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Tailoring the optical and spectroscopic properties of ascorbic acid via solvation with DMSO: A theoretical study using different quantum models

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ABSTRACT

The anti-oxidizing properties and physiological action of ascorbic acid have recently attracted considerable research attention. This study employs dimethyl sulfoxide (DMSO) solvent to examine the interaction of solvent molecules and the resulting structural modifications in ascorbic acid through trial and error with three quantum solvation models (CPCM, IEFPCM, and SMD). DMSO was selected from the models to analyze changes in the optical bandgap and spectroscopic properties using first-principles methods. Geometry optimization was performed at two different levels of theory: Hartree-Fock (HF) and density functional theory (DFT). The DFT method was employed with a 6–311 G/B3LYP basis set to yield the ground-state energy. The electronic orientation was investigated through potential energy mapping, while spectroscopic analysis encompassed ultraviolet (UV–VIS) and nuclear magnetic resonance (NMR) techniques. Additionally, Fourier transform infrared spectroscopy was used to gain a deeper understanding of the chemical structures of the compound. The findings shed light on the DMSO-Ascorbic acid interactions and revealed structure-property correlation.

1. Introduction

Ascorbic acid, also known as vitamin C, is a vital natural organic substance which may be found in several fruits and vegetables [1–5]. It comprises an organic molecule having the chemical formula $C_6H_8O_6$ that has four stereoisomers and six chiral carbon atoms [6–11]. Vitamin C is an essential micronutrient for humans. Unlike other animals, humans cannot naturally produce it due to which its demand needs to be fulfilled from foods or supplemented by other sources [12–18]. It is categorized as an antioxidant [19–22]. It may offer stronger benefits when oxidative stress is increased. The infections in humans and animals produce reactive oxygen species (ROS) which are oxidizing substances that activate phagocytes [23–29]. These reactive species play a crucial role in deactivating viruses and killing bacteria [30–34]. The biological processes in the body benefit greatly from the frequent consumption of acid through fruits and vegetables [35–37]. The presence of ascorbic acid in blood plasma is 10 times lower than that in white blood cells, which is clear evidence that it plays an important role in the immune system of the body in the cells [38–40]. Vitamin C also influences virus replication, interferon production, T-lymphocyte maturation, and phagocyte maturation in the laboratory. The inability of the human body to synthesize ascorbic acid motivates researchers to explore alternative ways of producing it [41–42].

The spatial arrangement of the atoms in ascorbic acid in the solid phase has been investigated via different structural and vibrational analysis techniques [42–45]. Dopamine has aromatic ring-like structures similar to ascorbic acid. Nasidi et al. studied the effects of halogen doping on dopamine and investigated the role of the band structure in detail [46].

In this study, three quantum models are extensively studied to analyze the effect of dimethly sulfoxide (DMSO), the solvent was selected due to its laboratory and industrial applications as solvents for many gases, synthetic fibres, paint, hydrocarbons, salts and natural products. This paper shows the effect of DMSO solvent on ascorbic acid and it is investigated in detail using three quantum models (i) conductor-like polarizable continuum model (CPCM) [47], (ii) integral equation

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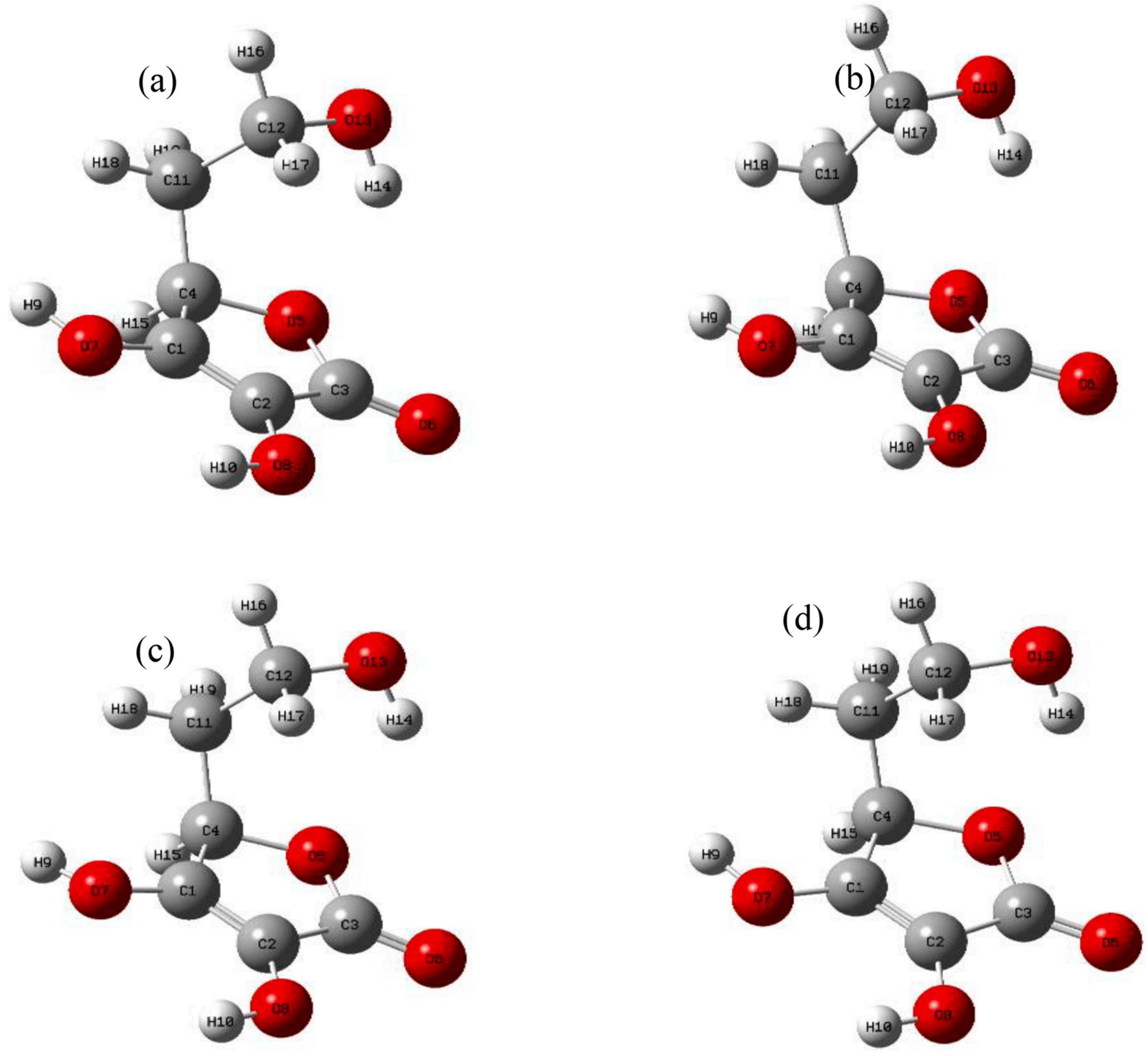

Fig. 1. The geometry optimized structure of (a) ascorbic acid (b) in DMSO (CPCM) (c) in DMSO (IEFPCM) (d) in DMSO (SMD).

