Chem Rev Lett 6 (2023) 415-427

Review Article

Chemical Review and Letters
journal homepage: www.chemrevlett.com
ISSN (online): 2645-4947 (print) 2676-7279

Epinephrine Compound: Unveiling Its Optical and Thermochemical Properties via Quantum Computation Methods

Rebaz Obaid Kareem[1,*], Mehmet Hanifi Kebiroğlu[2], Othman Abdulrahman Hamad[3], Omer Kaygili[4], and Niyazi Bulut[4]

[1]*Physics Department, College of Science, University of Halabja, 46018, Halabja, Iraq*
[2]*Department of Opticianry, Darende Bekir Ilicak Vocational School, Malatya Turgut Ozal University, Malatya, Türkiye*
[3]*University of Raparin, College of Science, Department of Chemistry46012, Sulamani, Iraq*
[4]*Department of Physics, Faculty of Science, Firat University, 23119, Elazig, Türkiye*

ARTICLE INFO

Article history:
Received 18 October 2023
Received in revised form 17 December 2023
Accepted 17 December 2023
Available online 26 October 2023

Keywords:
Epinephrine
Physicochemical
thermochemistry
Optical properties
NCI
RDG

ABSTRACT

This study employs Density Functional Theory (DFT) methodology to comprehensively investigate the structural and physicochemical characteristics of epinephrine, a molecule of physiological relevance. By employing DFT approaches, a more precise description of epinephrine's structure and properties is achieved compared to prior studies. A detailed examination of epinephrine's structure and various properties, such as the Highest Occupied Molecular Orbital (HOMO), Lowest Unoccupied Molecular Orbital (LUMO), Band Gap (BG), Density of States (DOS), Fourier-Transform Infrared Spectroscopy (FT-IR), Ultraviolet (UV) absorption, and Natural Bond Orbital (NBO) analysis. Furthermore, we explore non-covalent interactions (NCI) through the examination of Reduced Density Gradient (RDG) and Molecular Electrostatic Potential (MEP) maps. Incorporating FT-IR results, we delve into the vibrational properties of epinephrine, highlighting C-H vibrations at 3700, 3176.20, and 2986.14 cm^{-1}, along with specific vibrational modes of the benzene ring at 1558.43 and 1461.14 cm^{-1}. Additionally, we provide a comprehensive analysis of epinephrine's thermochemical properties at temperatures ranging from 100 to 200 K under constant pressure conditions (1 atm), including optical transitions. This comprehensive investigation enhances our understanding of epinephrine's structure and properties, paving the way for a more profound comprehension of its biological and pharmacological significance.

1.Introduction

The neurotransmitter norepinephrine (NE) is involved in the reuptake of released NE into nerve terminals in both the brain's central noradrenergic and peripheral sympathetic synapses. Many severe forms of psychosis and mental disease are linked to dysregulation of this neurotransmitter. Norepinephrine transporter (NET) inhibitors are promising new pharmacological targets for the treatment of a wide variety of psychiatric and neurological conditions [1]. Norepinephrine, also known as noradrenaline, is a neurotransmitter and hormone that plays a crucial role in the sympathetic nervous system, which is responsible for the "fight or flight" response in the body. It is chemically related to adrenaline (epinephrine) and is produced and released by certain nerve cells and the adrenal glands [2, 3].

For half a century, researchers have speculated that NE plays a crucial role in the pathophysiology [4], NE plays a crucial role in brain development, and research suggests that people with depression, withdrawal symptoms, and other conditions may have abnormal levels [2]. Moreover, NE is a chemical messenger carrying

Corresponding author.; e-mail: obedrebaz9@gmail.com
https://doi.org/ 10.22034/CRL.2023.421325.1253

messages between nerve cells [5]. Cell bodies in the locus coeruleus give birth to noradrenergic pathways that spread throughout the brain and spinal cord. When it comes to where they send their signals, NE neurons project to the limbic system [6], in addition to the frontal cortex. The amount of plasma NE is proportional to the degree of hypertension and sympathetic activity. The fact that NE is secreted by sympathetic nerve terminals is well known. As the sympathetic outflow rises, so does the amount of circulating NE [7, 8].

The effects of NE on brain inflammation, oxidative stress, and protein function are substantial [9]. We can only hypothesize about the connection between stress-related increases in NE and the resulting symptoms of re-experiencing, such as intrusive recollections and nightmares, but they are likely linked to the improved encoding of memory for arousing and unpleasant experiences. NE is also involved in the capacity to focus attention on relevant inputs. Increased "signal to noise ratio" refers to the fact that when NE is introduced into sensory cortical neurons, the neurons become more responsive to phasic sensory input while their tonic spontaneous discharge patterns remain unaltered or are reduced [10, 11]. Over a decade, researchers came to agree that the catecholamine NE played a crucial role in affective disorders like depression because its dysregulation contributed to symptoms like impaired attention, concentration, memory, arousal, and sleep. Some, if not all, cases of depression have been linked to low levels of norepinephrine and other catecholamines at strategically placed adrenergic receptors in the brain [4]. Swedish scientist Ulf von Euler discovered one of the first known neurotransmitters, norepinephrine in the brain in the 1940s [12]. In 1959, Rosenblatt et al. were among the first to propose that shifts in brain NE may play a role in depression.

