MOLECULAR GEOMETRY, HOMO-LUMO ANALYSIS AND MULLIKEN CHARGE DISTRIBUTION OF 2,6-DICHLORO-4-FLUORO PHENOL USING DFT AND HF METHOD†

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Phenolic compounds are used in human diet, commonly present in plants. Foremost polyphenolic compounds found in plants are flavanols, flavonoids, flavonones, iso-flavones, phenolic acids, flavonoids, chalcones, lignans etc. These compounds possess antimicrobial, antiviral and anti-inflammatory properties along with high antioxidative activity. The antioxidative activity of phenolic compounds depends on their structure. The polyphenols are very useful for the treatment of inflammation, cancer, anti-ageing purposes in cosmetic formulations, and nutraceutical applications. This article focused on substituted phenol, taking into concern their potential health benefits. The recent rise in machine-learning methods has engendered many advances in the molecular sciences. Using desired level of electronic structure theory from density functional theory, we can calculate the properties (electronic structure, force field, energy) of atomistic systems. The full electron density carries with it a considerable computational cost. While the DFT calculation loses accuracy when the molecule is either extended or compressed, Δ-DFT corrects these errors. Here, molecular point group symmetries are used to obtain chemical accuracy. The optimal 2,6-dichloro-4-fluoro phenol molecular geometry was derived using the 6-311+G (d, p) basis set and DFT/B3LYP (density functional theory) and Hartree-Fock (HF) techniques. A detailed interpretation of Homo-Lumo analysis of 2,6-dichloro-4-fluoro phenol is also listed. Using the 6-311+G (d, p) basis set and the Hartree-Fock (HF) method, the Mulliken charge distribution of this molecule has also been computed.

Keywords: *Homo-Lumo; Mulliken charge; 2,6-dichloro-4-fluoro phenol*
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INTRODUCTION

An essential method for analyzing the structure of organic molecules is vibrational spectroscopic analysis. The halogen derivatives of phenol find interesting application in agriculture and pharmaceutical field [1-6]. Studying their molecular characteristics and the nature of the reaction mechanism is crucial for understanding specific biochemical mechanisms and in the compound assessment [7,8]. The complete interpretation of spectroscopic studies pointed out that in aromatic compounds, phenol is on†e of the most important organic molecules in all aspects. Phenol and derivatives of phenol have broadly used as a solvent and synthetic intermediate in computational chemistry. The vibrational spectra of alkyl, halogen substituted phenols have undergone extensive research by numerous researchers [8-12]. To explore the effect of chlorine, bromine, fluorine and methyl substituents in phenol, a detailed vibrational and spectroscopic study seems attractive. So, this study includes the vibrational spectra, Homo-Lumo and Mulliken charge analysis of 2,6-dichloro-4-fluoro phenol.

EXPERIMENTAL DETAILS & COMPUTATIONAL DETAILS

In the present study we adopted density functional theory (DFT) to theoretically predict molecular geometry Homo-Lumo and Mulliken charge distribution. DFT studies have been accepted as a popular approach for molecular computation. All the calculations have been done using the Gaussian 09 program package [13]. First, a semi-empirical approach was used to derive the optimal geometry, and then by applying DFT Becke–Lee–Young–Parr composite of exchange correlation (B3LYP) functional using the 6-311+G (d, p) basis set. Finally, the geometry optimizations were carried out at the same level by using DFT-B3LYP hybrid functional and HF using 6-311+G (d, p) basis set [14, 15]. The vibrational problem was set-up in terms of symmetry and internal coordinates. The calculations have been done using the completely optimized geometry by assuming C1 point group symmetry. Using the GAUSSVIEW molecular visualization program [16], the values were made with a great degree of confidence along with available related molecules.

