PHYSICS AND CHEMISTRY
OF SOLID STATE
V. 26, No.1 (2025) pp. 158-165

Section: Chemistry

DOI: 10.15330/pcss.26.1.158-165

Vasyl Stefanyk Precarpathian
National University

ФІЗИКА І ХІМІЯ ТВЕРДОГО ТІЛА
Т. 26, № 1 (2025) С. 158-165

Хімічні науки

PACS: 31.15.E

ISSN 1729-4428 (Print)
ISSN 2309-8589 (Online)

Mohd Amin Mir[1], Maythem Mahmoud[2], Kim Andrews[2], Arunima Nayak[3],
Nupur Kukretee[3], Shreya Kotnala[4]

Experimental, Spectroscopic, Computational and Molecular Studies of Plant Growth Promotor 2-Naphthylacetic Acid

[1]Department of Mechanical Engineering, Prince Mohammad Bin Fahd University, Al-Khobar, Saudi Arabia,
mohdaminmir@gmail.com;
[2]Department of Mathematics & Natural Sciences, Prince Mohammad Bin Fahd University, AL Khobar, Saudi Arabia;
[3]Department of Chemistry, Graphic Era Deemed to be University, Dehradun, India;
[4]Department of chemistry, School of Basic & Applied Sciences, Shri Guru Ram Rai University Dehradun, India

The bioactive compound 2-Naphthylacetic Acid was the subject of theoretical experiments using DFT-B3LYP techniques with 6-311++G(d,2p) basis sets. Computational analysis included the calculation of 2-Naphthylacetic Acid's geometrical parameters, molecular characteristics, and vibrational spectra. Density Functional Theory was used to carry out geometrical optimizations. When the calculated vibrational spectra and optimized molecular geometry were matched to experimental results, significant agreement was found. Furthermore, for the aforementioned compound, DFT characteristics like, chemical hardness, total energy, chemical potential, and electrophilicity were calculated. The relative stability and reactivity of the compounds under study were predicted using these descriptors.

Keywords: 2-Naphthylacetic Acid, DFT-B3LYP, Computational Studies, DFT, stability.

Received 25 April 2024; Accepted 23 January 2025.

Introduction

The basic chemical properties of aromatic compounds are widely used to characterize them, and because of their adaptability in changing molecular geometry and substituent modifications, it is possible to customize the properties of materials for particular uses [1]. Low molecular weight materials are made up of molecules with regular size and a consistent structure. Polycyclic aromatic hydrocarbons (PAH) are unique in this group; they have well-established chemical and physical properties together with a significant molecular weight [2]. A subclass of PAH known as linear acenes has attracted a lot of interest in the field of electronic technology [3–4]. These compounds with pi-electron conjugated bonding system is critical to semiconductor characteristics. Charge carrier transit in molecular material layers depends on crystal packing, intermolecular interactions, and molecular structure [5]. In order to simulate the electrical characteristics of organic materials for theoretical research, the charge transfer transit mechanism must be empirically validated. Free molecules redistribute their charge in the condensed state, especially in crystals, to promote the van der Waals forces' formation and affect the charge states of the component atoms. As such, both intramolecular and intermolecular components are involved in the mechanism of chemical bond formation in molecular crystals. This mechanism is typically defined using quantum chemistry software, such as Gaussian09 [7], which can do density functional theory (DFT) computations [6]. In crystalline samples at low temperatures, the mobility and concentration of carriers in naphthalene and its derivatives are usually investigated. Utilizing the Hall effect approach and the photon impulse-generated instantaneous currents method, charge carrier mobility tests for monocrystalline naphthalene samples produced drift mobility values for holes in the order of 10^{-1} cm^{-2} at room temperature. Similar mobility values were found in charge transport in acenes monocrystals using ab initio theoretical study [9]. Specifically, investigations of the electrical characteristics of thin films consisting of naphthalene replaced with noncomplex chemical groups at room temperature are scarce. With a range of biological actions, naphthalene and its compounds are important structural elements in many natural things and medications [10], [11]. Therefore, it is very important to investigate new approaches for creating 2-Naphthylacetic Acid with certain substitution patterns. This paper presents the molecular and crystal structures of 2-Naphthylacetic Acid as well as single crystal X-ray diffraction, UV, and infrared research. DFT is used to analyze the title molecule's conformation with respect to a chosen torsion angle. Furthermore, using DFT/B3LYP with the 6-31G(d,p) basis set, the molecular structure, geometry, frontier molecular orbitals, molecular electrostatic potential, total molecular energies, dipole moments, nonlinear optical properties were examined. Results from experiments and theoretical calculations are compared in this paper.