Also cognizant of these findings in 1959, Pare and Sandler1 sought to treat depressive individuals with L-dopa, a precursor of norepinephrine. In 1963, Klerman et al. administered DL-dopa to seven persistently depressed individuals and addressed the potential role of dopamine and norepinephrine in this condition at length. In 1964, Schildkraut et al examined the impact of antidepressants on the excretion of 3-methoxy-4-hydroxymandelic acid in the urine of depressed individuals [13].

Using hydrogen bond interaction, we want to simulate NP's dynamic function in the presence of amino acids and alcohols [14]. However, the addition of a second OH group considerably enhances the reactivity towards radicals, even though all three isomers of NE show promise as molecules with potential antiradical activity. The most reactive location is the p-OH group, as can be shown. The lowest value is 319 kJ mol^{-1}, which is in good agreement with the actual and theoretical Figs for OH band. This value is 26 kJ mol^{-1} greater for octopamine, demonstrating that hydrogen bonding stabilizes the structure of the NE radical [15].

Electrochemical in vivo monitoring of NE using microfiber electrodes is commonplace because NE is a crucial catecholamine neurotransmitter in the mammalian central nervous system. The human body does this fascinating oxidation of these substances [16]. Phenylpropanolamine is a powerful, selective NE releaser. It also has some dopamine-releasing effects [17]. Norepinephrine has been defined as modulatory due to its post-synaptic actions on a cellular and neural circuit level. NE enhances responses generated in target cells by both excitatory and inhibitory afferent input [18]. The activity of NE is constrained by its absorption into the cytoplasm through the NET, which is found on the plasma membrane of noradrenergic neurons. The first publication to propose pharmaceutical control of the NET was in 1983.

Imipramine, a tricyclic antidepressant, was one of the early antidepressants available. These medications inhibit neurotransmitter NE reuptake by binding to the NET. By adjusting synaptic norepinephrine levels, NET inhibitors cure psychiatric and neurological problems, and their interaction with norepinephrine reuptake helps treat depression and attention-related disorders [19, 20]. Patients treated with norepinephrine fared better than those treated with dopamine, according to an Ameta-Analysis. The current understanding is that norepinephrine is one of several neurotransmitters involved in depression, and medications that target norepinephrine can be effective in treating depression. High doses of norepinephrine may have an effect, although it is unknown what such doses might be [20, 21].

The current understanding is that norepinephrine is one of several neurotransmitters involved in depression, and medications that target norepinephrine can be effective in treating depression.

During the progression of this study effort, DFT methodology contributes to the investigation of the structural and physicochemical characteristics of epinephrine by providing a powerful computational approach to predict and analyze its molecular geometry characteristics (HOMO, LUMO, BG, DOS, UV, and NBO, thermochemical, and optical properties) are studied.

2. Computational Method

All of the Epinephrine compound calculations for this present study were carried out using the quantum program known as Gaussian 5.0.9 version. The software application known as the Gauss View 5.0 package was used to estimate the initial geometries of the chemical compounds. Further, the Gaussian 09W was employed for output calculations using a DFT technique, and a variety of basis sets (SDD) were used in order to optimize the geometrical properties of the epinephrine molecule [22].

We evaluated the optimized molecules' global and local features by doing computations. Theoretical computations were run to learn more about the physical parameters and electronic characteristics of this compound, including its E_{HOMO}, E_{LUMO}, band gap of energy (Egap), ionization energy (IE), electron affinity (EA), absolute electronegativity (χ), global hardness (η), global softness (S), global electrophilic (ω), electro accepting (ω^+), electro donating (ω^-), and fraction of electrons transferred (ΔN_{max}) [23-27]. In addition, optical properties (Optical BG with the indirect and direct transition, thermochemical properties (heat capacity, entropy, and thermal energy have also been investigated at 100, 120, 140, 160, 180, and 200 K and standard pressure 1 atm have been calculated. Finally, this article describes the theory of non-covalent interactions (NCI) and the technique RDG.

3.Result and Discussion

3.1.Geometry Optimization

As shown in Fig 1, the best shape was generated by running the Gaussian program in conjunction with the DFT/ SSD basis set to the structure of the Epinephrine compound. Molecules possess their special orbitals that are distinct from the orbitals that are seen in atoms. The energy that is connected to a certain initial molecule shape is the focus of the first step of a geometry optimization technique that is useful for this approach. Epinephrine was shown to have the best geometrical optimization in Fig 1 [26]. Both the chemical and biological activity of organic compounds is directly tied to the geometry of their molecular orbitals HOMO, and LUMO, in addition to the type of these molecular orbitals (MOs) [28].