RESULT AND DISCUSSION
Molecular Geometry

Fig. 1 depicts the 2,6-dichloro-4-fluoro phenol's optimized molecular structure. The idealized molecular geometry depicts an isolated molecular entity with a point of equilibrium at the potential energy levels; the closure was confirmed by excluding imaginary vibrational wave numbers.
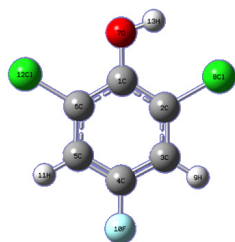
Figure 1 Molecular geometry of
2,6-dichloro-4-fluoro phenol.

The predicted bond lengths and angles, in addition to the geometrical characteristic for the 2,6-dichloro-4-fluoro phenol molecular unit in the solid phase, and the B3LY/6-311+G (d, p) optimized molecular unit are reported in Table 1. The 2,6-dichloro-4-fluoro phenol enhanced structural parameters computed by DFT using the B3LY/6-311+G (d, p) boundary condition are comparable with the atomic number scheme shown in Fig. 1.

There are two C-Cl bond lengths, six C-C bond lengths, one C-F bond length, one O-H bond length, two C-H bond lengths, and one C-O bond length in the title molecule. Table 1 displays the computed values of all bond lengths using Gaussian program in the current assignment.

Based on the estimation, the bond length order is (C3–C4<C4-C5<C2-C3<C5-C6<C1-C2<C1–C6) from the bond length order, it is clear that the benzene ring's hexagonal structure is slightly skewed. The bond angles C2-C1-C6 and C3-C4-C5 deviate from the standard hexagonal angle of 120° by 117.074° and 122.0141°, respectively. This is due to the substitution of Cl, F, and oxygen, group attached to C2, C6, C4, and C1 of the ring. The geometrical parameters evaluated serve as the foundation for the calculation of many other characteristics, including vibratory frequencies as well as other spectroscopic features of the molecule.

Table 1. Optimized geometrical parameters of 2,6-dichloro-4-fluoro phenol by DFT-B3LYP and HF method with 6-311++G(d,p) basis set.

S.No.	Bond length	Value (A⁰)		Bond angle	Value(⁰)	
		DFT	HF		DFT	HF
1	C1-C2	1.401	1.3867	C2-C1-C6	117.074	117.2542
2	C1 -C6	1.403	1.392	C2-C1-O7	123.6347	123.8141
3	C1-O7	1.3487	1.3351	C6-C1-O7	119.2913	118.9317
4	C2-C3	1.3887	1.3821	C1-C2-C3	122.6242	122.322
5	C2-Cl8	1.7602	1.7442	C1-C2-Cl8	117.8555	118.8152
6	C3-C4	1.384	1.3706	C3-C2-Cl8	119.5202	118.8628
7	C3-H9	1.0809	1.0721	C2-C3-C4	117.8876	118.2229
8	C4-C5	1.3857	1.3762	C2-C3-H9	121.3628	121.0386
9	C4-F10	1.3489	1.3241	C4-C3-H9	120.7496	120.7386
10	C5-C6	1.3889	1.3782	C3-C4-C5	122.0141	121.7399
11	C5-H11	1.0811	1.0722	C3-C4-F10	119.0016	119.2263
12	C6-Cl12	1.7455	1.7324	C5-C4-F10	118.9843	119.0339
13	O7-H13	0.9666	0.9421	C4-C5-C6	118.826	118.9212
14				C4-C5-H11	120.339	120.3072
15				C6-C5-H11	120.8349	120.7717
16				C1-C6-C5	121.574	121.5399
17				C1-C6-Cl12	118.857	119.2769
18				C5-C6-Cl12	119.5689	119.1832
19				C1-C7-H13	108.8655	111.1338
For numbering of atom refer Fig. 1						

Homo–Lumo Energy

The ability to provide electrons is characterized by the HOMO (Highest Occupied Molecular Orbital) energy, the competence to receive electrons is characterized by the LUMO (Least Unoccupied Molecular Orbital), and the gap between HOMO and LUMO specifies the chemical stability of molecules. Because it is a measurement of electron conductivity, the difference in energy between the HOMOs and LUMOs is an important criterion in understanding about features of molecular electric propagation. The energy values of LUMO and HOMO and their energy gap govern a molecule's kinetic stability, chemical responses, spontaneous polarizability, and chemical hardness-softness. [17-19].