I. Materials and Methods

1.1. Experimental

Polycyclic aromatic compounds, namely 2-Naphthylacetic Acid, a derivative of naphthalene, were subjected to spectral measurements. The KBr pellet approach was utilized to get the Infrared (IR) spectra on a BRUKER-ALPHA-PLATINUM-ATR-IR6V spectrometer, covering a wavelength range of 400-4000 cm^{-1}.

1.2. Computational Method

The Gaussian-03 program was utilized to perform Density Functional Theory computations. The conventional 6-311++ G(d,2p) basis set and the Becke-3Lee-Yang-Parr (B3LYP) functional were employed [12]. In order to describe all stationary points as minima, the optimal structural parameters—which are essential for vibrational wave number computations—were ascertained at the Hartree-Fock (HF) and DFT levels. The optimized geometry that resulted from allowing all parameters to relax and achieving convergence during the calculations is indicative of minimum energy, as indicated by wavenumber calculations' lack of imaginary values. Gauss View 3.07 was used for the display and study of molecular parameters, such as optimal molecular geometry, lowest unoccupied molecular orbital (LUMO), highest occupied molecular orbital (HOMO), and their energy gap difference. To learn more about the structural characteristics and chemical reactivities of the compounds with the titled names, the optimal geometry of these molecules was examined together with a number of molecular attributes, including bond length, bond angle, dipole moment, and many global descriptors.

II. Results and Discussion

2.1. Molecular Geometry

DFT/B3LYP was used to optimize the molecular geometry of 2-Naphthylacetic Acid using the 6-311++G(d,2p) basis set. The experimental values derived from X-ray diffraction were compared with the calculated bond lengths and bond angles. It was found that the molecule had a dipole moment of 7.0975 Debye and a total energy of -1171.6621 a.u. The benzene ring's bond distances, which varied between 1.35 and 1.43 Å, closely matched experimental values, demonstrating the accuracy of DFT techniques. Due to basis set approximations and environmental factors, the O-H bond length showed a slight departure from conventional values (0.98 Å). Tables 1 and 2 display the compound's optimized structural characteristics, which were determined via DFT/B3LYP calculations using the 6-311++ G(d,2p) basis set. Figure 1 shows an illustration of the 2-Naphthylacetic Acid optimized geometry.

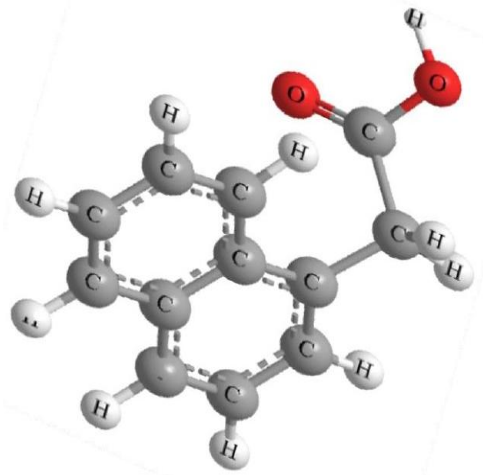

Fig. 1. The optimized geometry 2-Naphthylacetic Acid.

Table 1.
Optimized Structure Parameters of 2-Naphthylacetic Acid by DFT method

File Name	2-Naphthylacetic Acid
File Type	nsa.chk
Calculation Type	Freq
Calculation Method	B3LYP
Basis Set	6.311++G(D,2P)
Charge	0
Spin	singlet
Total Energy	-1171.66211931
Dipole moment	7.0975

The bond lengths, bond angles, and dihedral angles for 2-Naphthylacetic Acid are presented in Table 2-3. The total energy of 2-Naphthylacetic Acid is found to be -1171.6621 atomic units at the DFT/B3LYP level with the 6-311++G(d,2p) basis set, and its dipole moment is 7.0975 Debye. Interestingly, every C-C bond in the benzene ring has a length between 1.35 and 1.43 Å. The carbon-carbon bond distances range from 1.38 to 1.42 Å, while the carbon-hydrogen (C-H) bond distances are almost uniform and almost equal to 1.08 Å. Among the noteworthy findings are that the O-H bond length in 2-Naphthylacetic Acid varies from the typical bond length of 0.98 Å, falling between 0.93-0.96 Å. The C=O bond length in the DFT approach is 1.216 Å, while the conventional bond length is 1.21 Å. In the phenyl ring, all C-C-C bond angles range from 118 to 120 degrees. Remarkably, the bond angle values remain relatively unchanged in the presence of COOH group in the naphthalene ring. The majority of bonds have dihedral angles that are roughly 180 degrees, and the substituent present on the naphthalene ring has little effect on these values.

Table 2.