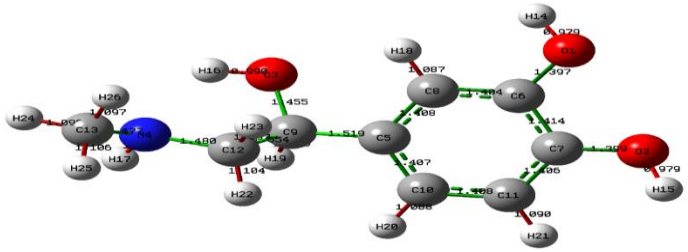
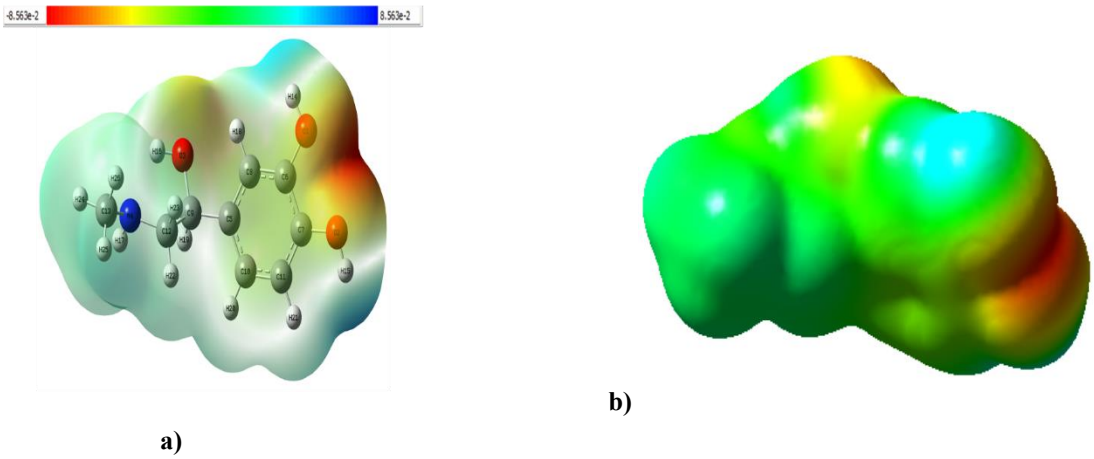


Fig 1. Geometrical optimization Epinephrine

Table 1. Initial Parameters

Name	Definition	Length (Å)	Name	Definition	Length (Å)	Name	Definition	Length (Å)
R1	R(1,6)	1.3973	R11	R(5,9)	1.5190	R21	R(11,21)	1.0896
R2	R(1,14)	0.9795	R12	R(5,10)	1.4071	R22	R(12,22)	1.1042
R3	R(2,7)	1.3988	R13	R(6,7)	1.4144	R23	R(12,23)	1.0972
R4	R(2,15)	0.9793	R14	R(6,8)	1.4040	R24	R(13,24)	1.0963
R5	R(3,9)	1.4546	R15	R(7,11)	1.4056	R25	R(13,25)	1.1055
R6	R(3,16)	0.9901	R16	R(8,18)	1.0873	R26	R(13,26)	1.0966
R7	R(4,12)	1.4800	R17	R(9,12)	1.5544			
R8	R(4,13)	1.4767	R18	R(9,19)	1.1050			
R9	R(4,17)	1.0215	R19	R(10,11)	1.4079			
R10	R(5,8)	1.4083	R20	R(10,20)	1.0879			



a) **b)**

Fig 2. **a)** The 3-D ESP map. **b)** The color scale (red- yellow-green-blue)

3.2 Natural Bond Orbital (NBO) Analysis

Because of its ability to provide understandable chemical representations of complicated quantum mechanical electronic structure data, natural bond orbital (NBO) analysis is a potent analytical method. NBO techniques include a group of algorithms that may be used to predict basic bonding ideas from theoretical frameworks like Hartree-Fock (HF), Density Functional Theory (DFT), and others [29, 30]. The study of hybridization, covalent and non-covalent impacts in polyatomic wave functions gave rise to the development of Natural Bond Orbital (NBO) analysis. According to NBO analysis, a given wave function may be ideally transformed into a localized form that corresponds to the one-center (lone pairs) and two-center (bonds) components of the chemist's Lewis structure depiction. The analysis focuses on orbital interactions between molecules, especially the transfer of charges in complexes [31]. The NBO included both donors and acceptors from NBOs [32].

NBO analysis results are shown in Fig 2. Table 1 summarizes the electronic structures and geometric features of the epinephrine compound, including the initial parameters (Angstroms and Degrees) Epinephrine, Color Range from 0.979 to 1.554. For neutral molecules, the sum of all atoms' NBO values is zero, while for charged varieties, the sum equals the total charge. When the NBO value is negative, the atom has a partial negative charge because its electron density is higher than neighboring atoms. When the NBO value becomes positive, the atom has a partial positive charge.

The electrostatic potential (ESP) Map may be affected by factors such as a higher electron affinity, dipole moment, or electronegativity. The energy of attraction between a positive unit charge and a collection of electrons or molecules is called the ESP map. As shown in Fig 2a, the color scale (red- yellow-green-blue) in ESP maps only shows the corresponding charge distribution of a molecular structure or comparable molecules; it does not represent the NBO charge value of an atom. Changing surface potential values could affect the color scale of ESP maps. Epinephrine (left to right) ESP diagrams. The colors on the map correspond to the surface potential ranges (8.56 e-2 (red) to +8.56 e+2 (blue)). In this graphic, greater red values indicate a higher electronic density, whereas lower blue values indicate a lower density, as discussed in the context of molecular orbital theory shown in Fig 2b. In conclusion, one may state that the right hand has a great deal of electrical density due to the color red. Combining NBO evaluation with ESP maps may help researchers match the chemical structure and reactivity of reagents, which neither approach alone could give [33].Molecular electrostatic potential (MEP) maps are color-coded representations of the electrostatic potential around a molecule. The MEP map can be used to identify regions of the molecule that are electron-rich (red) or electron-poor (blue). This information can be used to predict how the molecule will interact with other molecules [34].

