

CHEMISTRY & BIOLOGY INTERFACE

An official Journal of ISCB, Journal homepage; www.cbijournal.com

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

Vishnu A. Adole^{a,*}, Ravindra H. Waghchaure^{a,c}, Bapu S. Jagdale^{a,b}, Thansing B. Pawar^a

^aDepartment of Chemistry, Loknete Vyankatrao Hiray Arts, Science and Commerce College Panchavati, (Affiliated to SP Pune University, Pune) Nashik-422 003, India

^bDepartment of Chemistry, Arts, Science and Commerce College, (Affiliated to SP Pune University, Pune) Manmad -423 104, India

^cDepartment of Chemistry, Arts, Commerce and Science College, (Affiliated to SP Pune University, Pune) Karanjali -422 208, India

Corresponding author: vishnuadole86@gmail.com

ORCID ID: <https://orcid.org/0000-0001-7691-7884>

Received 13 June 2019, Accepted 12 January 2020

Abstract: Dihydropyrimidinone is one of the most noteworthy organic structures because of its huge scope of biological properties. Several derivatives of pyrimidine have been used as medicinal agents such as sedatives and hypnotics. In this work, a biologically important ethyl 4-(4-isopropylphenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate (IPPC) was synthesized; the structure of the compound was confirmed by using Fourier-transform infrared spectroscopy (FTIR), Proton nuclear magnetic resonance (¹H NMR), Carbon nuclear magnetic resonance (¹³C NMR), Distortionless Enhancement by Polarization Transfer (DEPT), and High-resolution mass spectrometry (HRMS) techniques. For an in-depth molecular structure description some quantum-chemical calculations have been accomplished by using density functional theory method with a basis set 6-311++G(d,p). The vibrational absorption bands were calculated and the scaled values are compared with the experimental FT-IR spectrum. Various structural and quantum chemical parameters have been computed and discussed for a better understanding of the electronic and chemical behaviour of IPPC. Furthermore, the molecular electrostatic potential (MEP) and some thermodynamic functions were also explored using theoretical calculations.

Keywords: DFT, 6-311++G(d,p), HOMO-LUMO, Molecular electrostatic potential, ethyl 4-(4-isopropylphenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate

Introduction

Dihydropyrimidinones (DHPM's) are crucial compounds with a wide variety of reported biological activities. An excellent biological profile of DHPM's includes properties like cancer treatment [1-3], Calcium channel inhibition [4, 5] antioxidant [6, 7], antiviral [8], antifungal [9], antibacterial [10-12], antidiabetic [13], antiulcer [14], and anti-inflammatory activity [15]. Importantly, the building blocks of nucleic acids (**Fig 1**); thymine (**1**), cytosine (**2**) and uracil (**3**) are pyrimidine containing scaffolds. Other vital molecules that contain pyrimidine nucleus are riboflavin (**4**), thiamine (**5**) and folic acid (**6**).

The quantum calculations derived from Density Functional Theory (DFT) have found to be influential in various branches of modern science [16-18]. Indeed various quantum chemical parameters can be investigated

using spectroscopic and quantum chemical calculations based on DFT. DFT calculations can be performed to study various vibrational bands and thus exact vibrational assignments can be easily carried out for experimental data. Importantly information about electron and chemical bonding in a molecule can easily be explored based on the DFT experiments. The fields like organic synthesis, catalysis, photoelectronic and solution chemistry can be studied on atomic and molecular levels by using DFT models [19-22]. The DFT/B3LYP method has been employed in the past for the computation of various structural and spectroscopic properties [23]. In continuation of our past work and by considering these crucial perspectives, a fruitful endeavour has been made to research basic parameters like total energy, electron density in highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO), charge density, absolute electronegativity (χ), softness (σ),