Table 1
Comparison showing the optimization of basis set for Hartree-Fock versus DFT in ascorbic acid.

Basis set	Hartree-Fock (eV)	DFT (eV)
STO-3G	0.801	0.700
3–21G	6.254	4.895
6–31G	7.050	5.146
6–31G*	7.050	5.146
6–311G	7.286	1.147
LanL2DZ	7.272	5.129
LanL2MB	0.806	1.674
SDD	7.459	5.247

formalism polarizable continuum model (IEFPCM) [48] and (iii) solvation model based on Density (SMD) [49] In these models, the solute effect of the molecule of interest, which is released into a space where the solvent charge is stabilized, is examined. [50] The difference between IEFPCM and CPCM is in the method used to define this space. [51] SMD is a model that uses a continuous model to determine the charges on the molecular surface of the solute. In addition, SMD has proven to be an effective solvation model [49]. The molecular structure was optimized using a 6–311 G/B3LYP basis set to achieve the geometry of the ground-state energy. The electronic and optical properties were determined, and the optimized molecules were solvated with DMSO using the three models to investigate the improvement in its effectiveness. The findings of this study revealed that the bandgap is sensitive to the solvent. The IEFPCM model is found to be the best solvent model for ascorbic acid.

2. Computational method

This study was carried out to study dimethyl sulfoxide (DMSO) molecules (see Fig. 1) as solvent using Gaussian 09 code, whereas the plot of the spectroscopic properties and graphical presentation of the results was performed via Origin package. The ground-state molecular optimization of the molecule was computed using the density functional theory (DFT) method together with a 6–311 G basis set through B3LYP functionals. This methodology is an established theoretical strategy to investigate the geometries and band structure of materials with more than one covalent electron. Two methods were used with eight basis set to compute the ground-state energy of the molecule. The choice of DFT/B3LYP/6–311 G level of theory was driven by its ability to provide accurate and comprehensive information about molecular structures and properties. The findings of this study contribute to a better understanding of the interactions between DMSO and ascorbic acid, establishing a valuable structure-property correlation. The calculated values

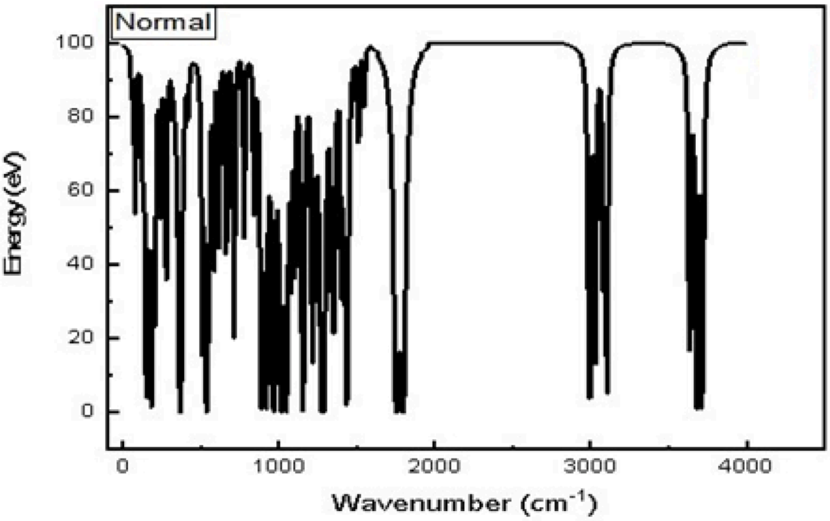

Fig. 2. The FT-IR of ascorbic acid.