Bond distances of 2-Naphthylacetic Acid

Bond	Bond Distance-DFT	Bond Distance-(experimental)
C_1- C_2	1.375	1.359
C_2- C_3	1.418	1.418
C_3- C_4	1.430	1.406
C_4-C_5	1.419	1.418
C_5-C_6	1.374	1.359
C_3-H_3	2.163	2.157
C_1-H_1	1.081	1.073
C_2-H_2	1.082	1.073
C_3-C_{10}	1.421	1.422
C_4-C_{11}	1.419	1.421
C_5-H_5	1.079	1.073
C_6-H_6	1.078	1.073
C_{11}-H_{11}	1.081	1.071
C_{12}-H_{12}	1.080	1.071
C_{12}-O_{13}	1.513	1.470
H_{14}-O_{14}	1.463	1.427

Table 3.

Bond angles of 2-Naphthylacetic Acid

Bond	Bond Angle(o)-DFT	Bond Angle (Experimental)
C_1-C_2-C_3	119.75	119.60
C_2-C_3-C_4	117.85	117.97
C_3-C_4-C_5	118.01	118.23
C_4-C_5-C_6	119.72	119.61
H_1-C_1-C	95.35	95.29
H_1-C_1-C_2	119.02	119.09
H_1-C_1-C_3	119.35	119.38
C_2-C_3-C_{10}	121.35	121.08
C_3-C_4-C_{11}	118.10	6118.21
H_4-C_4-C_5	117.77	117.89
C_5-C_6-C_{12}	119.10	119.25
C_{13}-C_{12}-C_5	119.14	119.25
C_{13}-C_3-C_{10}	120.03	119.85
H_{11}-C_{11}-C_4	119.18	118.82
H_{12}-C_{12}-C_{10}	119.55	119.46
O_{13}-H_{13}-H_{14}	105.20	105.52

2.2. Mulliken Atomic Charge

Table 4 displays the distribution of Mulliken atomic charges for 2-Naphthylacetic Acid. Since Mulliken charges are sensitive to the probability density, they are obtained from the local electron density and heavily rely on the basis set and functional. Significantly, the oxygen atom has the highest negative charge of -0.426, which is more than the -0.057 atomic charge of the oxygen atom in the phenolic OH group. With the exception of C3 and C4, which are involved in the benzene ring fusion, all carbon atoms are negatively charged. It's interesting to note that in the 6-311++G(d,2p) basis set, the net positive charge of all hydrogen atoms is between 0.136 and 0.208, with H11 showing a higher value of almost 0.249.

Table 4.

The calculated Mulliken atomic charge distribution of 2-Naphthylacetic Acid

ATOM	Atomic charge-DFT
C_1	-0.219
C_2	-0.629
C_3	0.727
C_4	0.167
C_5	-0.129
C_6	-0.079
H_7	0.090
C_8	-0.227
C_9	-0.150
C_{10}	0.139
C_{11}	0.230
C_{12}	-0.269
H_{14}	0.141
H_{15}	0.187
H_{16}	0.187
O_{13}	-0.320
O_{14}	-0.341

There were notable variations in the distribution of charges, according to the Mulliken charge study. The oxygen atom had the largest negative charge (-0.426 e), highlighting its potent electronegative properties. Because of their involvement in benzene ring fusion, carbon atoms C3 and C4 showed a slightly positive charge distribution. The hydrogen atoms' positive charges, which ranged from 0.136 to 0.208 e, added to the molecule's overall stability.

2.3. Vibrational Analysis

Vibrational analysis is an effective approach for learning about the structure of molecules. The theoretical and actual infrared (IR) spectra of 2-naphthylacetic acid are shown in Figures 2-3. Vibrational frequency assignments and other characteristics were found for the optimal structure in the gas phase using the molecular visualization tool Gauss View 5.0. The assignments of basic modes were examined by comparing the calculated and experimental results. Two variables account for the disparities, even though the computed frequencies for the major number of modes normally trend slightly higher than the actual values. Environmental influences could be involved in the first place. Secondly, the estimated value is a harmonic oscillation, however the experimental value indicates a harmonic oscillation. The assigned vibrational bands for both theoretical and experimental values are given in Table 5. The graph between the calculated and experimental modes, as presented in Fig. 2-3, allows one to evaluate the linearity with respect to experimental and calculated frequencies for 2-Naphthylacetic Acid. The title chemical exhibits an aromatic C-H stretching vibration about 2900-3010 cm^{-1}. This observation is consistent with the calculated theoretical value of 3100-

32500 cm^{-1} in DFT and 3150-3300 in HF. Observed at 1123 cm^{-1}, the α, α' C-H bending corresponds with the theoretically estimated value (1380 cm^{-1} in DFT). In 2-Naphthylacetic Acid, the estimated O-H stretching frequency (DFT) is 4100 cm^{-1}, and the equivalent experimental value is detected at 3550 cm^{-1}. The theoretical value (1767 cm^{-1} in DFT) is linked to the experimental C=C frequency of stretching 1725cm^{-1}. Approximately 1554 cm^{-1} is the observed C-H bending vibration, which agrees with the theoretically calculated value of 1546 cm^{-1} in DFT and 1515 in HF. The theoretical value (627 cm^{-1} in DFT) and the observed C=O symmetric stretching vibration (644 cm^{-1}) are in close alignment. By using the DFT approach, the estimated asymmetric C=O stretching vibration is found at 1046 cm^{-1}; the matching experimental value is found at 1049 cm^{-1}. Using the DFT approach, the theoretical values looks at 1285 cm^{-1} and the determined O-H bending values at 1250 cm^{-1}.