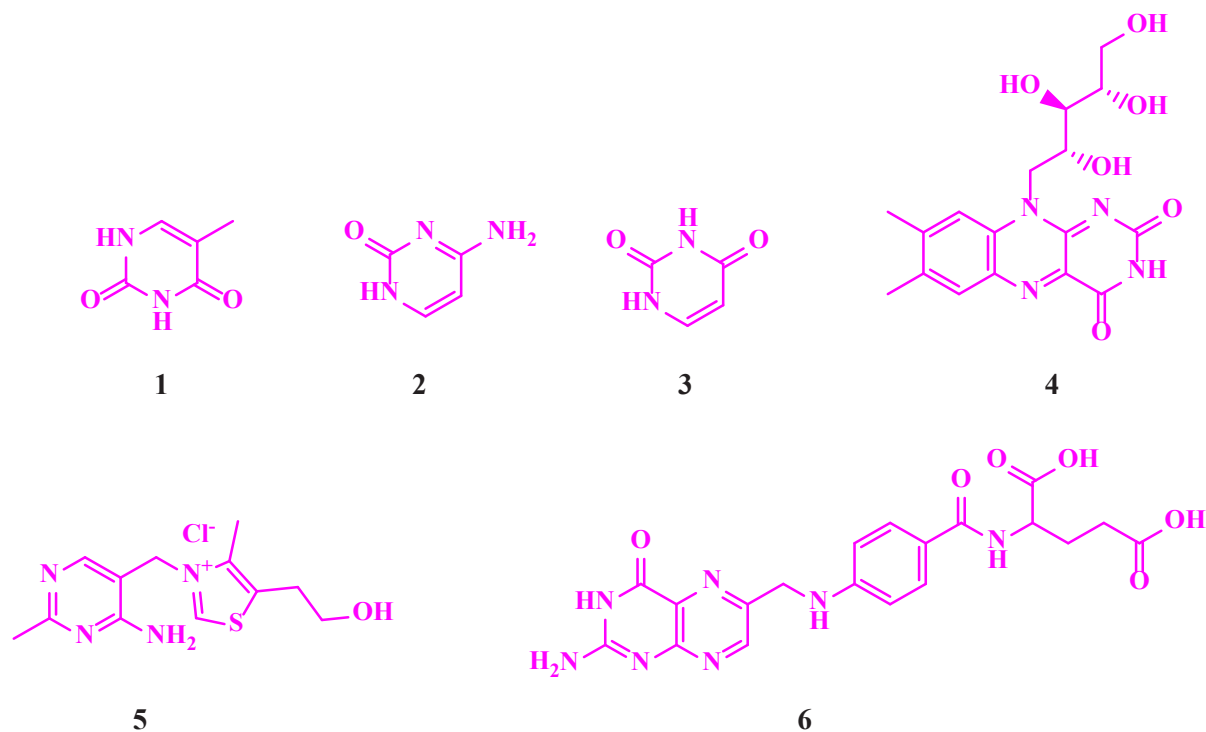


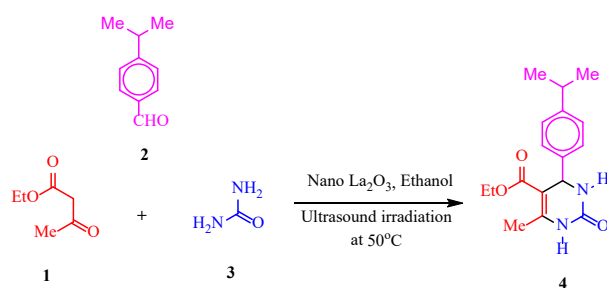
Figure 1 Some important compounds containing pyrimidine moiety

hardness (η) and electron transferred (ΔN) of the title molecule. To the best of our understanding, this is the first report on the DFT investigation of the title molecule. The point of this work was to show the theoretical examination of the IPPC. Moreover, the quantum-chemical estimations were utilized for a superior comprehension of the different properties.

MATERIALS AND METHODS

The chemicals with high purity were purchased from a local supplier (*Make: Avra synthesis and SD fine chemicals*). The chemicals were used as received without any further purification. The melting point was determined in open capillary and uncorrected. ^1H NMR and ^{13}C NMR spectra were recorded with a Bruker using CDCl_3 as a solvent, FT-IR spectra were obtained with potassium bromide pellets and HRMS were recorded on Bruker with ESI as a source. The reaction was monitored by thin-layer chromatography using aluminium sheets with silica gel 60 F254 (Merck). The physicochemical data is presented in **Table 1**.

Experimental procedure for the synthesis of ethyl 4-(4-isopropylphenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate (IPPC): Previously reported method has been employed for the synthesis of the title compound IPPC (**Scheme 1**) [24].