The high values of the energy gap indicate the ruggedness, whereas the small value displays the tenderness of the molecular structure. Since they require a significant amount of energy to excite, in comparison to soft molecules, hard molecules are not significantly polarizable [18-20]. A molecule is chemically reactive if it has a minimal or nonexistent HOMO-LUMO gap. The HOMO-LUMO gap illustrates the molecular fragility of the compound [20-21]. Additional quantity that is estimated is the electrophilicity index, which quantifies the energy loss experienced by a ligand as a result of the maximum electron flow between the donor and acceptor [17-18].

The energies of HOMO, LUMO, HOMO-1 (Second Highest Occupied Molecular Orbital), and LUMO-1 (Second Least Unoccupied Molecular Orbital) employ the TD-DFT approach for estimation. by employing the identical boundary conditions, as well as the related energy gap for 2,6-dichloro-4-fluoro phenol are shown in Table 2.

The equations are used to calculate some important properties are as follows (as given in Table 3):

Ionization Potential (I) = $-E_{HOMO}$

Electron Affinity (A) = $-E_{LUMO}$

Chemical Potential (μ) = $(E_{LUMO} + E_{HOMO})/2$

Global Hardness (η) = $(E_{LUMO} - E_{HOMO})/2$

Global Softness (S) = $1/\eta$
Electronegativity (σ) = $-\mu$
Electrophilicity Index (ω) = $\mu^2/2\eta$

These values will be same since the values of E_{HOMO} and E_{LUMO} are same for each basis set as shown in Table 3. Atomic orbital HOMO and LUMO compositions of the frontier molecular orbital for 2,6-dichloro-4-fluoro phenol are shown in Fig. 2 and Fig. 3 respectively.

Table 2. Energy values (eV) of 2,6-dichloro-4-fluoro phenol calculated by using TD-DFT/ B3LYP/6-311+G(d,p)

	HF/6-311+G(d,p)	**DFT/6-311+G(d,p)**
E_{HOMO}	-0.37157	-0.26498
E_{LUMO}	-0.08646	-0.04094
E_{HOMO-1}	-0.37321	-0.27095
E_{LUMO-1}	-0.11511	-0.02031
ΔE	0.28511	0.22404
∂E	0.2581	0.19064
$\Delta E = E_{LUMO} - E_{HOMO}, \partial E = E_{LUMO+1} - E_{HOMO-1}$		

Table 3. Calculated Ionization potential (I), Chemical potential (μ), Electron affinity (A), Global hardness (η), Global softness (S) in eV^{-1}, Electronegativity (σ) and Electrophilicity index (ω) using DFT and HF with 6-311+G(d,p) basis sets.

Parameters	**B3LYP/6-311+G(d,p) Values in (eV)**	**HF/6-311+G(d,p) Values in (eV)**
E_{HOMO}	-0.26498	-0.37157
E_{LUMO}	-0.04094	-0.08646
Ionization Potential (I)	0.26498	0.37157
Electron Affinity (A)	0.04094	0.08646
Chemical Potential (μ)	-0.15296	-0.229015
Global Hardness (η)	0.11202	0.142555
Global Softness (S)	8.92697733	7.01483638
Electronegativity (σ)	0.15296	-0.229015
Electrophilicity Index (ω)	0.10443118	0.183956614