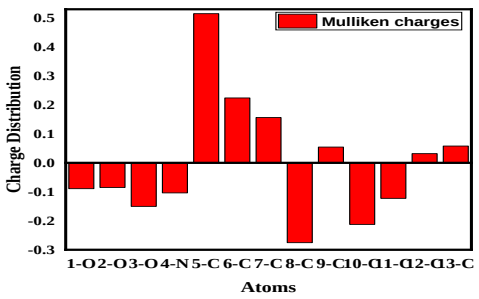


Fig 3. Mulliken charges with hydrogens summed into heavy atoms

According to Fig 3, the assignment of atomic charges is one of the important characteristics that must be considered when characterizing the activity of a chemical. According to the data, the DFT approach reveals that epinephrine had a greater atomic charge. The fact that the oxygen in the epinephrine molecule has a larger atomic charge than the other atoms in the molecule implies that it may have potential sites for nucleophilic moieties and may interact with weak electronic molecules. However, nitrogen atoms had a higher electrophilic reaction, similar to that of radical species [35].

3.3 Thermochemistry

This research estimated this chemical's thermodynamic properties parameters at different temperatures using DFT using the SSD basis, as shown in Table 2. These thermodynamic possessions characteristics consist of entropy (S), molar heat capacity (Cv), and thermal energy (E). The values of those variables have a one-to-one correspondence with the temperatures being monitored. In addition, when temperatures rise, there is a corresponding increase in the oscillation and vibration of atomic particles.

The final formulae for computing the components of physicochemical values detected by Gaussian are produced by the three equations that make up this equation system. The entropy (S) that each component provides may be determined using that component's partition function and plugged into equation (1) [36]:

$$S=R\left(ln(q_t q_e q_r q_v e) + T\left(\frac{\partial \ln q}{\partial T}\right)_V\right) \quad (1)$$

The total internal thermal energy, which is symbolized by the symbol (E) and may be calculated using equation (2), can also be determined with the use of the partition function: $E=NK_BT^2\left(\frac{\partial \ln q}{\partial T}\right)_V$ (2)

Lastly, equation (3) suggests that the energy may be used to determine the total heat capacity (Cv):

$$Cv=\left(\frac{\partial E}{\partial T}\right)_V \quad (3)$$

The quantity of heat needed to increase the temperature by 1 °C per unit of mass is known as its heat capacity or specific heat. Specific heat helps determine processing temperatures and heat requirements and separates composites [37]. Epinephrine's thermodynamic properties at varying temperatures provide a comprehensive understanding of the molecule's energy landscape, stability, and response to thermal changes, as well as a variety of environmental and physiological conditions. This understanding contributes to the characterization of the molecule's thermodynamic stability and reactivity.

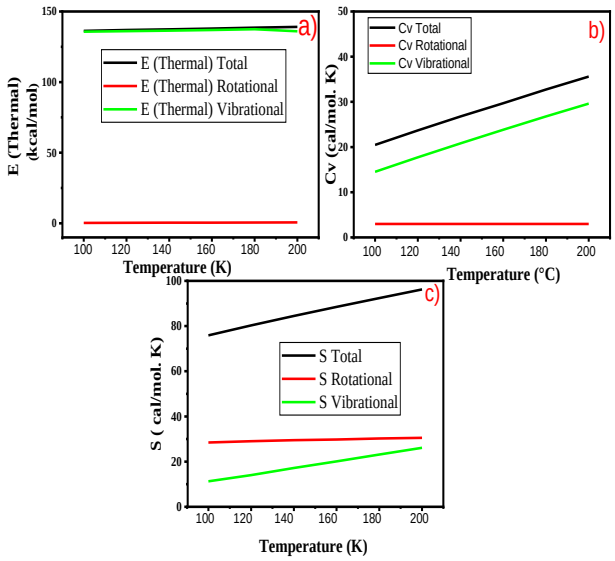


Fig 4. Thermal investigation: a) thermal energy, b) heat capacity, c) entropy

Entropy (S) is the probability distribution of a system's microstates. A microstate is a system's molecular and atom arrangement. The computation of the thermal energy considers the sum of the kinetic energies of all of the atoms that collectively make up the structure of this molecule. The energy that is held by an item or system as a result of its temperature is referred to as its thermal energy. Thermal energy always moves from the body with the higher temperature to the body with the lower temperature whenever there is a temperature differential between the two objects [38]. As shown in Table 2, A system that has a low entropy has fewer potential microstates than one that has a high entropy since the former has a greater number of possible microstates. As shown above Table 2, the value total E thermal > vibrational> rotational. Since translational energy E_t is usually far bigger than vibrational (E_v) and rotational energies (E_r), the total thermal energy of a material is often greater than these three (vibrational, rotational, and translational) energies. The value of total Cv > vibrational > rotational, is because translational Cv is connected to particle movement as a whole, whereas vibrational and rotational Cv are linked to molecule mobility.Temperature affects the translational Cv

vibrational, and rotational Cv ratio. Translational heat capacity is usually greater at greater temperatures. Because molecules move quickly at higher temperatures, as illustrated in Fig 4. The E thermal of a material may become stable (constant) with rising temperature at extremely low temperatures. On the other hand, another cause is quantum effects. The quantum effects of particles may be important at extremely low temperatures [39]. Quantum effects may localize atoms, reducing their velocity and vibration.