Scheme1 Synthesis of IPPC

Table 1 Physicochemical data of synthesized title molecule IPPC^a

Entry	Time (min)	Yield (%) ^b	M.P. (°C)
1	45	94	144

[a] Reaction conditions: 1 (0.01 mmol), 2 (0.01 mmol), 3 (0.01 mmol) under ultrasound irradiation at 50 °C

[b] Isolated yield of pure product

Spectral data of IPPC - M. F.: $\text{C}_{17}\text{H}_{22}\text{N}_2\text{O}_3$; Pale yellow crystals; m.p. 176 °C; **FT-IR** (cm^{-1}) - 3224.98, 3101.54, 2939.52, 1712.79, 1651.07, 1589.34, 1234.44, 786.96; **^1H NMR** (400MHz, DMSO-d_6); δ (ppm) - 1.17 (t, 3H) 1.22 (d, 3H), 2.32 (s, 3H), 2.87 (sept, 1H), 4.08 (q, 2H), 5.37 (d, 1H), 5.90 (s, 1H), 7.15 (d, 2H), 7.23 (d, 2H), 8.54 (s, 1H); **^{13}C NMR** (100 MHz, DMSO-d_6); δ (ppm) -14, 17, 24, 34, 55, 60, 101, 126, 127, 141, 146, 149, 154, 166; **HRMS**- (m/z): $[\text{M}+\text{H}]$ – *Calculated*: 303.1708, *Observed*: 303.1704.

Computational details

DFT calculations were performed on an Intel (R) Core (TM) i5 computer using Gaussian-03(W) program package without any constraint on the geometry [25]. The geometry of the title compound was optimized by DFT/B3LYP method using the 6-311++G(d,p) basis set. Vibrational bands were calculated at the same level of theory for the optimized structure and the obtained frequencies were scaled by an empirical factor 0.96 [16]. Vibrational band assignments were made using the Gauss View 4.1 molecular visualization program. To investigate the reactive sites of the title compound, the molecular electrostatic potential (MEP) was computed using the same method. All the calculations were carried out for the optimized structure in the gas phase.

Results and discussion

Spectral analysis of IPPC

The synthesized compound IPPC was characterized by FT-IR, ^1H NMR, ^{13}C NMR, and HRMS methods. The spectral investigation confirms the structure of the compound. In FT-IR spectrum (Fig. 9), the important bands (in cm^{-1}) are 3224.98 (N-H), 3101.54 (sp^2 C-H), 2939.52 (sp^3 C-H), 1712.79 (C=O, ester), 1651.07 (C=O, amide), 1589.34 (C=C), 1234.44 (C-O), 786.96 (Ar bending). There are ten types of protons present in IPPC as predicted by the ^1H NMR spectrum. It confirms the *p*-disubstituted pattern for aromatic ring which shows the ortho coupling of aromatic protons. The two NH protons displayed singlets at 5.90 and 8.54 ppm. The presence of vicinal coupling in the ethyl and isopropyl group has been confirmed from the ^1H NMR spectrum. The ^{13}C NMR spectrum confirms the presence of protonated and non-protonated carbon signals. The chemical shift value 166 and 154 ppm indicates carbonyl functional groups of amide and ester respectively. The high-resolution mass spectrum is depicted in which indicates the exact molecular weight and a molecular formula of a compound. The experimental value of $[\text{M}+\text{H}]^+$ peak is 303.1708 which is in correct agreement with the theoretical value (303.1704).

Molecular geometry

The optimized molecular structure is shown in Figure 2. The structural parameters like bond lengths and bond angles for the title molecule have been established by the DFT/B3LYP method with the 6-311++G (d, p) as basis set and are presented in Table 2. The title molecule IPPC consists of two six-membered rings. The DFT calculation predicts the benzene ring is planar (as expected) while another ring is non-planar. The molecule IPPC is an asymmetric top molecule and possesses the C1 point group symmetry. The self-consistent field (SCF) energy of the title molecule at the DFT/B3LYP method with the 6-311++ G (d, p) as basis set is found to be - 996.5631 a.u. with dipole

moment 3.9470 Debye. Amongst aromatic ring carbon-carbon double bond lengths, C5-C6 has the highest bond length (1.4013 Å) and C4-C5 has the lowest (1.391 Å). The olefinic carbon-carbon (C11-C13) bond length is 1.36 Å. Both the carbonyl groups are having nearly same bond length as predicted by this method. The C-N bond length for C12-N31 and C12-N33 are 1.4021 and 1.3587 Å respectively. The C35-C37 bond has the highest bond length which is 1.5397 Å.