2-Naphthylacetic Acid's vibrational spectra were measured experimentally and contrasted with values calculated using DFT. There was a good agreement between the aromatic C-H stretching vibration appearing at 2900-3010 cm^{-1} (experimental) and 3100-3250 cm^{-1}

Table 5.

Experimental and DFT assisted Vibrational frequencies of 2-Naphthylacetic Acid

S. N.	Assigned pattern	Vibrational frequencies (experimental) (cm^{-1})	Vibrational frequencies DFT method (cm^{-1})
1	Asymmetric C-H stretching	3110	3173
2	Symmetric C=C stretching	1622	1632
3	Symmetric C=O stretching	1238	1225
4.	C-H stretching	864	857
5.	In plane C-H bending	825	818
6	Asymmetric C-H stretching	769	778
7	Symmetric C-C stretching	684	669
8	Symmetric C=O stretching	644	635
9	Symmetric C-O stretching	569	553
10	Symmetric C=C stretching	1502	1540
12	In-plane C-H bending	1269	1286

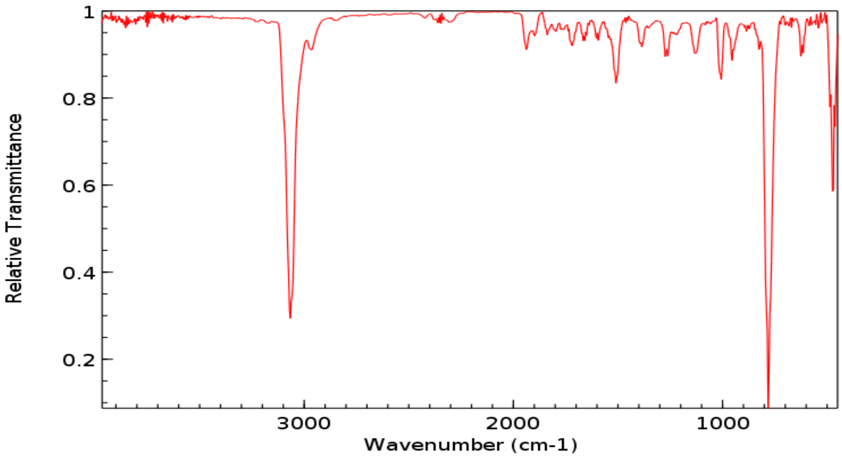

Fig. 2. Experimental FT IR Spectrum of 2-Naphthylacetic Acid.

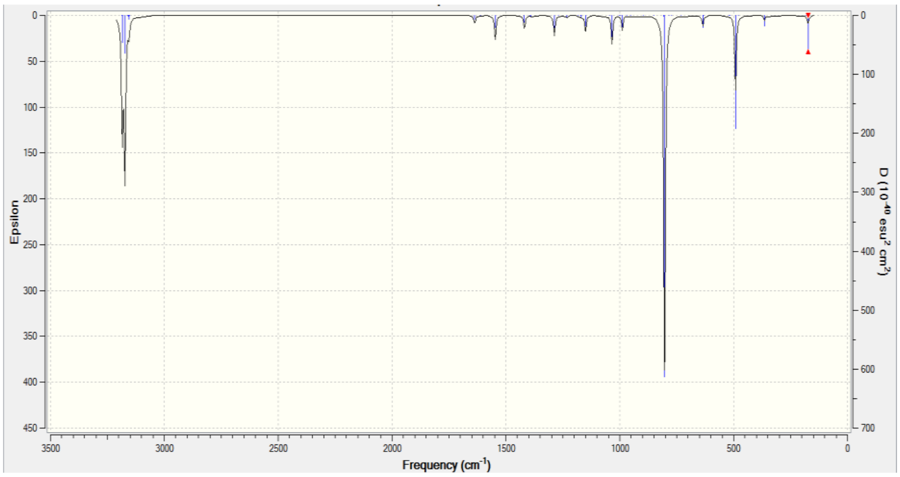

Fig. 3. FT IR Spectrum of 2-Naphthylacetic Acid by DFT method at B3LYP/6-311++G level.