3.4 Nuclear Magnetic Resonance Spectroscopy

A logical extension of these ideas is the introduction of additional NMR dimensions that depend on molecular properties such as size, shape, mass, and charge that are not explicitly included in spin Hamiltonians. These overall molecular properties are not well represented in conventional NMR, as spin interactions tend to be quite local. Therefore, dispersion based on such properties can provide new information as well as a means for editing NMR spectra. The problem is to identify ways that molecular properties influence NMR spectra or can be made to affect NMR spectra [40]. The DTF/ SSD basis set has been used to investigate chemical shift C, H, O, and N epinephrine, as illustrated in Using the DFT method, the order of C NMR chemical Shielding (ppm) is very dependent on the molecular position, ordering the chemical Shielding (ppm) from high to small is as follows 9-C >11-C > 8-C > 10-C > 5-C > 7-C > 6-C. The H NMR Shielding: 17-H> 32-H> 26-H> 25-H> 24-H> 22-H> 15-H> 14-H> 16-H> 19-H> 21-H> 20-H> 18H. 4-N -NMR chemical shifts for the epinephrine molecule's single nitrogen atom may also be expected by utilizing ammonium as a substitute for an organic solvent.

3.5 UV–Visible analysis

To improve the Epinephrine molecule's ground-state electron configuration. It is approximated using the DFT approach at the (B3LYP/SSD level) for the electronic excitation in the low energy state. Calculations using the DFT approach demonstrated that there is just one transition in the invisible area of electromagnetic radiation. In the computation of UV-visible wavelengths, the kind of basis set is more significant than the number of peaks for determining the accuracy of the peaks position. Transition and absorption spectra show that the highest absorption wavelength parallels the electronic transition from HOMO to LUMO [41].

Table 4. Peak information of Epinephrine

Wavelength (nm)	Strength
254.15	0.0468
221.29	0.0779
213.91	0.0345

The oscillator strength of an ultraviolet (UV) absorption band indicates how much light a molecular structure absorbs at a wavelength. Table 4 and Fig 5 show the maximum strength molecular structure absorbed at 221.29 nm and 0.0779 strength. This result is totally in agreement with a recent study [35].

Table 2. Research estimated this chemical's thermodynamic

This is because the substance's particles do not have enough energy to vibrate or spin.

Temperature (K)	Total			Rotational			Vibrational		
	E kcal/ mol	Cv cal/ mol.K	S cal/ mol.K	E kcal/ mol	Cv cal/ mol.K	S cal/ mol.K	E kcal/ mol	Cv cal/ mol.K	S cal/ mol.K
100	136.30	20.48	75.89	0.29	2.98	28.48	135.70	14.52	11.31
120	136.89	23.68	80.27	0.35	2.98	29.02	136.10	17.72	14.02
140	137.32	26.78	84.46	0.41	2.98	29.48	136.48	20.81	17.21
160	137.88	29.70	88.50	0.47	2.98	29.80	136.90	23.82	20.10
180	138.51	32.73	92.41	0.53	2.98	30.23	137.44	26.77	23.16
200	139.10	35.60	96.20	0.59	2.98	30.50	136.00	29.60	26.10

Table 3. Chemical shifts of Epinephrine

Method	Shielding (ppm)	Method	Shielding (ppm)
18-H	25.0894	7-C	45.1287
20-H	26.1986	5-C	54.8930
21-H	26.2766	10-C	72.0546
19-H	28.5470	8-C	74.0868
16-H	28.6199	11-C	74.3839
14-H	28.6247	9-C	113.7552
15-H	28.9186	12-C	126.4355
22-H	30.0443	13-C	152.8365
24-H	30.1690	1-O	198.6911
25-H	30.1873	2-O	203.6644
26-H	30.3512	4-N	220.3560
23-H	30.6504	3-O	263.9360
17-H	32.8230		
6-C	42.7779		

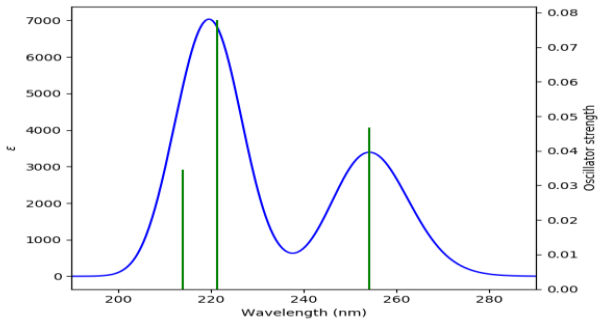


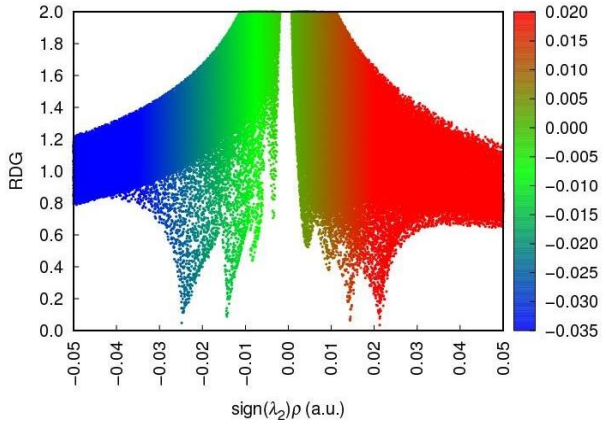
Fig 5. UV–Visible analysis of Epinephrine