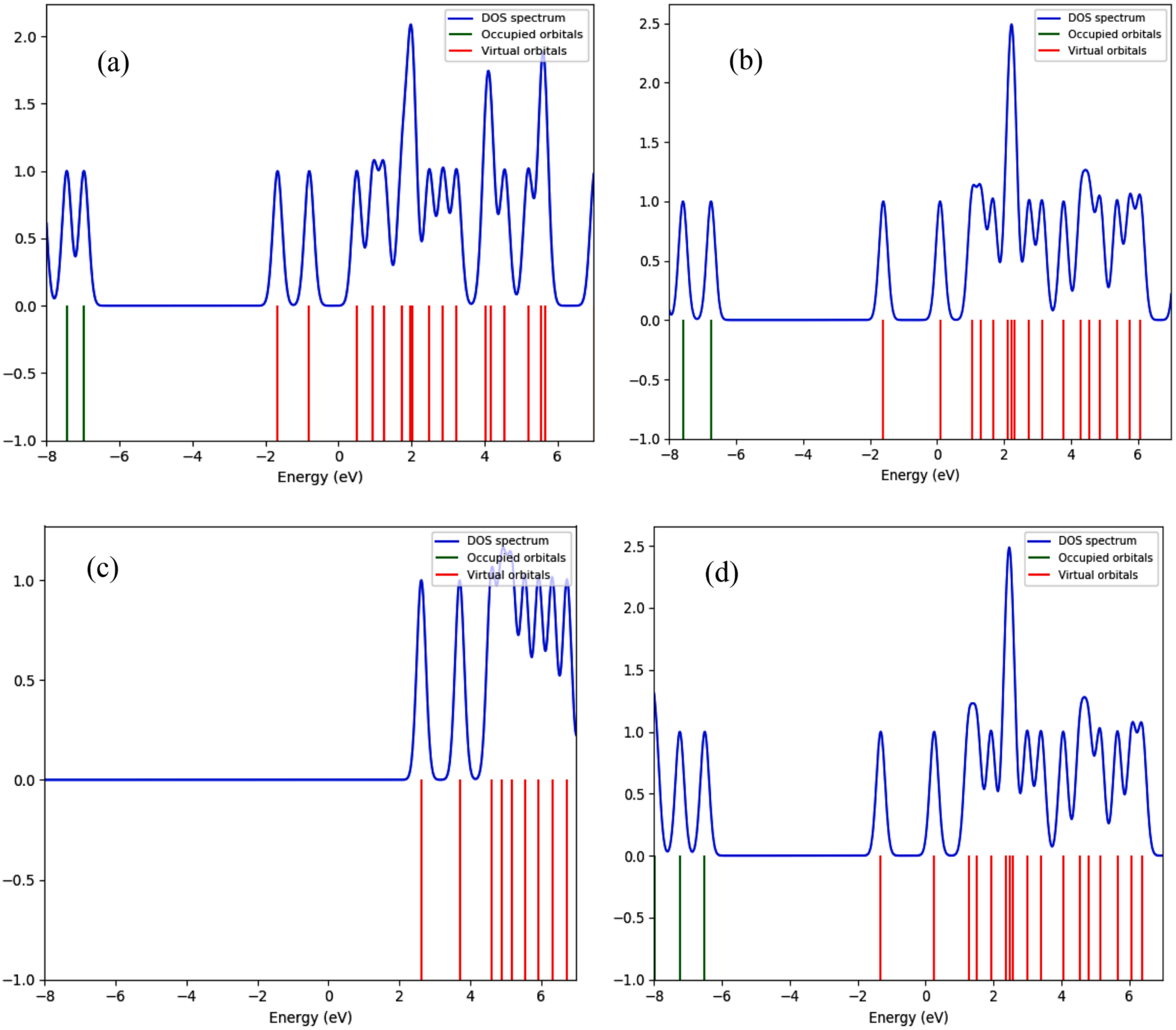

Fig. 3. The calculated density of states of (a) ascorbic acid (b) DMSO (CPCM) (c) DMSO (IEFPCM) (d) DMSO (SMD).

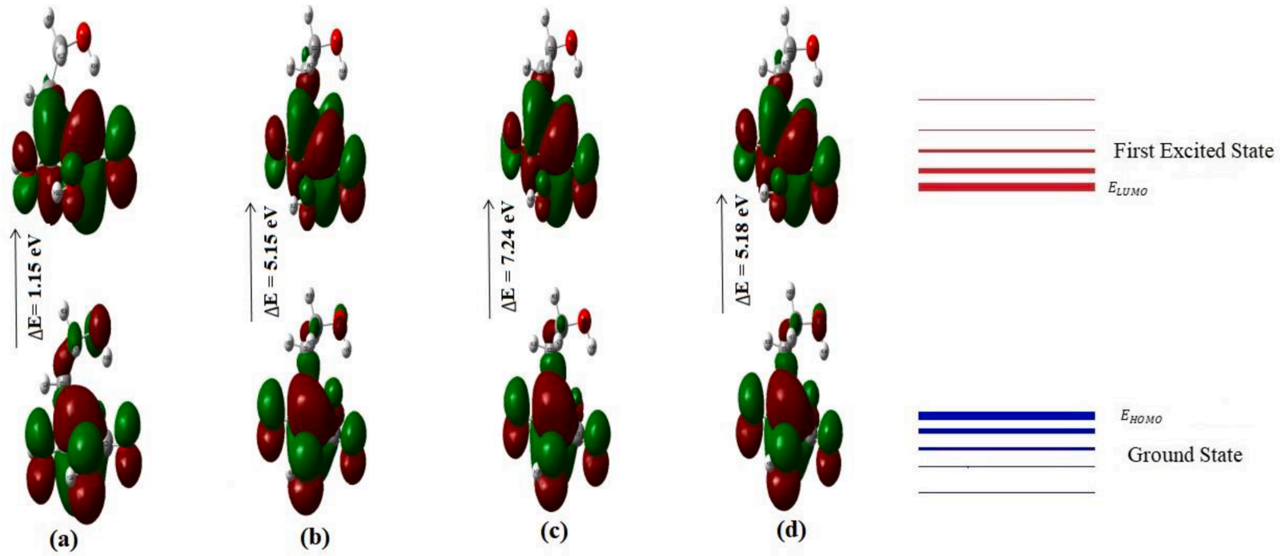

Fig. 4. The homo and lumo of (a) ascorbic acid (b) in DMSO using CPCM (c) in DMSO using IEFPCM (d) in DMSO using SMD.

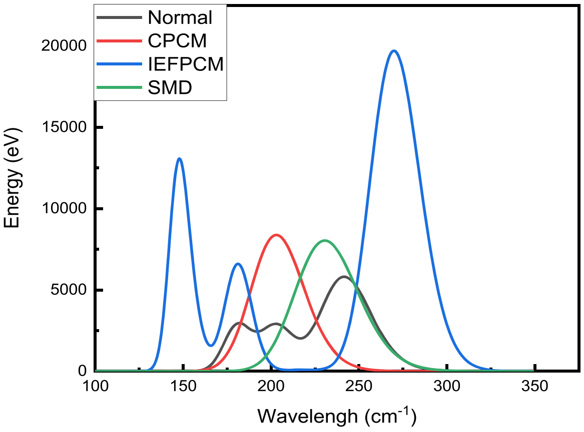

Fig. 5. The comparison of calculated UV–vis absorption spectra of ascorbic acid determined by using models CPCM, IEFPCM, and SMD.

of energy are in agreement with the literature which points to the validity of the results being reported. To observe the effect of the solvents on the titled molecule, the UV–VIS and FT-IR were calculated before and after the solvation with DMSO using different models. The chemical shift and environments were also determined using nuclear magnetic resonance (NMR) when the solvated with the solvent. The same basis set was implemented to plot the three-dimensional plot of the highest occupied molecular orbitals (HOMO) and lowest unoccupied molecular orbital (LUMO).

Table 1 clearly shows the energy difference between the HOMO and LUMO during the optimizaition of the title molecule. The energy comparison was made between the basis and 6–311 G was selected. The selection of the basis set was due to the fact 6–311 G is the basis that is close to the literature value. Eight basis sets were used for the compilation of the lowest ground-state energy after which the appropriate basis set for the remaining analysis was used to test the two approaches, Hartree-Fock (HF) and density functional theory (DFT), in this work. The comparison of energies as a function of basis sets computed at two levels of theory is given in Table 1. The eight basis were used to show a clear comparison and difference between the bandgap energies of the title molecule relative to their respective basis set.