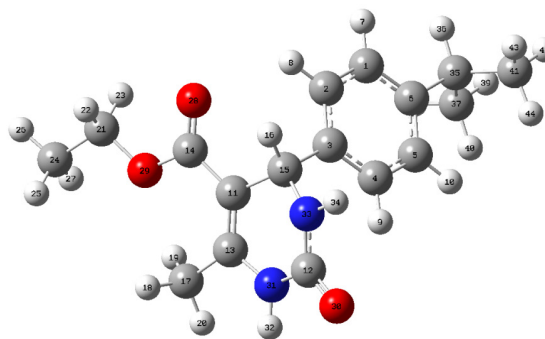


Figure 2 Theoretical optimized geometric structure (front view) of IPPC by DFT/B3LYP method 6-311++G(d,p) basis set

Table 2 Optimized geometrical parameters of IPPC by DFT/ B3LYP with 6-311++G(d,p) basis set

Bond lengths (Å)					
C1-C2	1.3946	C12-O30	1.2192	C21-C29	1.4486
C1-C6	1.3968	C12-N31	1.4021	C24-H25	1.0926
C1-H7	1.0858	C12-N33	1.3587	C24-H26	1.0933
C2-C3	1.3956	C13-C17	1.5067	C24-H27	1.0925
C2-H8	1.0841	C13-N31	1.3855	N31-H32	1.0088
C3-C4	1.3999	C14-O28	1.217	N33-H34	1.0099
C3-C15	1.5316	C14-O29	1.357	C35-H36	1.096
C4-C5	1.391	C15-H16	1.0908	C35-C37	1.5397
C4-H9	1.0843	C15-N33	1.4685	C35-C41	1.5394
C5-C6	1.4013	C17-H18	1.091	C37-H38	1.093
C5-H10	1.0849	C17-H19	1.0889	C37-H39	1.0942
C6-C35	1.5217	C17-H20	1.0922	C37-H40	1.0941
C11-C13	1.36	C21-H22	1.0924	C41-H42	1.0942
C11-C14	1.4677	C21-H23	1.0921	C41-H43	1.093
C11-C15	1.5265	C21-C24	1.5154	C41-H44	1.0941
Bond angles (°)					

C2-C1-C6	121.4038	C11-C14-O28	123.1842	C14-O29-C21	115.95
C2-C1-H7	119.2173	C11-C14-O29	114.9048	C12-N31-C13	125.0634
C6-C1-H7	119.3788	O28-C14-O29	121.9099	C12-N31-H32	113.4764
C1-C2-C3	120.7088	C3-C15-C11	112.7192	C13-N31-H32	119.4596
C1-C2-H8	119.8765	C3-C15-H16	107.3223	C12-N33-C15	124.9098
C3-C2-H8	119.4054	C3-C15-N33	112.6082	C12-N33-H34	113.8699
C2-C3-C4	118.2258	C11-C15-H16	107.2855	C15-N33-H34	117.5969
C2-C3-C15	119.9585	C11-C15-N33	109.4152	C6-C35-H36	106.7385
C4-C3-C15	121.815	H16-C15-N33	107.1779	C6-C35-C37	111.8988
C3-C4-C5	120.8338	C13-C17-H18	110.8478	C6-C35-C41	112.0029
C3-C4-H9	120.2046	C13-C17-H19	111.1477	H36-C35-C37	107.3691
C5-C4-H9	118.958	C13-C17-H20	110.4247	H36-C35-C41	107.4149
C4-C5-C6	121.2334	H18-C17-H19	106.9561	C37-C35-C41	111.1025
C4-C5-H10	118.8523	H18-C17-H20	108.4699	C35-C37-H38	111.1702
C6-C5-C10	119.9135	H19-C17-H20	108.8838	C35-C37-H39	110.5931
C1-C6-C5	117.5941	H22-C21-H23	107.6765	C35-C37-H40	111.3083
C1-C6-C35	120.7739	H22-C21-C24	111.9835	H38-C37-H39	108.1702
C5-C6-C35	121.6318	H22-C21-O29	108.7179	H38-C37-H40	107.7849
C13-C11-C14	126.0596	H23-C21-C24	111.9825	H39-C37-H40	107.6695
C13-C11-C15	119.8151	H23-C21-O29	108.692	C35-C41-H42	110.5965
C14-C11-C15	114.1143	C24-C21-O29	107.7039	C35-C41-H43	111.2018
O30-C12-N31	120.9161	C21-C24-H25	111.2366	C35-C41-H44	111.3314
O30-C12-N33	125.3167	C21-C24-H26	109.541	H42-C41-H43	108.1435
N3-C12-N33	113.7416	C21-C24-H27	111.1489	H42-C41-H44	107.6642
C11-C13-C17	127.4268	H25-C24-H26	108.1286	H43-C41-H44	107.7556
C11-C13-N31	118.7247	H25-C24-H27	108.5422	-	-
C17-C13-N31	113.8478	H26-C24-H27	108.1426	-	-