(a)	**(b)**

Figure 2. Atomic orbital HOMO compositions for 2,6-dichloro-4-fluoro phenol using (a) DFT/6-311+G(d,p) and (b) HF/ 6-311+G(d,p)
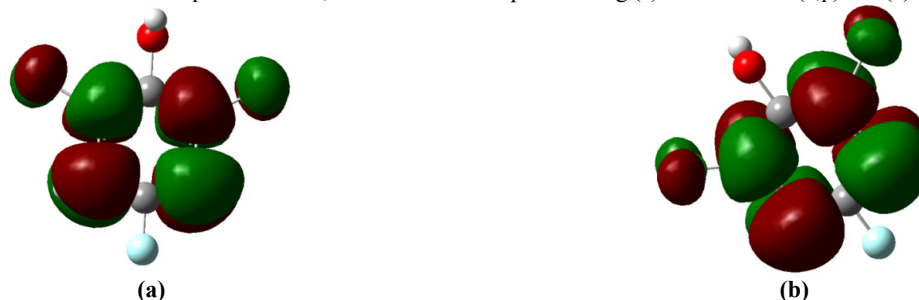

(a)	**(b)**

Figure 3. Atomic orbital LUMO compositions for 2,6-dichloro-4-fluoro phenol using (a) DFT/6-311+G(d,p) and (b) HF/ 6-311+G(d,p)

Mulliken Charges

By applying the basis sets HF/6-311+G (d, p) and B3LYP/6-311+G (d, p) in a Mulliken population analysis, Mulliken charges have been approximated [20-30]. Fig. 4 depicts the 2,6-dichloro-4-fluoro phenol mulliken charges. The 2,6-dichloro-4-fluoro phenol atoms' Figure 4 illustrates the positive and negative charge distribution of this article.

Table 5. Mulliken charges of 2,6-dichloro-4-fluoro phenol computed by HF/6-311+G(d,p) and B3LYP/6-311+G(d,p) basis sets

S.No.	**Atom**	**HF/6-311+ G(d,p)**	**DFT/6-311+ G(d,p)**
1	C	0.422709	0.322090
2	C	-0.396267	-0.346824
3	C	-0.212681	-0.177132

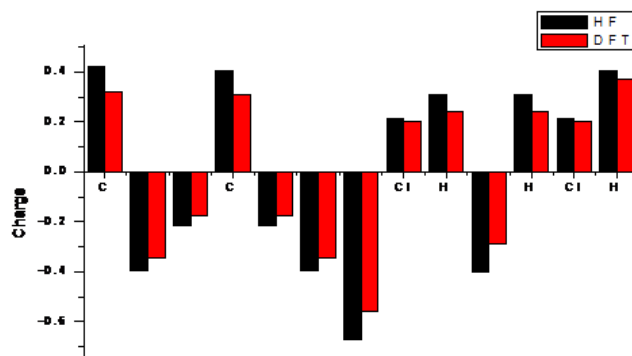| S.No.	Atom	HF/6-311+ G(d,p)	DFT/6-311+ G(d,p)
4	C	0.402539	0.311973
5	C	-0.212681	-0.177132
6	C	-0.396267	-0.346824
7	O	-0.669420	-0.559410
8	Cl	0.216720	0.201306
9	H	0.309530	0.242573
10	F	-0.397307	-0.286088
11	H	0.309530	0.242573
12	Cl	0.216720	0.201306
13	H	0.406873	0.371590

Figure 4. Mulliken charges distribution of 2,6-dichloro-4-fluoro phenol calculated by HF/6-311+G(d,p) and B3LYP/6-31+G(d,p) basis sets.

CONCLUSIONS

The 2,6-dichloro-4-fluoro phenol atom's improved molecular geometry was predicted at the B3LYP level using the 6-311+G (d, p) basis set. As a result, only admissible variations from the research observations were included in the task, which was presented at a higher level with a larger boundary condition. Transmission of charge occurs inside the molecular structure, as evidenced by the computed HOMO and LUMO energies. In order to understand the compound, the 2,6-dichloro-4-fluoro phenol's Mulliken Charge has additionally been measured.