3. Result and discussion

This study uses spectroscopic methods including ultraviolet (UV), Fourier transform spectroscopy (FT-IR), and nuclear magnetic resonance (NMR) to analyze the effects of doping the named compound with halogens on the bandgap and density of states. The calculated density of states for ascorbic acid, DMSO using CPCM, IFPCM and SMD are shown in Fig. 3.

3.1. The molecular orbital

The compound studied herein has 47 molecular orbitals which can be used to analyze the band structure and other important properties. The investigation of molecular orbitals is very important because it explains the electron distribution in ascorbic acid [37–40]. Fig. 3 clearly shows the bandgap energy of ascorbic acid and then solvated with the three quantum models.

The orbitals in the ascorbic acid that are already occupied by the electrons are forty-seven [52]. It can be seen from Fig. 3 that the highest occupied molecular orbitals (HOMO) resided on the portion of the ring while at the same time the lowest unoccupied molecular orbital (LUMO) totally resides and is localized on the ring part. The energy difference between the HOMO and LUMO can be described as the bandgap energy. To form a correlation between the chemical reaction and biochemical systems, the bandgap energy is used as a probe. Additionally, a molecule with a small-valued band gap is called a soft molecule. Soft molecules can be more polarizable and have higher chemical reactivity in addition to low kinetic stability [53–54]. It is understood from Fig. 4 that ascorbic acid has more chemical stability in the IEFPCM model.

The change in the bandgap energy takes places due to interaction between the solvents (DMSO) molecules during the reaction. Among the three models, IEFPCM was selected to be the best solvent for ascorbic acid as it has values very close to the literature. This result is a clear indication that the bandgap energy of ascorbic can be controlled using solvents as shown in Fig. 3.

3.2. UV–Vis spectroscopy

Ultraviolet spectroscopy (UV–VIS) is used for the determination of the molecular structures in this study. The absorption intensity of the materials was calculated as a function of wavelength as shown in Fig. 5. The IEFPCM model exhibited the highest absorption intensity 19,700 eV at a wavelength of 286 cm^{-1}. The CPCM peaked with an intensity 8350

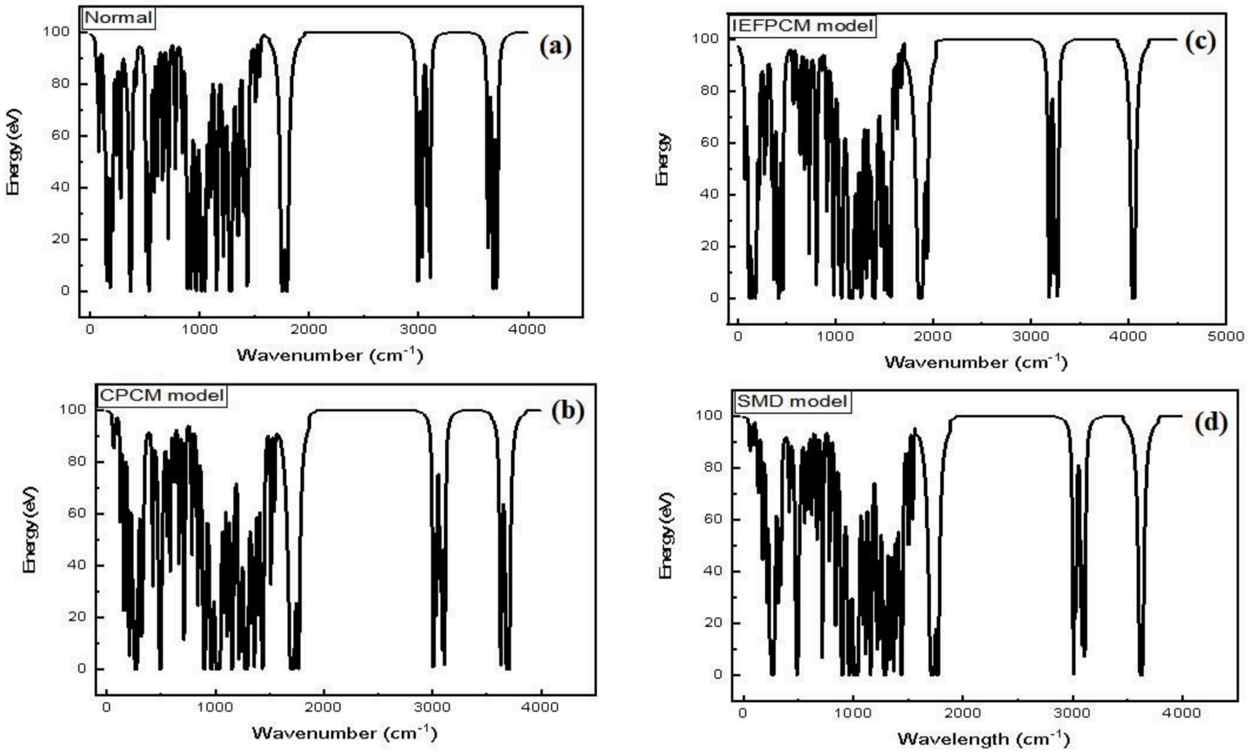

Fig. 6. The FT-IR of (a) ascorbic acid (b) in DMSO using CPCM (c) in DMSO using IEFPCM (d) DMSO using SMD.

eV and at the same time SMD model peaked with an intensity 8035 eV with corresponding values of wavelengths as 200 cm^{-1} and 232 cm$^{-1,}$ respectively. The calculations carried out using IEFPCM highest absorption peak due to which it seems to be a suitable model for solvating ascorbic acid. In addition, it is understood from these results that Ascorbic acid has absorption peaks in the middle UV region in all models.