These optical characteristics are cornerstones with broad applications in areas such as lens design, material analysis, and the development of innovative optical technologies including glass. Explaining and expressing the chemical properties of molecules relies frequently on the fact that their band gap energies belong to the UV-visible spectrum. This property depends on photons with energies equal to or greater than its band gap energy stimulating electrons from the valence band (VB) to the conduction band (CB). Fig 6, shows optical band gaps (BG_{opt}) with an energy of around 4.30 eV using Tauc plot, and indirect electronic transition method. The BG_{opt} energy is the minimal energy needed to excite a semiconductor electron from the VB to the CB.

The physical explanation for an optical band gap is the smallest quantity of energy that a photon must possess for it to be absorbed by a material. This minimal amount of energy is called the optical band gap. In the epinephrine molecule, the transition from the VB level to the CB level requires energy of 4.30 eV. In conclusion, absorption of light requires that its energy be larger than or equal to the energy of the molecule's band gap. The difference in energy between the HOMO and the LUMO constitutes the band gap. When a molecule absorbs a photon, an electron is stimulated from the HOMO to the LUMO energy level.

3.6 Non-Covalent Interactions (NCI)

The non-covalent interactions theory (NCI) is an innovative theoretical tool used to describe intermolecular interactions and evaluate the nature of weak interactions; it provides a more detailed picture of



molecular systems. The NCI index is based on the reduced density gradient (RDG) and has been detailed in several research publications. The RDG function, as noted here, s(r), is an essential dimensionless quantity in DFT used to describe the deviation from a standardized electron distribution and related to the electron density ρ(r) and its first derivative by equation (4):

$$s(r) = \frac{1}{2\left(3\pi^2\right)^{1/3}} \frac{\left|\nabla_{p(r)}\right|}{p(r)^{4/3}}$$

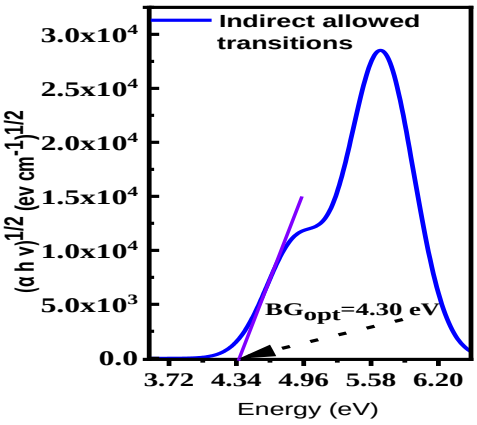


Fig 6. Optical investigations indirect allowed transition using a Tauc plot.

To determine the type of interaction, the sign of the second eigenvalue of the Hessian can be used, and this can give information about bonded and non-bonded interactions. At the location of non-covalent interactions, the higher values of the density are related to a stronger interaction [42].

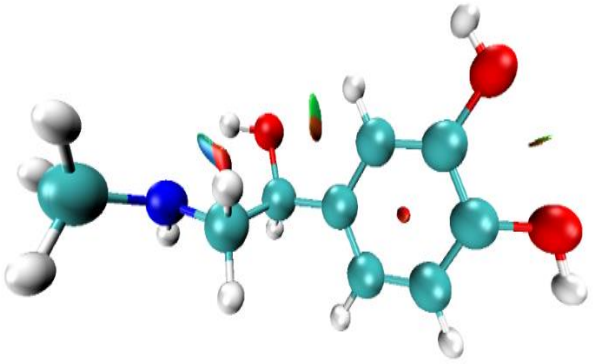


Fig 8. The RDG iso-value of Epinephrine

The RDG scatter graphs of epinephrine complexes are shown in Figs 7 and 8. The blue colors are at the left of Fig 7. The computed NCI regions of the Epinephrine compound indicate the hydrogen-bonding interaction. A hydrogen bond is usually dipole–dipole attractive. It is stronger than Van der Waals but weaker than covalent bond strength. Van der Waals forces attract molecules of neutrality with modest electrostatic forces (F_e). NCI has four categories: i) Van der Waals force attracts and repels permanent, immediate, and induced dipoles among atoms or molecules. ii) Hydrogen bonds are formed when one electronegative atom interacts with another via a hydrogen atom that is connected to a strongly electronegative atom, for example (H interaction with N, O). iii) Electrostatic interactions are those

Fig 7. The computed NCI regions of Epinephrine

between ions or dipoles with opposing charges, such as (Na^+) and (Cl^-) ions. iv) Hydrophobic interactions are the result of nonpolar molecules' reluctance to bond with water [43-45]. The green colors are relative to weak noncovalent interactions such as π-π staking and van der Waals interactions; the red colors or positive regions are related to steric clashes. Fig 8. The RDG iso-value of epinephrine shows clearly that the iso-surface forms blue disks between the hydrogen bond acceptor and donor atoms in the considered solutions of urea. The color green represents the van der Waals interaction, but the color red is associated with the steric cyclic effect. The study of non-covalent interactions using RDG and MEP maps gives a complete picture of the type and location of non-covalent interactions in the epinephrine molecule. When looking at complexes, hydrogen bonds are considered the main interaction in the epinephrine complexes, and van der Waals interactions are molecules. NCI theory explains epinephrine's non-covalent interactions, revealing its structural stability, molecular recognition, physicochemical characteristics, and biological activity.