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REFERENCES

[1] R.A. Yadav, P. Rani, M. Kumar, R. Singh, P. Singh, and N.P. Singh, "Experimental IR and Raman spectra & quantum chemical studies of molecular structures, conformers & vibrational characteristics of L-ascorbic acid", Spectrochemica Acta A, **84**(1), 6 (2011). https://doi.org/10.1016/j.saa.2011.07.043

[1] V. Krishnakumar et al., "Vibrational and normal coordinate analysis of xanthine and hypoxanthine", Indian J. of Physics, **42(06)**, 411-418 (2004). http://nopr.niscpr.res.in/handle/123456789/26125

[2] V.K. Rastogi, V. Jain, M.A. Palafox, D.N. Singh, and R.A. Yadav, "The variation of enthalpy function and heat capacity of 2,6,4 DCFP", Spectrochemica Acta, **57**(A), 209 (2001). https://doi.org/10.1016/S1386-1425(00)00327-9

[3] V. Krishnakumar, and V. Balachandran, "FTIR, FT-Raman spectral analysis and normal coordinate calculations of 2-hydroxy-3-methoxy-benzyldehyde-thio-semicarbozone", Indian J. of Pure and Appl. Physics, **42**, 313-318 (2004). http://nopr.niscpr.res.in/bitstream/123456789/9583/1/IJPAP%2042%285%29%20313-318.pdf

[4] S. Gunasekaran, and P. Abitha, Indian J. of Pure and Appl. Physics, **43**, 329-334 (2005). http://nopr.niscpr.res.in/bitstream/123456789/8791/1/IJPAP%2043%285%29%20329-334.pdf

[5] S. Chaudhary, Ph. D. Thesis, "Spectral investigation and thermodynamic functions of some aromatic molecules", C.C.S Univ. 2001.

[6] V. Krishnakumar, and R.J. Xavier, "FT-Raman and FT-IR spectral studies of 3-mercapto-1,2,4 triazole", Indian J. of Pure and Appl. Phys. **41**, 95-112 (2003). http://nopr.niscpr.res.in/bitstream/123456789/25035/1/IJPAP%2041%282%29%2095-99.pdf

[7] Fu. Aiping, Du. Dongmei, and Z. Zhengyu, "Study of formamide-meyhonal dimer with ab initio and density function theory methods", Journal of Quantum Chemistry, **97**, 865-875 (2004). https://doi.org/10.1002/qua.10796

[8] A. Altum, K. Gölcük, and M. Kumru, Journal of Molecular Structure, **637**, 155 (2003). https://doi.org/10.1016/S0166-1280(03)00531-1

[9] V. Krishnakumar, and R. Ramasamy, "Spectral and normal coordinate analysis of 6-methoxy purine", Indian J. of Pure and App. Physics, **40**, 252-255 (2002). https://www.researchgate.net/publication/279895257_Spectral_and_normal_coordinate_analysis_of_6-methoxy_purine

[10] B.S. Yadav et al., "FT-IR spectroscopic studies of 2-hydroxy-4-methyl pyrimidine hydrochloride" Asain journal of chemistry, **20**(1), 273-276 (2008).https://asianjournalofchemistry.co.in/user/journal/viewarticle.aspx?ArticleID=20_1_43

[11] V. Krishnakumar et al., "Normal coordinate analysis of vibrational spectra of 2- methyliodine and 5-hysdroxyinolane", Indian J. of Pure and Appl. Physics, **41**, 85-99 (2003). https://www.semanticscholar.org/paper/Normal-coordinate-analysis-of-vibrational-spectra-Krishnakumar-Xavier/bb1c9858cca12a0d182404e34ec3db17af178eb8

[12] R.L. Frost, Y. Xi, S.J. Palmer, G.J. Millar, K. Tan, and R.E. Pogson, "Vibrational spectroscopy of synthetic stecorite H(NH₄)Na(PO₄)·4H₂O", Spectrochimica Acta A, **84**(1), 269-274 (2011). https://doi.org/10.1016/j.saa.2011.09.040