Mulliken atomic charges

Mulliken atomic charges are based on the electron density. The Mulliken atomic charges of the title molecule are calculated by DFT/B3LYP method with a 6-311++G(d,p) basis set in the gaseous phase are given in **Table 3**. Mulliken atomic charges reveal that all the hydrogen atoms have a net positive charge but H32 atom has the highest positive charge (0.342696) than other hydrogen atoms. This can be ascribed to the hyperconjugation (σ -conjugation) effect. The C3 atom has the highest net positive charge (1.088443).

Table 3 Mullikan atomic charges

Atom	Charge	Atom	Charge
1 C	-0.722841	23 H	0.181037
2 C	-0.506338	24 C	-0.614947
3 C	1.088443	25 H	0.148507
4 C	-0.275032	26 H	0.151269
5 C	-0.643042	27 H	0.153458
6 C	0.647103	28 O	-0.257541
7 H	0.152600	29 O	-0.113188
8 H	0.202248	30 O	-0.320497
9 H	0.186746	31 N	-0.217081
10 H	0.169039	32 H	0.342696
11 C	0.035746	33 N	-0.261307
12 C	0.130577	34 H	0.335449
13 C	0.189553	35 C	0.084751
14 C	-0.369359	36 H	0.180907
15 C	0.283984	37 C	-0.676522
16 H	0.280702	38 H	0.140144
17 C	-0.969110	39 H	0.146833
18 H	0.211975	40 H	0.150979
19 H	0.208422	41 C	-0.675687
20 H	0.103530	42 H	0.146719
21 C	0.087127	43 H	0.140998
22 H	0.191560	44 H	0.149391

Global reactivity descriptors

The **Table 4** represents electronic parameters of title molecule. The Frontier orbitals (**Fig 3**), HOMO and LUMO are very essential to assess the reactivity/stability of molecules further E_{HOMO} and E_{LUMO} are linked with electron-donating and electron-accepting potentials respectively. Amongst the orbitals that contain electrons, the HOMO is the highest in energy, and of the orbitals that don't, the LUMO is the

lowest in energy. This implies they are closest in energy out of all orbitals in the molecule. The smaller is the energy gap between HOMO and LUMO, greater is the stability of a molecule. The lower HOMO-LUMO energy gap (0.18343 a.u.) demonstrates the inevitable charge transfer interactions taking place within the molecule.

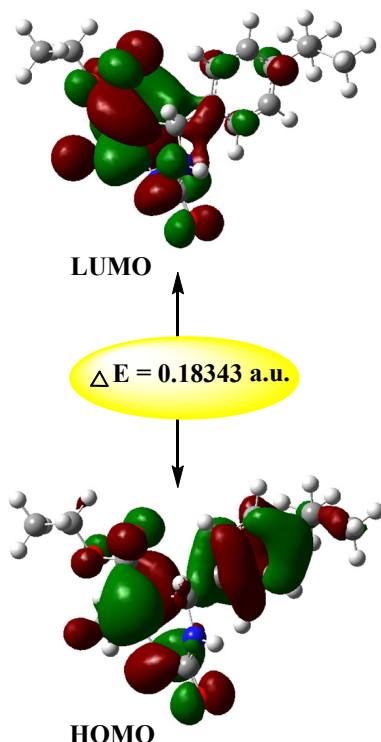


Figure 3 The HOMO and LUMO plots of the title compound by DFT/B3LYP method with 6-311++ G (d, p) basis set.

All Global reactivity descriptors are depicted in **Table 5**. The donor-acceptor behavior of synthetic framework can be successfully foreseen with the guide of absolute hardness and global softness parameters. These two parameters correspond to the gap between the HOMO and LUMO energies and related to the stability of the chemical structure. The ionization capacity of an electron is determined by its chemical potential value and it is furthermore associated with its χ . The nucleophilic and electrophilic ability is governed by the value of the electrophilicity index. Our outcome shows

that the title molecule IPPC has a higher value of electrophilicity index and thus it is a good electrophile. The donor and accepted electron charge can be processed by the greatest measure of electronic charge.