(DFT). Due to hydrogen bonding effects in the experimental settings, the experimental O-H stretching frequency was determined to be 3550 cm^{-1}, while the theoretical value was 4100 cm^{-1}. At 644 cm^{-1} (experimental) and 627 cm^{-1} (DFT), the C=O symmetric stretching was seen with little variation.

2.4. Frontier Molecular Orbitals

The LUMO and HOMO also known as frontier molecular orbitals, are essential to comprehending UV-VIS spectra as well as optical and electrical characteristics. Chemical reactivity, optical polarizability, kinetic stability, and chemical hardness/softness of a molecule are all determined by the energy gap between HOMO and LUMO [13]. Using the 6-311++G(d,2p) basis set, HOMO and LUMO energies as well as the energy gap for cm^{-1} were computed at the B3LYP level. At the DFT (B3LYP)/6-31++G(d,2p) level, the HOMO-LUMO energy gap of cm^{-1} represents the molecular activity. Using the DFT approach, the energy value of the HOMO and LUMO of 2-Naphthylacetic Acid in the gaseous phase are determined to be -0.215 eV and -0.057 eV, respectively. Figure 4 shows these numbers as well as the corresponding graphic representations. The computed energy difference between HOMO and LUMO is 0.158 eV, which sheds light on potential charge transfer interactions inside the molecule that may affect its biological activity. The molecular electrostatic potential map and continuous map of 2-naphthylacetic acid are shown in Figure 5. Studying the areas where electrophiles are drawn (a sign of dominant electron distribution effects) is made easier with the help of this image. The largest positive zone is displayed in blue throughout the bulk of the MEP, indicating the optimal site for nucleophilic assault, while the maximum negative region is shown in red throughout, representing the preferred site for electrophilic attack. When examining the connection between molecular structure and physiochemical parameters, MEP diagrams are helpful [14].

To assess electronic characteristics, HOMO-LUMO analysis was done. There was an energy gap of 0.158 eV since the calculated HOMO energy was -0.215 eV and the LUMO energy was -0.057 eV. Its prospective uses in optoelectronics may be increased by a lower energy gap, which indicates good charge transfer capabilities and moderate chemical reactivity. Its moderate reactivity was supported by molecular electrostatic potential maps, which showed areas of nucleophilic (red) and electrophilic (blue) assault.

2.5. Chemical Reactivity Parameters

In the fields of chemistry and biology, Density Functional Theory (DFT) is a useful technique for calculating molecular characteristics and providing qualitative insights into a range of phenomena [15]. Ionization energy and electron affinity values are the basis

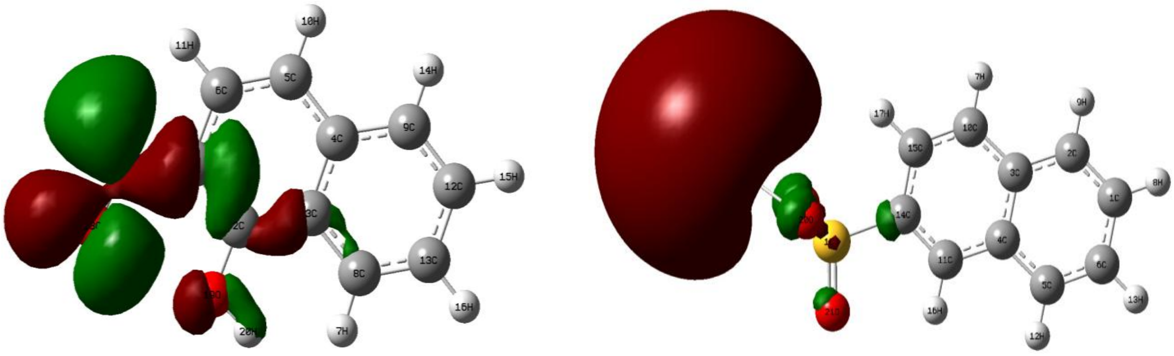
(a) (b)

Fig. 4. The HOMO and LUMO orbitals 2-Naphthylacetic Acid.

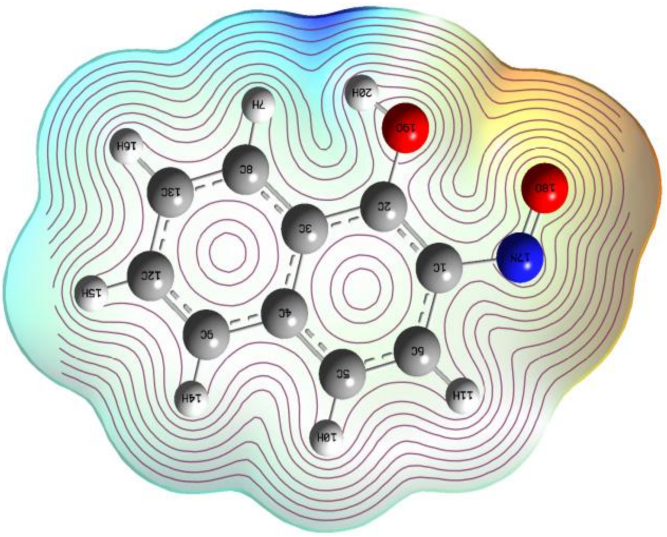
Fig. 5. The molecular electrostatic potential surface of 2-Naphthylacetic Acid.