3.3. *FT-IR spectroscopy*

The Fourier transform infrared (FT-IR) is a spectroscopic technique which is used to functional groups present in a molecule. The FTIR calculations of ascorbic acid before and after solvation were carried out using Gaussian 09 with 6–311 G/B3LYP basis set. The C—C, C=C, and C—H bonds in Figs. 2 and 6 were analyzed to explore the benzene rings that are present. It has been reported that ascorbic acid's typical carbon hydrogen (C—H) stretching vibrations take place at a wavelength of about 3000 cm^{-1} and can exhibit moderate bands (multiplicity) when compared to typical C—H stretching vibrations [16–18]. The C—H bond in ascorbic acid's vibrational modes is present in this experiment between 3065 and 3124 cm^{-1}. Due to its conformity with the literature, this shows that the base set chosen is accurate. Aliphatic C—H has stretching vibrations at approximately 2750 cm^{-1} [36], whereas it was found to be about 2867–2973 in this work, which points to an agreement with the literature. The observed peaks at about 1259, 1193, and 1147 cm^{-1} bands are attributed to in-plane bending vibration in the ascorbic acid. The results obtained theoretically in this work confirm that B3LYP computed values are close to the true value, which indicates the worth of the IEFPCM model for the molecule under investigation. The C—C vibrations exhibited different peaks due to the nature of the ascorbic acid as it has resonating benzene ring (mesomeric effect) attached to it.

3.4. *NMR spectroscopy*

The nuclear magnetic resonance (NMR) is a spectroscopic technique that can be used to determine the chemical environments of the atoms present in a particular molecule. In this work, the NMR calculations were carried out to investigate the chemical positions of protons and carbons before and after the process of solvation. The NMR results calculated on ascorbic acid (solvated and non-solvated) obtained when solvated with CPCM, IEFPCM, and SMD are shown in Fig. 7. Nasidi et al. investigated the halogen doping of ascorbic acid and discovered that there is always a change in the orientation of carbon and proton of a complex molecule when the doped with the halogens [10]. The orientation of the molecules changes when solvated due to interaction with solvent molecules depending on the models of the solvents. The normal ascorbic acid has range −200–300 ppm but changes to −150 to 300 ppm, −100 to 400 ppm and −150 to 300 ppm when solvated with DMSO in CPCM, IEFPCM, and SMD models respectively. Figs. 7a–d show the comparison of the chemical shift that occur when ascorbic acid that was solvated with the three quantum models. In fig B, by looking at the result there is highest absorbtion from −100 to 400 ppm due to the fact the IEFPCM model is the suitable model for controlling the bandgap and electronic activites of the ascorbic acid. At the same time, the other models (CPCM and SMD) have the same absorbtion from −150 to 300 ppm.

3.5. *Potential energy surface (PES)*

The potential energy map is extremely useful as it shows exactly shows the orientations, movements, and concentrations of electrons in a molecule. The distribution of electrons in a molecule can be described by the potential energy map as the red color indicates electron rich areas while blue signifies electron poor areas. In this work, the concentrations of the electrons are along the oxygen atom in the normal ascorbic acid shown in Fig. 8. Oxygen is the most electronegative atom in the structure, and it attracts the electrons towards it. This is why areas around oxygen appear to be red while other areas appear to be blue indicating electron poor areas. But when the titled molecule was solvated with DMSO, the arrangements of the electrons changed due to interactions with the molecules of the solvents. This observation is useful as it provides more light in the configuration of the electrons. The interaction is

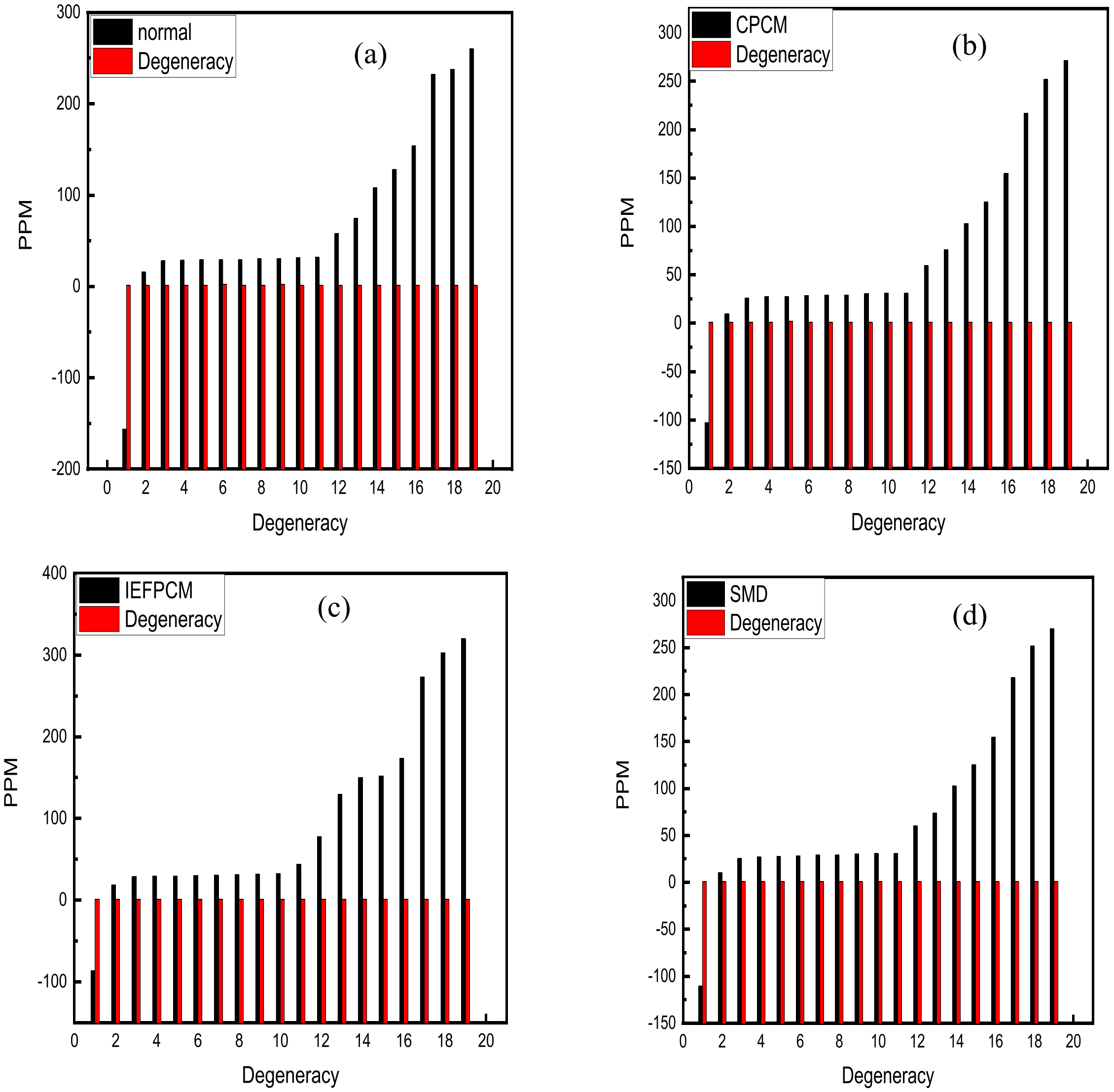

Fig. 7. The calculated NMR results (a) ascorbic acid (b) in DMSO using CPCM (c) in DMSO using IEFPCM (d) in DMSO using SMD.

more intense in IEFPCM models which makes it a more suitable solvent than the other models (CPCM and SMD).

