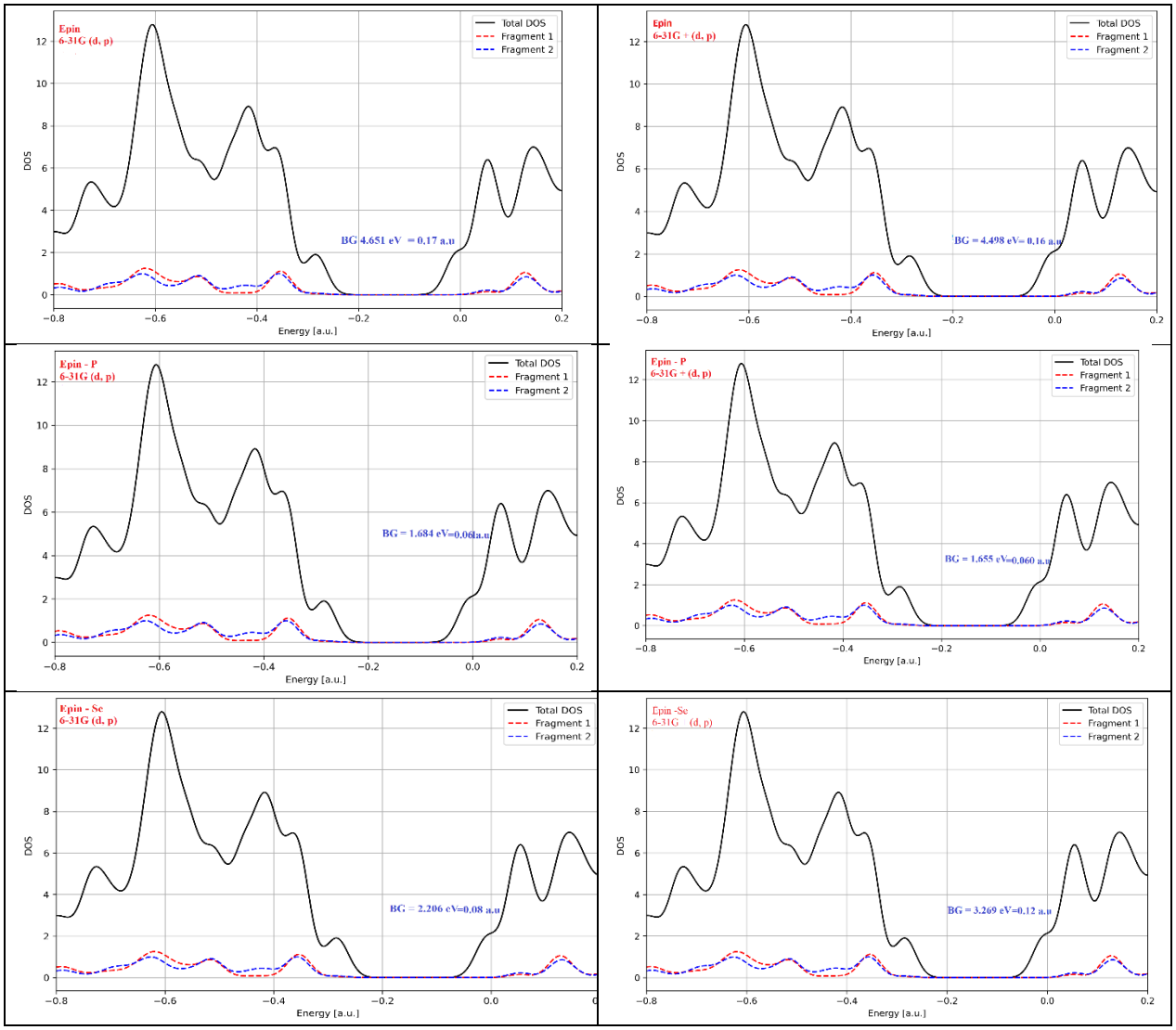

Fig. 4 – Total Energy (a.u), the density of state (DOS) using Fragments 1, and 2.

CONCLUSION

In conclusion, our thorough analysis using Gaussian program simulations with DFT/6-31G(d,p), and 6-31G+(d,p) basis sets on Epinephrine compounds provided essential insights into their molecular characteristics. The examination of molecular orbitals, including HOMO and LUMO, alongside ground state energy assessments, revealed the intricate relationship between molecular structure and chemical behavior. Specifically, the investigation of front molecular orbitals (FMOs) shed light on electronic structure and reactivity. Calculated HOMO-LUMO energy gaps using DFT/B3LYP methodology offered valuable information on molecular stability and reactivity, with protonation decreasing the band gap energy, indicating increased reactivity and decreased stability. The ranking of molecular hardness and softness further elucidated reactivity trends, with Epin -P demonstrating the highest softness and reactivity. Optical properties analysis unveiled relationships between refractive index, dielectric constant, optical electronegativity, and HOMO-LUMO energy gap, with consistent trends observed across different equations. Epin -P exhibited the highest refractive index, followed by Epin -Se and Epin. The dielectric constant correlated with refractive index values, indicating a linked behavior. Optical electronegativity played a role in discerning bonding types, with lower $\Delta\chi^*$ values corresponding to higher refractive indices, highlighting its relationship with HOMO-LUMO energy gap. Density of states (DOS) analysis provided insights into energy composition within units, with slight variations observed in epinephrine molecule substitutions, indicating potential impacts on electronic spectra and molecular properties.

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