Table 4 Electronic parameters of title molecule

E_{Total} (a.u.)	E_{HOMO} (eV)	E_{LUMO} (eV)	ΔE (eV)	I (eV)	A (eV)
-996.5631	-6.8289	-1.4375	-4.99	6.8289	1.4375

Note: Abbreviations: I, ionization potential; A, electron affinity

Table 5 Global descriptors of title molecule

χ (eV)	η (eV)	σ (eV ⁻¹)	ω (eV)	Pi (eV)	ΔN_{max} (eV)	Dipole moment (Debye)
4.1332	2.6957	0.3710	3.1686	-4.1332	1.5332	3.9470

Note: $\chi = (I + A)/2$; $I = -E_{\text{HOMO}}$ & $A = -E_{\text{LUMO}}$; $\eta = (I - A)/2$; $\sigma = 1/\eta$; $\omega = \text{Pi}^2/2\eta$; $\text{Pi} = -\chi$; $\Delta N_{\text{max}} = -\text{Pi}/\eta$. Abbreviations: χ , electronegativity; η , absolute hardness; σ , global softness; ω , global electrophilicity; Pi, chemical potential; ΔN_{max} , maximum no. of electron transferred

Vibrational assignments

The title molecule IPPC has 44 atoms and therefore has 126 fundamental modes of vibration as per $3N-6$ formula. The theoretical IR spectrum is depicted in **Fig 4**. The vibrational frequencies are calculated for IPPC at B3LYP level using basis set 6-311++G (d,p) have been represented in the **Table 5**. IPPC contains two carbonyl groups, olefinic C=C, N-H, C-O bond, etc. The various modes of vibrations are given in **Table 6**. In experimental FT-IR spectrum (**Fig 5**), the important IR absorption signals (in cm⁻¹) are 3224.98, 3101.54, 2939.52, 1712.79, 1651.07, 1589.34, 1234.44 and 786.96. The first two absorption bands are due to N-H and C-H stretching vibrations respectively. The

stretching frequency at 1712.79 and 1651.07 are due to ester and amide carbonyl group stretching vibrations. The stretching vibrations 1589.34 is ascribed to the C=C stretching. The IR signal at 1234.44 cm^{-1} suggests C-O stretching. The present study indicates there is good correlation between computed and experimental IR vibrations.

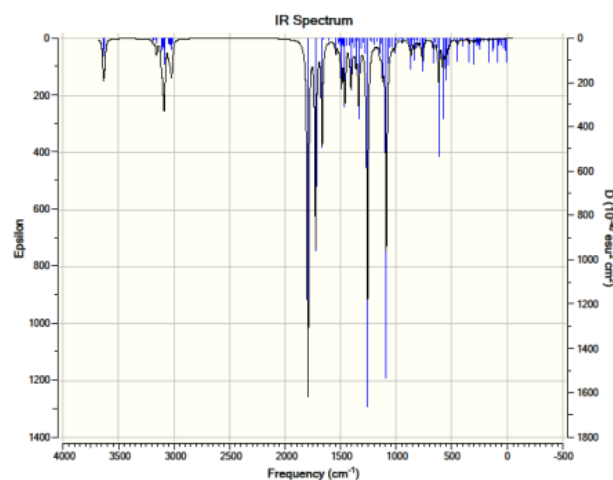


Figure 4 Theoretical IR spectrum of IPPC by DFT/B3LYP method with the 6-311++G(d,p) as a basis set

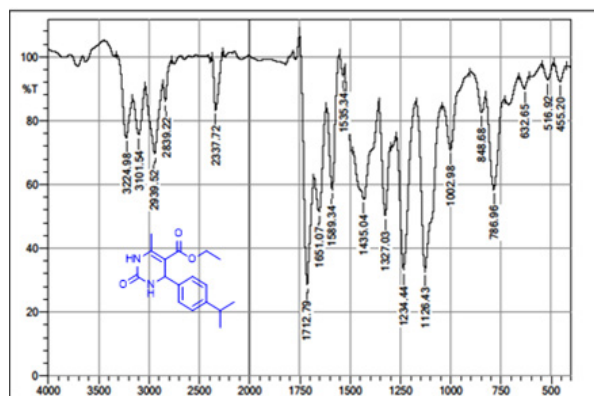


Figure 5 Experimental FT-IR spectrum of the title compound obtained on Shimadzu - FTIR

Table 5 Selected experimental and theoretical vibrational assignments calculated at 6-311++G(d,p) level