for important chemical reactivity parameters, such as electronegativity, chemical potential, hardness, softness, and electrophilicity index. The reciprocal of hardness, or S, is a measure of a compound's reactivity [16]. As shown in the table 6, the ionization energy (IE) is written as IE = -εHOMO, while the electron affinity (EA) is written as EA = -εLUMO. Both are obtained from the HOMO and LUMO orbital energies. Chemical potential, electronegativity, and chemical hardness can all be computed using a molecule's HOMO and LUMO energy values [17]. The Gaussian 03 software was used for all calculations [18]. Working equations for group electronegativity, group hardness, softness, and other related properties can be obtained from the above formulae. Table 6 shows the final results for the named compounds' ionization potential, electronegativity, hardness, softness, and electrophilicity index [19, 20]. A more reactive nucleophile is indicated by a lower value of the electrophilicity index in Table 6, while a higher ω value indicates a good reactive electrophile. Utilizing the DFT/B3LYP/6-311G (d, 2p) level, the global reactivity descriptors ionization energy, electron affinity, chemical hardness, chemical softness, chemical power, and electrophilicity index were examined in order to get knowledge about the reactivity and stability of the molecule. The aforementioned compounds showed a linear comparison between their electrophilicity and electron affinity with substituted naphthalene showing lower softness values.

Table 6.

HOMO and LUMO energy gaps and their Comparison by DFT methods

S. N.	Properties	2-Naphthylacetic Acid
1	HOMO Energy(eV)	-0.215
2	LUMO Energy (ev)	-0.057
3	Energy Gap between HOMO-LUMO	-0.158
4.	Complete Hardness	0.177
5.	Ionization power	0.215
6	Electron Affinity	0.057
7	Electronegativity (I+EA)/2	0.528
8	Chemical potential	-0.528
9	Total Softness	-3.428
10	Total Electrophilicity	0.054

To ascertain the stability of the molecule, the chemical reactivity indices were calculated. Moderate electron-donating capacity is shown by the ionization energy of 0.215 eV. Limited electron-accepting nature is supported by an electron affinity of 0.057 eV. A balanced reactivity is suggested by the electronegativity of 0.528 eV. Its moderate nucleophilicity is confirmed by its electrophilicity index of 0.054 eV.

The frontier molecular orbitals, particularly the Highest Occupied Molecular Orbital (HOMO) and the Lowest Unoccupied Molecular Orbital (LUMO), play a crucial role in determining the electronic properties of molecules. The HOMO-LUMO energy gap, in particular, is indicative of a molecule's chemical reactivity, stability, and electronic transitions. The Density Functional Theory (DFT) calculations provide insightful parameters related to these properties for 2-Naphthylacetic Acid.

HOMO-LUMO Energy Gap and Reactivity

2-Naphthylacetic Acid has an energy gap of -0.158 eV since its HOMO energy is determined to be -0.215 eV and its LUMO energy to be -0.057 eV. In general, a narrower HOMO-LUMO gap indicates more polarizability, decreased kinetic stability, and higher chemical reactivity. A wider gap, on the other hand, indicates a molecule that is less reactive and more stable. 2-Naphthylacetic Acid is a promising option for optoelectronic or catalytic applications due to its intermediate stability and tendency for electronic transitions, as evidenced by the comparatively tiny gap seen here.

Chemical Hardness and Softness

The inverse characteristics of chemical hardness (0.177 eV) and overall softness (-3.428 eV) indicate how resistant a molecule is to variations in its electron distribution. The moderate hardness score indicates that 2-Naphthylacetic Acid has a balanced electrical nature that makes it appropriate for a range of chemical processes. It is neither too soft (prone to quick electron exchange) nor too hard (resistant to charge transfer).

Ionization Power and Electron Affinity

The electron affinity (0.057 eV) and ionization power (0.215 eV) demonstrate the molecule's propensity to gain or lose electrons. A reduced ionization power supports the molecule's moderate reactivity by indicating that it takes comparatively less energy to donate an electron. Its mild electrophilic nature is further supported by the electron affinity value, which indicates a limited propensity to receive electrons.

Electronegativity and Chemical Potential

The molecule's capacity to draw electrons to itself is shown by its electronegativity, which is 0.528 eV and is computed as (I+EA)/2. The stability of the molecule in an electronic environment is shown by the chemical potential (-0.528 eV), which is same in magnitude but opposite in sign. The entire chemical behavior of 2-Naphthylacetic Acid is influenced by its mild electron-withdrawing tendency, which is confirmed by these parameters.