4. Conclusion

In this research, the DMSO solvent effects on ascorbic acid were investigated using three quantum solvation models CPCM, IEFPCM, and SMD. The models selected in this study caused rearrangements in the electronic structure of the molecular orbitals thereby making a little change in the in the energy difference of highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO). The titled molecule was optimized by selecting 6–311 G/B3LYP basis set to achieve the geometry of the ground-state energy. The spectroscopic parameters were determined and then the optimized molecules were solvated with DMSO using three models to analyze the changes and investigate the improvement in its effectiveness through bandgap. It was found out the bandgap is sensitive to the solvent. This information is extremely useful as it can help us control the bandgap. It was understood that the chemical stability of the title molecule was highest in the IEFPCM model. The selection of the IEFPCM as the best solvent is as result obtained in the above calculation. The model has the highest peak in highest energy absorption when UV spectroscopy was carried out with peak around 19,700 eV and at the same time has the highest peak when UV spectroscopy was conducted. The potential energy map for the selected model shows that there is possible rearrangement of electronic structures when the solvation took place. The effect only occurs on this model as it didn’t happen on the other models.

Research data

No data was used for the research described in the article.

CRediT authorship contribution statement

Ibrahim Isah Nasidi: Investigation. **Emine Tanış:** Conceptualization, Supervision, Investigation. **Omer Kaygili:** Investigation, Writing – original draft. **Samia Naeem:** Investigation, Validation. **Abdul Majid:** Investigation, Writing – original draft. **Bilel Mehnen:** Investigation. **Niyazi Bulut:** Investigation, Writing – original draft.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

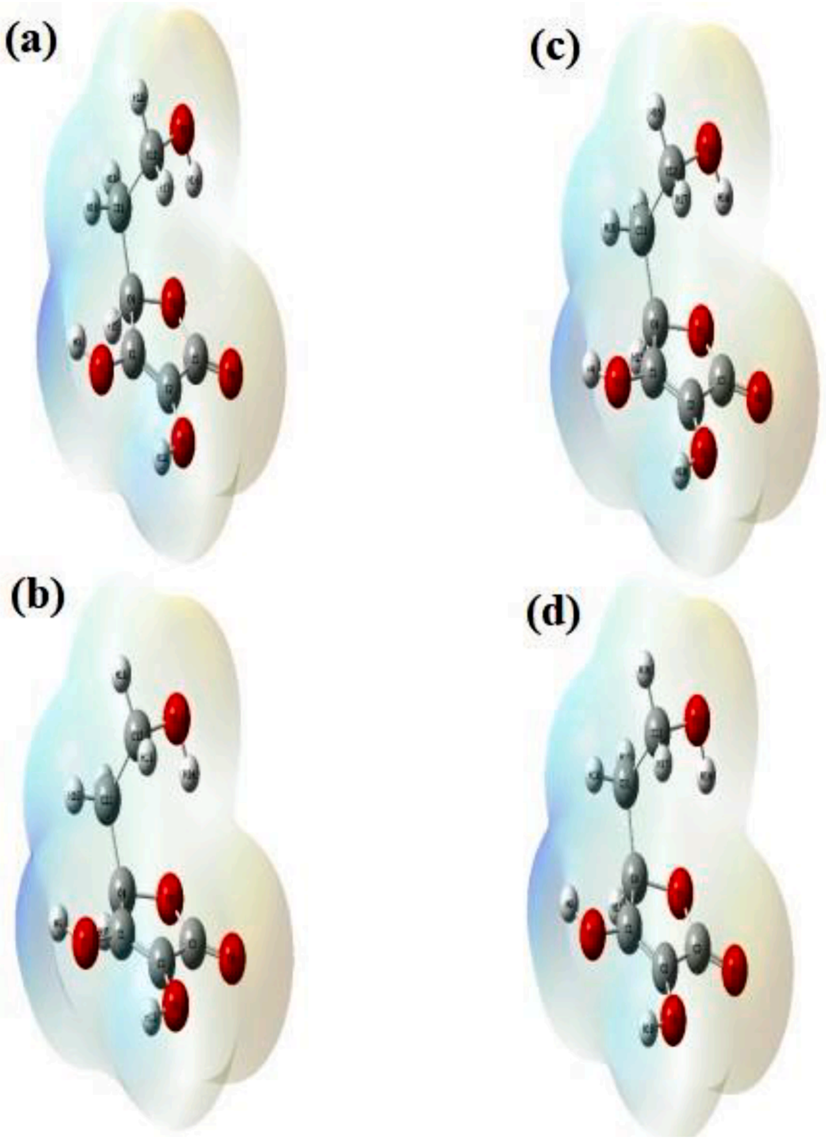

Fig. 8. The PES calculated for (a) ascorbic acid (b) DMSO using CPCM (c) DMSO using IEFPCM (d) DMSO using SMD.

Data availability

Data will be made available on request.

Acknowledgments

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References

[1] H. Lu, S. Xu, CDs-MnO2-TPPS ternary system for ratiometric fluorescence detection of ascorbic acid and alkaline phosphatase, ACS Omega 6 (2021) 16565–16572.

[2] C. Orek, B. Gündüz, O. Kaygili, N. Bulut, Electronic, optical, and spectroscopic analysis of TBADN organic semiconductor: experiment and theory, Chem. Phys. Lett. 678 (2017) 130–138.

[3] M. Said, Y. Datti, A. Nuhu, T. Buhari, B. Ahmed, Computational study of lawsonia inermis as potential and promising candidate for production of solar cell, Eur. J. Adv. Chem. Res. 2 (2021) 21–27.