Mode	Computed scaled frequencies (cm^{-1})	IR Intensity ($\text{km} \text{ mol}^{-1}$)	Observed frequencies (cm^{-1})	Assignments
126	3382	72.41	-	ν N31-H
125	3239	43.39	3224.98	ν N33-H
124	3064	2.23	3101.54	ν C2-H
123	3058	6.31	-	ν C4-H
119	2989	38.92	-	ν asym C21H ₂
110	2930	16	2939.52	ν sym C21-H ₂
104	1722	722.74	1712.79	ν C=O (ester)
103	1655	414.36	1651.07	ν C=O (amide)
102	1599	205.36	1589.34	ν C=C
99	1480	23.97	-	ρ C1-H-C2-H
92	1432	66.73	-	β N31-H
79	1307	38.05	-	γ C15-H
75	1244	0.79	-	t C21H ₂
73	1226	20.91	1234.44	ν C13-N31

ν - stretching; sym- symmetric; asym- asymmetric; def- deformation; β - In-plane bending; γ - out of plane bending; ρ - rocking; t - twisting

Molecular electrostatic potential

The Molecular Electrostatic Potential (MEP) for the title molecule IPPC was plotted by employing a 6-311++G(d,p) basis set and is depicted in Fig 6. The electrophilic and nucleophilic sites give an idea about the region of molecular interaction. The MEP suggests the high electron density is located near heteroatoms N and O atoms in the title molecule.

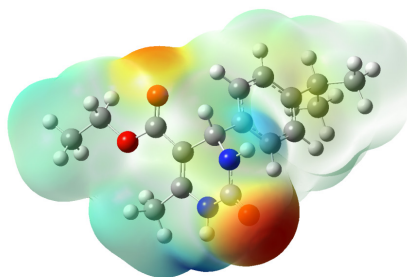


Figure 6 Molecular electrostatic potential of IPPC by DFT/B3LYP method with the 6-311++G(d,p) as a basis set

Thermodynamic properties

In light of the vibrational examination, the different thermodynamic properties were processed from the theoretical frequencies and are tabulated in **Table 6**. All the thermodynamic data revealed in the present research would be helpful for additional assessment and can be utilized to process the other thermodynamic energies as indicated by connections of thermodynamic parameters. In present investigation, the theoretical thermodynamic calculations based on vibrational data provided valuable insights on thermodynamic stability of the title molecule. Our study reveals that the molecule IPPC is thermodynamically stable.

Conclusions

In the present study, DFT/B3LYP method at 6-311++G(d,p) basis set has been used for the

exploration of various important structural, electronic and quantum chemical parameters of title molecule IPPC. The HOMO-LUMO energy gap energy supports the interaction of charge transfer within the molecule. An ideal correlation has been observed between the experimental and theoretical FT-IR data. The molecular electrostatic potential has been presented for the investigation of chemical reactivity. The Frontier Molecular Orbital study was used for the understanding of the charge transfer phenomenon within the molecule. Global chemical reactivity parameters were computed to determine the chemical nature of the title molecule.

Acknowledgments

Authors acknowledge Central instrumentation facility, Savitribai Phule Pune University, Pune for NMR and Mass spectral analysis. Authors

Table 6 Theoretically computed thermodynamic properties

Parameter	Value
E total (kcal mol ⁻¹)	245.026
Translational	0.889
Rotational	0.889
Vibrational	243.248
Heat Capacity at constant volume, Cv (cal mol ⁻¹ K ⁻¹)	83.519
Translational	2.981
Rotational	2.981
Vibrational	77.557
Total entropy S (cal mol ⁻¹ K ⁻¹)	168.056
Translational	43.014
Rotational	34.922
Vibrational	90.120
Zero point Vibrational Energy Ev ₀ (kcal mol ⁻¹)	230.930
Rotational constants (GHZ):	0.73819 0.12677 0.10964
E (RB3LYP) (a.u.)	-1304.6251
Dipole moment (Debye)	3.9470

also would like to thank Principals of Lokenete Vyankatrao Hiray Arts, Science and Commerce College Panchavati, Nashik and Arts, Science and Commerce College, Surgana for permission and providing necessary research facilities. The authors would like to express their sincere and humble gratitude to Prof. Arun B. Sawant for the Gaussian study. Dr. Aapoorva P. Hiray, Coordinator, MG Vidyamandir Institute, is gratefully acknowledged for the Gaussian package.

Conflict of interest

The authors declare that they have no conflict of interest.