Electrophilicity Index and Potential Applications

The molecule has a modest propensity to act as an electrophile, according to its total electrophilicity index of 0.054 eV. According to this characteristic, 2-Naphthylacetic Acid is more likely to behave in chemical reactions as a moderate nucleophile than a potent electrophile. Designing molecular systems for chemical synthesis, medicinal development, and electronic materials may benefit from such properties.

Conclusions

This work uses the 6-311++G(d,2p) basis set and DFT/B3LYP levels to investigate the optimal structures and properties of 2-Naphthylacetic Acid. Vibrational analysis of 2-Naphthylacetic acid was carried out using DFT-B3LYP methods using basis sets 6-311++G(d,2p). The effects of substituting –OH, CHO, and C=O with the ring were analyzed, and the oscillational frequencies of

2-Naphthylacetic acid with the given names were spoken about. In the DFT B3LYP/6-311++G(d,2p) technique, there was a good frequency match between the simulated and observed spectra. Minimal standard deviation was used to verify that theoretical and experimental wave numbers agreed, and qualitative agreement was noted between calculated and observed frequencies as well as different parameters like bond lengths, bond angles, and dihedral angles that were evaluated using both DFT and HF methods. To identify variations in the reactivity of the compound, energy characteristics such as the ionization energy (I), softness (S), electrophilicity (ω), and frontier orbital gap (ΔE) were calculated. All three compounds' energy separation between their HOMO and LUMO revealed details about the internal charge transfer interactions that affect the molecules' biological activity. The bioactivity of the molecule is supported by the decrease in the HOMO and LUMO energy gap. The idea of chemical reactivity was successfully applied to the reactivity indices determined using the DFT approach.

Mir M. Amin – Ph.D.;
Mahmoud Maythem – Ph.D.;
Andrews Kim – Ph.D.;
Nayak Arunima – Ph.D.;
Kukretee Nupur – Ph.D.;
Kotnala Shreya – Ph.D.