[4] S. Dutta, S. Pal, P. Panwar, R.K. Sharma, P.L. Bhutia, Biopolymeric nanocarriers for nutrient delivery and crop biofortification, ACS Omega 7 (2022) 25909–25920.

[5] E. Fereyduni, E. Vessally, E. Yaaghubi, N. Sundaraganesan, One-pot synthesis, FT-IR, NMR and density functional method (B3LYP) studies on 2- (cyclohexylamino)-2-oxo-1-(pyridin-2-yl)-ethyl benzoate, Spectrochim. Acta Part A 81 (2011) 64–71.

[6] C. Orek, P. Koparir, M. Koparir, Ncyclohexyl-2-[5-(4-*pyridyl*)- 4-(*p-tolyl*)-4H-1,2,4-*triazol*3-*ylsulfanyl*]-acetamide dihydrate: synthesis, experimental, theoretical characterization and biological activities, Spectrochim. Acta Part A 97 (2012) 923–934.

[7] T.S. Xavier, The effect of electron charge transfer in biological activity and vibrational wavenumbers of 2′- Deoxyuridine and 5-Fluoro-2′-Deoxyuridine: DFT approach, Solid State Sci. 13 (2011) 1906–1915.

[8] S. Demir, M. Dinçer, E. Şahan, et al., Molecular structure and vibrational and chemical shift assignments of 6-(2- hydroxyethyl)-2,3,4-triphenyl-2,6-dihydro-7H-pyrazolo[3,4- *d*]pyridazin-7-one by DFT and ab initio HF calculations, J. Mol. Struct. 985 (2011) 251–260.

[9] Y. Liu, C. Liu, J. Li, Comparison of vitamin C and its derivative antioxidant activity: evaluated by using density functional theory, ACS Omega 5 (2020) 25467–25475.

[10] I.I. Nasidi, O. Kaygili, A. Majid, N. Bulut, M. Alkhedher, S.M. ElDin, Halogen doping to control the band gap of ascorbic acid: a theoretical study, ACS Omega 7 (48) (2022) 44390–44397, https://doi.org/10.1021/acsomega.2c06075.

[11] I.I. Nasidi, et al., Structure determination of serotonin using quantum approximations, J. Phys. Chem. Funct. Mater. 3 (2) (2021) 41–47.

[12] I.I. Nasidi, H. Kebiroglu, A theoretical study on diphenehydramine molecule, J. Phys. Chem. Funct. Mater. 3 (2) (2019) 48–53.

[13] I.I. Nasidi, et al., Spectroscopic properties determination flavanol by quantum analysis, J. Phys. Chem. Funct. Mater. 3 (2) (2021) 36–40.

[14] I.I. Nasidi, et al., A theoretical study on anthracene molecule, J. Phys. Chem. Funct. Mater. 3 (2) (2019) 43–47.

[15] L.C. Bichara, E. Lanú s, G. Nieto, A. Brandán, Density functional theory calculations of the molecular force field of ascorbic acid, vitamin C, J. Phys. Chem. A 114 (2010) 4997–5004.

[16] H. Tanak, Crystal structure, spectroscopy, and quantum chemical studies of ( )-2-[(2 *Chlorophenyl*)*iminomethyl*]-4-trifluor-omethoxyphenol, J. Phys. Chem. A 115 (2011) 13865–13876.

[17] M.H. Kebiroglu, C. Orek, N. Bulut, O. Kaygili, S. Serhat Keser, T. Ates, Temperature dependent structural and vibrational properties of hydroxyapatite: a theoretical and experimental study, Ceram. Int. 43 (2017) 15899–15904.

[18] C. Liu, J. Sun, Impact of marine-based biomaterials on the immunoregulatory properties of bone marrow-derived mesenchymalstem cells: potential use of fish collagen in bone tissue engineering, ACS Omega 5 (2020) 28360–28368.

[19] S.A. Fahmy, N.K. Mahdy, H. Al Mulla, A.N. ElMeshad, M.Y. Issa, H.M.E.S. Azzazy, PLGA/PEG nanoparticles loaded with cyclodextrin-peganum harmala alkaloid complex and ascorbic acid with promising antimicrobial activities, Pharmaceutics 14 (2022) 142.

[20] H. Tajmir-Riahi, Coordination chemistry of vitamin C. Part I. Interaction of L-ascorbic acid with alkaline earth metal ions in the crystalline solid and aqueous solution, J. Inorg. Biochem. 40 (1990) 181–188.

[21] S. Cailotto, E. Amadio, M. Facchin, M. Selva, E. Pontoglio, F. Rizzolio, A. Perosa, et al., Carbon dots from sugars and ascorbic acid: role of the precursors on morphology, properties, toxicity, and drug uptake, ACS Med. Chem. Lett. 9 (2018) 832–837.

[22] N. Sugino, Reactive oxygen species in ovarian physiology, Reprod. Med. Biol. 4 (2005) 31–44.

[23] J. Hvoslef, P. Klaeboe, B. Pettersson, S. Svensson, J. Koskikallio, S. Kachi, Vibrational spectroscopic studies of L-ascorbic acid and sodium ascorbate, Acta Chem. Scand. 25 (1971) 3043–3053.

[24] C.Y. Panicker, H.T. Varghese, D. Philip, FT-IR, FT-raman and SERS spectra of vitamin C, Spectrochim. Acta, Part A 65 (2006) 802–804.

[25] A. Ruetenik, A. Barrientos, Dietary restriction, mitochondrial function and aging: from yeast to humans, Biochim. Biophys. Acta 1847 (2015) 1434–1447.

[26] H. Gökce, N. Öztü rk, M. Taş an, Y. Alpaslan, G. Alpaslan, Spectroscopic characterization and quantum chemical computations of the 5- (4-pyridyl)-1 -1,2,4-triazole-3-thiol molecule, Spectrosc. Lett. 49 (2016) 167–179.

[27] M.N. Arshad, I. Shafiq, M. Khalid, A.M. Asiri, Exploration of the intriguing photovoltaic behavior for fused indacenodithiophene. based A-D-A conjugated systems: a DFT model study, ACS Omega 7 (2022) 11606–11617.

[28] M.P. Andersson, P. Uvdal, New scale factors for harmonic vibrational frequencies using the B3LYP density functional method with the triple-ζ basis set 6-311+ G (d, p), J. Phys. Chem. A 109 (2005) 2937–2941.