[13] M. Karabacak, M. Cinar, Z. Unal, and M. Kurt, "Spectroscopic and computational studies on 3-methyl aniline", Mol. Struct. **982**, 22-27 (2010). https://doi.org/10.1016/j.molstruc.2010.07.033

[14] V.P. Gupta, and P. Tandon, "Conformational and vibrational studies of isomeric hydrogen cynide tetramers by quantum chemical methods", Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy, **89**, 55-66 (2012). https://doi.org/10.1016/j.saa.2011.12.030

[15] M.J. Frisch et al., Gaussian 09 Revision A.02, Gaussian, Inc., Wallingford CT, 2009.

[16] A. Abhas et al., Spectrochimica Acta Part A, **21**, 376-383 (2015). https://doi.org/10.1016/j.saa.2014.11.024

[17] Samuel Tetteh et al, Electronic Spectra of *ortho*-Substituted Phenols: An Experimental and DFT Study", Hindawi Journal of Spectroscopy, **1**, 1-10 (2018). https://doi.org/10.1155/2018/4193657

[18] F.A. Pasha, H.K. Srivastava, Y. Beg, and P.P. Singh, "DFT Based Electrophilicity Index and QSAR study of Phenols as Anti Leukaemia Agent", American Journal of Immunology, **2**(1), 23-28 (2006). https://thescipub.com/pdf/ajisp.2006.23.28.pdf

[19] M. Bogojeski, L. Vogt-Maranto, M.E. Tuckerman, K.-R. Müller, and K. Burke, "Quantum chemical accuracy from density functional approximations via machine learning", Nature Communication, **11**, 5223 (2020). https://doi.org/10.1038/s41467-020-19093-1

[20] J. Teotia et al., "Ultraviolet Absorption Spectra, Solvent Effect and Non-Linear Optical Properties of 2-Amino-4,6 dimethylpyridine by Hartee-Fock and Density Functional Theory", Asian Journal of Chemistry, **28**(10), 2204-2210 (2016). https://doi.org/10.14233/ajchem.2016.19928

[21] S. Kumar, R. Kumar, J. Teotia, and M.K. Yadav, "Experimental & theoritical (ab initio & DFT) analysis of UV-Vis spectra, thermodynamic functions & nonlinear optical properties of 2-chloro-3,4-dimethylbenzyl dehyde", Journal of Advances in Physics, **8**(2), 2122-2134 (2015). https://rajpub.com/index.php/jap/article/view/1519/pdf_158

[22] S. Kumar, Surbhi, and M.K. Yadav, "Optimized Molecular Geometries, Internal Coordinates, Vibrational Analysis, Thermodynamic properties, First Hyper Polarizability and Homo-Lumo Analysis of Duroquinone using Density Functional Theory and Hartree-Fock Method.", Russian Journal of Physical Chemistry B, **15**, S22–S31 (2021). https://doi.org/10.1134/S1990793121090116

[23] H. Kumar, N. Choudhary, Varsha, N. Kumar, Suman, and R. Seth, "Phenolic compounds and their health benefits: A review", Journal of Food Research and Technology April-June, **2**(2), 46-59 (2014). https://www.researchgate.net/profile/Harish-Kumar-96/publication/350966390_Phenolic_compounds_and_their_health_benefits_A_review/links/607d535b8ea909241e0cf38c/Phenolic-compounds-and-their-health-benefits-A-review.pdf

[24] X. Xiang, Z.-X. Zhao, and H.-X. Zhang, "A theoretical study based on DFT calculations on the different influence of functional groups on the C–H activation process *via* Pd-catalysed β-X elimination", Royal Society of Chemistry, **12**, 26116-26122 (2022). https://doi.org/10.1039/D2RA03506E