References

1. TU Mayer, TM Kapoor, SJ Haggarty, RW King, SL Schreiber, TJ Mitchison, *Science*, 286, **1999**, 971.
2. CM Wright, RJ Chovatiya, NE Jameson, DM Turner, G Zhu, S Werner, DM Huryn, BW, Day, JM Pipas, P Wipf, JL Brodsky, *Bioorg. Med. Chem.*, 16, **2008**, 3291.
3. BP Kumar, G Sankar, RN Baig, S Chandrashekaram, *Eur. J. Med. Chem.*, 44, **2009**, 4192.
4. KS Atwal, GC Rovnyak, J Schwartz, S Moreland, A Hedberg, JZ Gougoutas, MF Malley, DM Floyd, *J. Med. Chem.*, 33, **1990**, 1510.
5. KS Atwal, GC Rovnyak, SD Kimball, DM Floyd, S Moreland, BN Swanson, JZ Gougoutas, J Schwartz, KM Smillie, MF Malley, *J. Med. Chem.*, 33, **1990**, 2629.
6. J Kim, T Ok, C Park, W So, M Jo, Y Kim, M Seo, D Lee, S Jo, Y Ko, I Choi, *Bioorg. Med. Chem. Lett.*, 22, **2012**, 2119.
7. M Mansouri, A Movahedian, M Rostami, A Fassihi, *Res. Pharm. Sci.*, 7, **2012**, 257.
8. A Vasconcelos, PS Oliveira, M Ritter, RA Freitag, RL Romano, FH Quina, *J. Biochem. Mol. Toxicol.*, 26, **2012**, 155.
9. P Sharma, N Rane, VK Gurram, *Bioorg. Med. Chem. Lett.*, 14, **2004**, 4185.
10. AR Trivedi, VR Bhuva, BH Dholariya, DK Dodiya, VB Kataria, VH Shah, *Bioorg. Med. Chem. Lett.*, 20, **2010**, 6100.
11. RK Yadlapalli, OP Chourasia, K Vemuri, M Sritharan, RS Perali, *Bioorg. Med. Chem. Lett.*, 22, **2012**, 2708.
12. N Tewari, VK Tiwari, RC Mishra, RP Tripathi, AK Srivastava, R Ahmad, R Srivastava, BS Srivastava, *Bioorg. Med. Chem.*, 11, **2003**, 2911.
13. A Barakat, MS Islam, AM Al-Majid, HA Ghabbour, HK Fun, K Javed, R Imad, S Yousuf, MI Choudhary, A Wadood, *Bioorg. Med. Chem.*, 23, **2015**, 6740.
14. M Ahmad Bhat, MA Al-Omar, AM Naglah, *J. Enzyme Inhib. Med. Chem.*, 33, **2018**, 978.
15. R Tammi, JA Ripellino, RU Margolis, M Tammi, *J. Invest. Dermatol.*, 90, **1988**, 412.
16. AB Sawant, RS Nirwan, *Indian J. Pure & Appl. Phys.*, 50, **2012**, 308.
17. TB Pawar, BS Jagdale, AB Sawant, VA Adole, *J. Chem., Biol. Phys. Sci.*, 7, **2017**, 167.
18. N Sundaraganesan, G Elango, S Sebastian, P Subramani, *Indian J. Pure & Appl. Phys.*, 47, **2009**, 481.
19. WJ van Rensburg, PJ Steynberg, MM Kirk, WH Meyer, GS Forman, 691, **2006**, 5312.
20. K. Rizwan, M. Zubair, N. Rasool, T. Mahmood, K. Ayub, N. B. Alitheen, M. N. Aziz, M. N. Akhtar, S. M. Bukhary, V. U. Ahmad, M. Rani, *Chem. Central J.* 12, **2018**, 49.
21. ZR Akerling, JE Norton, KN Houk, *Org. Lett.*, 6, **2004**, 4273.
22. AB Sawant, SG Wagh, *Indian J Pure & Appl. Phys.*, 56, **2018**, 405.
23. N Sundaraganesan, E Kavitha, S Sebastian, JP Cornard, M Martel, *Spectrochim. Acta, Part A: Mol. Biomol. Spectrosc.*, 74, **2009**, 788.
24. VA Adole, TB Pawar, PB Koli, BS Jagdale, *J. Nanostruct. Chem.*, 9, **2019**, 61.
25. MJ Frisch, GW Trucks, HB Schlegel, et al., *Gaussian 03, Revision E.01*, Gaussian, Inc, Wallingford CT, USA 2004.