3.7 FT-IR Vibrational Spectroscopic Analysis

Fourier transform infrared (FT-IR) spectroscopy is based on measuring the absorption of multicolored infrared light. Functional groups in a given molecule are identified according to their vibrational modes at different IR frequencies. Utilizing infrared spectroscopy as a tool makes it feasible to determine which functional groups contribute to the formation of hydrogen bonds inside the molecule. FT-IR measurements depend on changes in dipole moment [46-48]. FT-IR dependent on the amount of the compounds [45, 49, 50].

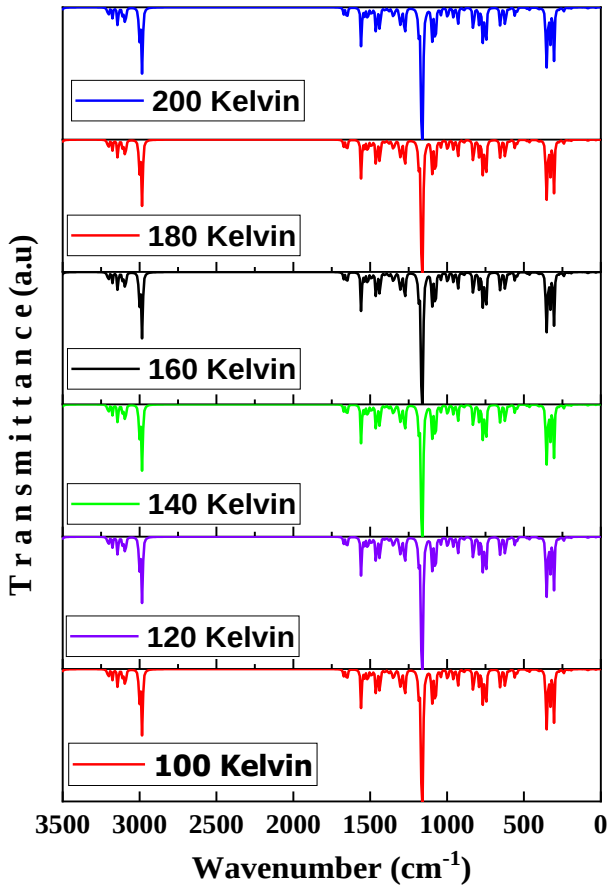


Fig 9. FTIR results of the Epinephrine compound using DFT/SSD method

As can be seen in Fig 9. A compound's characteristics have been evaluated by measuring the vibrational bond of the C–H, CH2, C-C, CH3, N-H, and OH using DFT/ SSD basis set at 120 Kelvin degrees. Because of the weaker contact between C-H compared to the interaction between C-C, the C-H stretching vibration for aromatic molecules was typically reported in the range 1461.14 cm^{-1} (interaction C-C > C-H) [35]. The N-H vibration of the nitrogen atom at 3523 cm^{-1}. The O-H vibrational stretching at 3700 cm^{-1}, and vibrational bending at 1461.14 cm^{-1}, and 350 investigated. The CH3 symmetrical stretching at 2981.52 cm^{-1}. CH2 vibrational bending at 3001.72 cm^{-1}. The benzene ring was vibrated at 1558.43, and 1451.14 cm^{-1}. This finding is in agreement with the results of previous research [35, 51, 52]. In conclusion, small changes in the peaks as a result of the complicated relationship between the quantized energy levels of vibrational techniques, thermal expansion impacts, anharmonicity, and other factors that influence the molecular structure of the Epinephrine compound in FTIR as a result of temperature changes. An additional factor is electronegativity. When two atoms with differing electronegativities combine, the resulting bond does not result in an equal distribution of electrons between the atoms. FT-IR spectroscopy displays significant vibrational properties of epinephrine, which offer extensive information on the compound's functional groups, bond connectivity, intermolecular interactions, and structural features.

3.8 Computed electron structure

Frontier molecular orbitals (FMOs) and molecular electrostatic potential (MEP) maps are two powerful tools for understanding the reactivity and properties of molecules. Frontier molecular orbitals are the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO). They are responsible for most of the chemical reactivity of a molecule. The energy gap between the HOMO and LUMO is called the HOMO-LUMO gap energy. A smaller HOMO-LUMO gap indicates a more reactive molecule, as it is easier for electrons to be excited from the HOMO to the LUMO. Fig 10 shows the HOMO, LUMO energy diagram Epinephrine compound, SDD basis set, and BG values using the DFT method. The HOMO value is -5.698 eV and the LUMO value is -0.101 eV. The BG value is 5.597 eV. Table 5 shows the equations and the value of the quantum chemical descriptors calculated for Epinephrine. This result is supported by a literature study using a DFT/3-21G basis set to an Epinephrine compound (5.84 eV) [35].