[25] S. Bhandari, R. Khatun, T.S. Khan, D. Khurana, M.K. Poddar, A. Shukla, V.V.D.N. Prasada, and R. Bal, "Preparation of a nanostructured iron chromite spinel in the pure form and its catalytic activity for the selective oxidation of benzene to phenol: experimental and DFT studies", Journal of Green Chemistry, **24**, 9303-9314 (2022). https://doi.org/10.1039/D2GC02335K

[26] F. Maldonado, L. Villamagua, and R. Rivera "DFT Analysis of the Adsorption of Phenol on the Nonpolar (10$\bar{1}$0) ZnO Surface", J. Phys. Chem. C, **123**(19), 12296–12304 (2019). https://doi.org/10.1021/acs.jpcc.9b01906

[27] Sarvendra et al., "Vibrational spectroscopic investigation, first hyper polarizability & Homo Lumo analysis of tetrahydroxy-1,4 quinone hydrate using DFT and HF methods", Russian J. of Physical Chemistry B, **12**(3), 383-393 (2018).

[28] Seema et al., "Ultraviolet absorption spectra, solvent effect and Non- linear Optical properties of 1,2,4,5-tetrachloro-3-nitrobenzene by hartee-fock density functional theory" International journal of research and analytical reviews, **6**(2), 2241-2248 (2019). http://ijrar.org/viewfull.php?p_id=IJRAR19K3768

[29] S. Kumar, Surbhi, and M.K. Yadaw, S. Kumar, Surbhi, and M.K. Yadaw, "Ultraviolet Absorption spectra, solvent effect and non-linear optical properties of tetrahydroxy-1-4 quinone hydrate by HF and DFT theory", Asian Journal of Chemistry, **29**(10), 2241-2248 (2017). https://doi.org/10.14233/ajchem.2017.20741

МОЛЕКУЛЯРНА ГЕОМЕТРІЯ, HOMO-LUMO АНАЛІЗ ТА РОЗПОДІЛ ЗАРЯДУ МАЛЛІКЕНА 2,6-ДІХЛОР-4-ФТОРФЕНОЛА ЗА ДОПОМОГОЮ DFT ТА HF МЕТОДІВ

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Фенольні сполуки використовуються в раціоні людини, зазвичай присутні в рослинах. Основними поліфенольними сполуками, які містяться в рослинах, є флаваноли, флавоноїди, флавонони, ізофлавони, фенольні кислоти, флавоноїди, халкони, лігнани тощо. Ці сполуки мають антимікробні, противірусні та протизапальні властивості разом із високою антиоксидантною активністю. Антиоксидантна активність фенольних сполук залежить від їх структури. Поліфеноли дуже корисні для лікування запалень, раку, для запобігання старінню в косметичних рецептах і нутрицевтиках. Ця стаття присвячена замінним фенолам, враховуючи їх потенційну користь для здоров'я. Недавній розвиток методів машинного навчання породив багато досягнень у молекулярних науках. Використовуючи бажаний рівень теорії електронної структури з теорії функціоналу густини, ми можемо розрахувати властивості (електронну структуру, силове поле, енергію) атомістичних систем. Повна електронна густина несе з собою значні обчислювальні витрати. Хоча розрахунок DFT втрачає точність, коли молекула розтягується або стискається, Δ-DFT виправляє ці помилки. Симетрії груп молекулярних точок використовуються для отримання хімічної точності. Оптимальну молекулярну геометрію 2,6-дихлор-4-фторфенолу було отримано за допомогою базового набору 6-311+G (d, p) і методів DFT/B3LYP (теорія функціоналу густини) і Хартрі-Фока (HF). Також наведено детальну інтерпретацію аналізу Homo-Lumo 2,6-дихлор-4-фторфенолу. За допомогою базисного набору 6-311+G (d, p) і методу Хартрі-Фока (HF) було також обчислено розподіл заряду Маллікена цієї молекули.
Ключові слова: *гомо-люмо; заряд Маллікена; 2,6-дихлор-4-фторфенол*