[29] J.A. Montgomery Jr., M.J. Frisch, J.W. Ochterski, G.A Petersson, A complete basis set model chemistry. VI. Use of density functional geometries and frequencies, J. Chem. Phys. 110 (1999) 2822–2827.

[30] P. Bobadova-Parvanova, K.A. Jackson, S. Srinivas, M. Horoi, C. Köhler, G. Seifert, Scanning the potential energy surface of iron clusters: a novel search strategy, J. Chem. Phys. 116 (2002) 3576–3587.

[31] A. Hamd Hssain, B. Gündü z, A. Majid, N. Bulut, NTCDA compounds of optoelectronic interest: theoretical insights and experimental investigation, Chem. Phys. Lett. 780 (2021), 138918. No.

[32] A. Frisch, Gaussian 09W Reference, Gaussian, Inc., Wallingford, CT, 2009.

[33] K.A. Grice, R. Patil, A. Ghosh, J.D. Paner, M.A. Guerrero, E.J.M. Camacho, S. Patil, et al., Understanding the structure and reactivity of the C-S linkage in biologically active 5-arylthio-5 H- chromenopyridines, New J. Chem. 42 (2018) 1151–1158.

[34] A.E. Fazary, N.S. Awwad, H.A. Ibrahium, A.A. Shati, M.Y. Alfaifi, Y.H. Ju, Protonation equilibria of N-acetylcysteine, ACS Omega 5 (2020) 19598–19605.

[35] A. Jamal, S.H. Faizi, N. Dege, Synthesis, Structural Characterization, DFT calculations, and molecular docking of a novel quinoline derivative, J. Mol. Struct. (2023), 137251.

[36] M.M. Hossain, S.K. Shaha, F. Aziz, Antioxidant potential study of some synthesized N-heterocycles, Bangladesh Med. Res. Council Bull. 35 (2009) 49–52.

[37] A. Hashim, H. Abduljalil, H. Ahmed, Analysis of optical, electronic and spectroscopic properties of (biopolymer-SiC) nano-composites for electronics applications, Egypt. J. Chem. 0 (2019) 1659–1672.

[38] F. Pereira, K. Xiao, D.A. Latino, C. Wu, Q. Zhang, Aires-de-Sousa, J. Machine learning methods to predict density functional theory B3LYP energies of HOMO and LUMO orbitals, J. Chem. Inf. Model. 57 (2017) 11–21.

[39] V.A. Adole, R.H. Waghchaure, B.S. Jagdale, T.B. Pawar, Investigation of structural and spectroscopic parameters of Ethyl 4-(4-isopropylphenyl)-6-methyl-2-oxo-1, 2, 3, 4-tetrahydropyrimidine-5-carboxylate: a, DFT Study Chem.-Biol. Interact. 10 (2020) 22–30. Vol.

[40] R.A. Yadav, P. Rani, M. Kumar, R. Singh, P. Singh, N.P. Singh, Experimental IR and Raman spectra and quantum chemical studies of molecular structures, conformers and vibrational characteristics of L-ascorbic acid and its anion and cation, Spectrochim. Acta Part A 84 (2011) 6–21.

[41] T. Kurata, Y. Nishikawa, Chemical characteristics of dehydro-L-ascorbic acid, Biosci. Biotechnol. Biochem. 64 (2000) 1651–1655.

[42] F. Parenti, F. Tassinari, E. Libertini, M. Lanzi, A. Mucci, π-Stacking signature in NMR solution spectra of thiophene-based conjugated polymers, ACS Omega 2 (2017) 5775–5784.

[43] Z. Xu, W.K. Tang, Q. Zhou, S. Chen, C.K. Siu, G. Zhu, On the hydrolytic stability of unsymmetric platinum (iv) anticancer prodrugs containing axial halogens, Inorg. Chem. Front. 8 (2021) 3794–3802.

[44] C. Orek, J. Kłos, F. Lique, N. Bulut, Ab initio studies of the Rg-NO+ ($X1\sum+$) van der Waals complexes (Rg = He, Ne, Ar, Kr, and Xe), J. Chem. Phys. 144 (2016), 204303. No.

[45] T.O. Unimuke, H. Louis, E.A. Eno, E.C. Agwamba, A.S. Adeyinka, Meta-hybrid density functional theory prediction of the reactivity, stability, and IGM of azepane, oxepane, thiepane, and halogenated cycloheptane, ACS Omega 7 (2022) 13704–13720.

[46] I.I. Nasidi, C. Orek, O. Kaygili, N. Bulut, Computational study of doping in dopamine to control optical and spectroscopic properties, ACS Omega (2023).

[47] Y. Takano, K.N. Houk, Benchmarking the conductor-like polarizable continuum model (CPCM) for aqueous solvation free energies of neutral and ionic organic molecules, J. Chem. Theory Comput. 1 (2005) 70–77.

[48] R. Cammi, Molecular Response Functions For the Polarizable Continuum Model: Physical Basis and Quantum Mechanical Formalism, Springer, 2013.

[49] A.V. Marenich, C.J. Cramer, D.G. Truhlar, Universal solvation model based on solute electron density and on a continuum model of the solvent defined by the bulk dielectric constant and atomic surface tensions, J. Phys. Chem. B 113 (2009) 6378–6396.

[50] V. Barone, M. Cossi, Quantum calculation of molecular energies and energy gradients in solution by a conductor solvent model, J. Phys. Chem. A 102 (1998) 1995–2001.

[51] E. Cances, B. Mennucci, J. Tomasi, A new integral equation` formalism for the polarizable continuum model: theoretical background and applications to isotropic and anisotropic dielectrics, J. Chem. Phys. 107 (1997) 3032–3041.

[52] J.S. Al-O., Y.M.A. H, M.M. Kamal, M.E.L.G. Tarek, Geometry and electronic properties of Vitamin C, Turkish computational and theoretical chemistry, 2(1), 2018, 2602–3237.

[53] P.K. Chattaraj, B. Maiti, HSAB principle applied to the time evolution of chemical reactions, J. Am. Chem. Soc. 125 (2003) 2705–2710.

[54] V. Arjunan, L. Devi, R. Subbalakshmi, T. Rani, S. Mohan, Spectrochim. Acta A 130 (2014) 164.