[1] M. Borsenberger and D. S. Wiss, Organic Photoreceptor for Imaging Systems (Marcel Dekker, New York, 1993).
[2] J. Roncali, P. Leriche, and P. Blanchard, *Molecular Materials for Organic Photovoltaics: Small is Beautiful*, Adv. Mater., 26(23), 3821 (2014); https://doi.org/10.1002/adma.201305999.
[3] M. Amin Mir et.al. *The Molecular Structural Analysis of Biologically Important Catechol Molecule: An Integrative Perspective from Experiments and Futuristic Tools*. Current Organo-catalysis, 12, 17 (2023).
[4] Bernard Marciniak, Sylwester Kania, Ewa Różycka-Sokołowska, Janusz Kuliński *Electronic properties of chosen naphthalene derivatives*. Molecular Crystals and Liquid Crystals, 743(1), 103 (2022); https://doi.org/10.1080/15421406.2022.2055254.
[5] K. Yoshizawa, *An orbital rule for electron transport in molecules*. Acc. Chem. Res., 45(9), 1612 (2012); https://doi.org/10.1021/ar300075f.
[6] I.A. Fedorov, Y.N. Zhuravlev, and V.P. Berveno, *Electronic structure and chemical bond in naphthalene and anthracene.* Phys. Chem. Chem. Phys., 13(13), 5679 (2011); https://doi.org/10.1039/C0CP02200D.
[7] M.A. Mir, *DFT, Hirshfeld Surface, Molecular Docking and Drug Likeness Studies of Medicinally Important Coumarin Molecule*. Arab J Sci Eng, 48, 7445 (2023); https://doi.org/10.1007/s13369-022-07476-z.
[8] D.H. Spielberg, A.I. Korn, and A.C. Damask, *Experimental and Theoretical Hall Mobilities of Holes and Electrons in Naphthalene*. Phys. Rev. B, 3(6), 2012 (1971); https://doi.org/10.1103/PhysRevB.3.2012.
[9] M. Amin Mir, *Molecular dynamic, Hirshfeld surface, molecular docking and drug likeness studies of a potent anti-oxidant, anti-malaria and anti-Inflammatory medicine: Pyrogallol"*. Results in Chemistry, 5, 100763 (2023); https://doi.org/10.1016/j.rechem.2023.100763.
[10] Zhi-Jun Zhang, Susan L Morris-Natschke, Yung-Yi Cheng. *Development of anti-influenza agents from natural products*. Med Res Rev., 40(6), 2290 (2020). https://doi.org/10.1002/med.21707.
[11] Minghua Chen, Sheng Lin, Li Li, Chenggen Zhu, Xiaoliang Wang, Yanan Wang, Bingya Jiang, Sujuan Wang, Yuhuan Li, Jiandong Jiang, Jiangong Shi. *Enantiomers of an indole alkaloid containing unusual dihydrothiopyran and 1,2,4-thiadiazole rings from the root of Isatis indigotica*. Org Lett., 14(22), 5668 (2012); https://doi.org/10.1021/ol302660t.
[12] N.R. Gonewar, V.B. Jadhav K.D. Jadhav, and R.G. Sarawadekar. *Theoretical calculations of infrared, NMR and electronic spectra of 2-nitroso-1, naphthol or 1-2 naphthoquinine-2 oxime and comparison with experimental data*. Research in Pharmacy 2(1), 18 (2012).
[13] C. Lee, W. Yang, R.G. Parr, Development of the Colle-Salvetti correlation-energy formula into a functional of the electron density. Phys. Rev. BB7, 785 (1998); https://doi.org/10.1103/physrevb.37.785.
[14] M. Senyel, O. Alver, C. Parlak, *NMR determination of solvent dependent behavior and XRD structural properties of 4-carboxy phenylboronic acid: A DFT supported study*. Spectrochim. Acta A., 71, 830. (2008).
[15] A. Suvitha, S. Periandy, S. Boomadevi, M. Govindaraja. *Vibrational frequency analysis, FT-IR, FT-Raman, ab initio, HF and DFT studies, NBO, HOMO–LUMO and electronic structure calculations on pycolinaldehyde oxime.* Spectrochimica Acta Part A: Molecular and Biomolecular spectroscopy, 117, 216 (2014); https://doi.org/10.1016/j.saa.2013.07.080.
[16] P. Geerlings, F. De Proft, W. Langenaeker, *Conceptual density functional theory*. W. chem Rev, 103, 1793 (2003); https://doi.org/10.1021/cr990029p.
[17] S. Renuga, M. Karthikesan, S. Muthu, *FTIR and Raman spectra, electronic spectra and normal coordinate analysis of N, N-dimethyl-3-phenyl-3-pyridin-2-yl-propan-1-amine by DFT method*. Spectrochim Acta Part A, 127, 439 (2014); https://doi.org/10.1016/j.saa.2014.02.068.
[18] M. Amin Mir. Biogenic Amines: Catalysis, Quality, and Safety Aspects of Food Items Consumed in Saudi Arabia. Current Organocatalysis, 11 (4), 310 (2024); https://doi.org/10.2174/0122133372285097240220062811.
[19] P.K. Chattaraj, and S. Giri, Stability, *Reactivity, and Aromaticity of Compounds of a Multivalent Super Atom*. Journal of Physical Chemistry A, 111, 11116 (2007); https://doi.org/10.1021/jp0760758.
[20] J. Padmanabhan, R. Parthasarathi, V. Subramanian, and P. Chattaraj, *Electrophilicity-Based Charge-Transfer Descriptor*. The Journal of Physical Chemistry, 111, 1358 (2007); https://doi.org/10.1021/jp0649549.

Мохд Амін Мір[1], Мейтем Махмуд[2], Кім Ендрюс[2], Аруніма Наяк[3], Нупур Кукреті[3],
Шрея Котнала[4]

Експериментальні, спектроскопічні, обчислювальні та молекулярні дослідження стимулятора росту рослин на основі 2-нафтилоцтової кислоти

[1]*Факультет машинобудування, Університет принца Мохаммада Бін Фахда,*
Аль-Хобар, Саудівська Аравія, mohdaminmir@gmail.com;
[2]*Департамент математики та природничих наук, Університет принца Мохаммада Бін Фахда,*
Аль-Хобар, Саудівська Аравія;
[3]*Хімічний факультет, університет Графічної ери, Дехрадун, Індія;*
[4]*Хімічний факультет, Школа фундаментальних і прикладних наук, Університет Шрі Гуру Рам Рай, Дехрадун, Індія*

Предметом теоретичних експериментів з використанням методів DFT-B3LYP з базисними наборами 6-311++G(d,2p) є біоактивна сполука 2-нафтилоцтова кислота. Розрахунковий аналіз включає розрахунок геометричних параметрів, молекулярних характеристик і коливальних спектрів 2-нафтилоцтової кислоти. Теорію функціоналу густини використано для проведення оптимізації геометрії. Розраховані вібраційні спектри та оптимізована молекулярна геометрія при зіставлені з експериментальними результатами вказали на значний збіг. Крім того, для вищезгаданої сполуки розраховано такі характеристики DFT, як хімічна твердість, повна енергія, хімічний потенціал і електрофільність. Відносна стабільність і реакційна здатність досліджуваних сполук передбачено за допомогою цих дескрипторів.

Ключові слова: 2-нафтилоцтова кислота, DFT-B3LYP, розрахункові дослідження, DFT, стабільність.