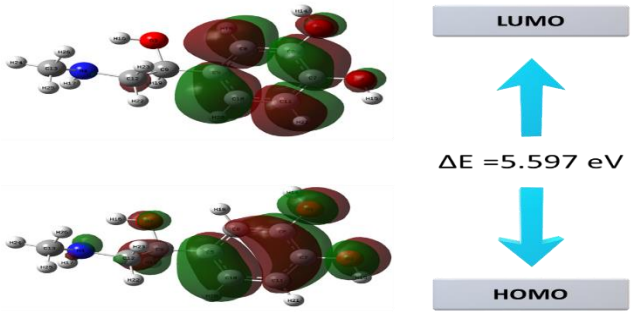


Fig 10. HOMO, LUMO energy diagram Epinephrine compound, using SDD basis set, and DFT method

Epinephrine has a powerful inhibitory activity that is dependent on the greatest HOMO energy values and E. Additionally, the negatively charged oxygen and carbon atoms in our compound gave a more effective inhibitor action. The donor-acceptor process, which relies on adsorption on a metal surface, works better when negatively charged heteroatoms are present. Epinephrine's large concentration of negatively charged atoms, in comparison to positively charged atoms, gives it potent anticorrosion properties [35]. Coordinated covalent bonding between the metal and the inhibitor is described by the value of electronegativity. The high BG energy value suggests that this molecule is relatively stable. The energy lost during the whole process of energy transmission between receivers and transmitters is quantified by the ω index. Many theoretical explanations and predictions about molecular properties and behavior have been made with DFT's help in this work. Electronic and molecular chemical potential (Pi) play important roles in the quantum chemical process, as does electronegativity (χ). Parr and Pearson used research on the significance of the chemical potential in the field of chemistry. They hypothesized that the chemical potential is an essential component in the charge transfer process, which is necessary for the explanation of chemical reactivity. Higher chemical potentials are related to weaker stability and faster reaction rates, whereas higher electronegativity values indicate that atoms and molecules are more capable of attracting electrons to themselves. In addition, the large value of the compound's BG is a factor in determining the size of the dipole moment [26, 53]. The FMOs and MEP maps reveal epinephrine's electrical structure and bonding, revealing its potential reactivity, physicochemical qualities, and biological activity. The MEP map shows the molecule's nucleophilic or electrophilic potential, whereas the HOMO-LUMO gap energy is critical for electron transfer processes

Table 5. The calculated quantum chemical descriptors for Epinephrine

Compound	Calculation Equation [26, 53]	Results
E_{HOMO} (eV)	---------	-5.698
E_{LUMO} (eV)	--------	-0.101
Gap Energy (eV)	$\Delta E_{Gap}(= E_{HOMO} - E_{LUMO})$	5.597
Ionization Energy (eV)	IA = -EHOMO	5.698
Electron Affinity (eV)	EA = -ELUMO	0.101
Hardness (eV)	$\eta = \frac{1}{2}\left[\frac{\partial^2 E}{\partial^2 N}\right]_{v(r)} = \frac{I-A}{2}$	2.798
Softness (eV^{-1})	$\langle\alpha\rangle = \frac{1}{3}\left[\alpha_{xx} + \alpha_{yy} + \alpha_{zz}\right] = \sigma = \frac{1}{\eta}$	0.357
Electronegativity (eV)	$\chi = \frac{IE + EA}{2} =$	2.899
Dipole moment (eV^{-1})	$\mu = -\chi = \left[\frac{\partial E}{\partial N}\right]_{V(r)} = -\left(\frac{I+A}{2}\right)$	-2.899
Electrophilicity (eV)	$\omega = \frac{\chi^2}{2\eta}$	1.501
Nucleophilicity index (eV)	$\varepsilon = \frac{1}{\omega}$	0.666
Nucleophiles (eV)	$\omega^{+} = \frac{(I+3A)^2}{16(I-A)}$	0.325
Electrodonating (eV)	$\boldsymbol{\omega^{-} = \frac{(3I+A)^2}{16(I-A)}}$	3.224
Nucleophilicity (eV)	$\Delta N_{max} = \frac{-\mu}{\eta}$	1.036

4.Conclusion

In conclusion, this study employed DFT calculations to model the chemical structure of epinephrine, and the resulting model was used to predict various properties of this compound. It was established that epinephrine acts as a donor molecule due to its high EHOMO value and low ELUMO value, resulting in significant inhibitory potential. The calculated BG value for epinephrine, using a DFT/SSD basis set, was determined to be 5.597 eV, which is in close agreement with the value of 5.84 eV reported in the literature using a DFT/3-21G basis set for epinephrine. Furthermore, our FT-IR results revealed specific vibrational modes of the benzene ring at 1558.43 and 1451.14 cm-1, which align with previous research findings. This affirms the accuracy and reliability of our approach. Additionally, the presence of hydrogen-bonding interactions in the epinephrine compound was detected. Moreover, our investigation into the thermodynamic properties of epinephrine highlighted that the total thermal energy (E thermal) predominates over vibrational and rotational energies. Translational energy (Et) was found to be significantly greater than both vibrational (Ev) and rotational energies (Er), consistent with typical energy distribution patterns in molecular systems. These results collectively enhance our understanding of epinephrine's chemical properties and its potential in various applications. Overall, this research sheds light on epinephrine's chemical characteristics and possible uses. This knowledge may help design novel compounds with better pharmacological and commercial qualities and better understand epinephrine's action in varied situations.

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