Asian Pub. Corp.

www.asianpubs.org

ARTICLE

Synthesis, Molecular Structure, HOMO-LUMO and Spectroscopic Investigation of (*E*)-1-(2,4-Dichloro-5-fluorophenyl)-3-(2,6-dichlorophenyl)prop-2-en-1-one: A DFT Based Computational Exploration

Vishnu A. Adole[1,✉], Ravindra H. Waghchaure[2], Thansing B. Pawar[3], Bapu S. Jagdale[1] and Kailas H. Kapadnis[3]

Asian Journal of Organic & Medicinal Chemistry

Volume: 5 Year: 2020
Issue: 3 Month: July–September
pp: 242–248
DOI: https://doi.org/10.14233/ajomc.2020.AJOMC-P285

Received: 23 June 2020
Accepted: 6 September 2020
Published: 15 September 2020

ABSTRACT

In present study, the synthesis, molecular structure, HOMO-LUMO and spectroscopic investigation of (*E*)-1-(2,4-dichloro-5-fluorophenyl)-3-(2,6-dichlorophenyl)prop-2-en-1-one (CFPCP) is reported. The structure of the title compound was affirmed based on FTIR, ^{1}H NMR & ^{13}C NMR spectroscopic techniques. The computational examination has been performed by employing density functional theory (DFT) method at B3LYP/6-311G++(d,p) basis set. The geometry of the title molecule has been optimized and established at the same level of theory. The various structural and quantum chemical parameters have been investigated for the title molecule at the 6-311G++(d,p) basis set. To explore the electron distribution, Mulliken atomic charges and molecular electrostatic potential surface are discussed. Besides, vibrational assignments were made and the scaled frequencies have been compared with the experimental frequencies. For the investigation of the absorption wavelength, excitation energy and the oscillator strength TD-DFT method using B3LYP/6-311G++(d,p) basis set is used. Some thermochemical functions have also been investigated using harmonic vibrational frequencies.

KEYWORDS

(*E*)-1-(2,4-Dichloro-5-fluorophenyl)-3-(2,6-dichlorophenyl)prop-2-en-1-one, DFT, 6-311++G(d,p), FMO.

Author affiliations:

[1]Department of Chemistry, Arts, Science and Commerce College (Affiliated to Savitribai Phule Pune University, Pune), Manmad-423104, India
[2]Department of Chemistry, Mahant Jamanadas Maharaj Arts, Commerce and Science College (Affiliated to Savitribai Phule Pune University, Pune), Karanjali-422208, India
[3]Research Centre in Chemistry, Loknete Vyankatrao Hiray Arts, Science and Commerce College Panchavati (Affiliated to Savitribai Phule Pune University, Pune), Nashik-422003, India

✉To whom correspondence to be addressed:

E-mail: vishnuadole86@gmail.com

Available online at: http://ajomc.asianpubs.org

INTRODUCTION

Chalcones serve as versatile intermediates for the synthesis of a variety of heterocyclic compounds with the diverse pattern of pharmacological properties [1-4]. The chalcone route is the most common to synthesize vital pharmacological motifs like pyrazolines [5], benzodiazepines [6], benzothiazepines [7], pyrimidines [8], *etc*. Natural as well as synthetic chalcone and their analogs exhibit an excellent variety of pharmacological and biological impacts [9-14]. They are found to demonstrate significant anticancer [15], antimycobacterial [16], antibacterial [17], antifungal [18], antiviral [19,20], anti-inflammatory [21], antitumour [22], antihypertensive [23,24], antioxidant [25-27] and anticonvulsant properties [28]. Importantly, the halogen bearing chalcones have been studied as pharmaco-

logically potent molecules [29,30]. Halogen bearing chalcones have been found display medicinal applications like modulators of multidrug resistance, antimicrobial agents, antidiabetic, antiproliferative, antioxidant, anti-inflammatory, anticancer and analgesic properties [31-37].

The role of green chemistry and its applications in organic synthesis has seen a tremendous rise in the past few years [38-40]. Many methodologies have been accounted for the synthesis of chalcones. However, still, the most simple and common reaction method for the synthesis of chalcone is Claisen-Schmidt condensation between an aromatic ketone and aromatic aldehyde. The methods like microwave and ultrasound irradiation are also adequate in terms of yield, time and purity. Theoretical chemistry is a great tool for the study of many molecular properties [41-45]. Along with this, the study on spectral properties has become easy access due to the theoretical calculations [46-57]. The DFT has been used for the investigation of many vital aspects in the past decade. The crucial facets like geometrical entities, reactivity positions, reaction pathways and study on spectral properties are the most studied *via* DFT computations. By looking at these crucial aspects discussed above, we wish to report the synthesis of the title compound, its structural and spectroscopic exploration by using DFT at B3LYP/6-311++G (d,p) basis set. The properties like bond length, bond angle, HOMO-LUMO energies and thermochemical functions have been discussed in the present research.

EXPERIMENTAL

All chemicals and solvents were purchased from Sigma laboratory, Nashik (Sigma-Aldrich, SD Fine chemicals and Avra Synthesis). Melting points were determined in open capillaries and are uncorrected. IR spectra were recorded on the Shimadzu-FTIR spectrophotometer using KBr pellets. ^{1}H NMR and ^{13}C NMR were recorded on BRUKER ADVANCE III HD NMR 500 MHz instrument. The progress of the reactions was monitored by TLC on Merck silica plates. All the apparatus were washed and dried in an oven before use.

Synthesis of the title compound: Previously reported [24] ultrasound method has been employed for the synthesis of the title compound CFPCP (**Scheme-I**). In a typical synthesis, 1-(2,4-dichloro-5-fluorophenyl)ethan-1-one (0.01 mol), 2,6-dichlorobenzaldehyde (0.01 mol) were mixed in a conical flask containing ethanol solvent. To this reaction mixture, 2 mL of 40% NaOH was added and the resulting mixture was exposed to ultrasound irradiation until formation of the title compound (checked by TLC). The contents of the flask were poured into the beaker containing crushed ice and acidified by using dilute HCl. The resulting crude product was filtered, dried and recrystallized to furnish white colour product. The structure of the title compound was confirmed based on FT-IR, PMR and CMR spectroscopic analysis.

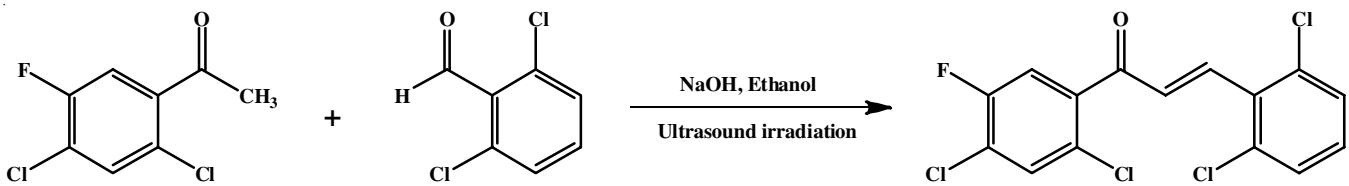
Computational investigation: DFT calculations were performed using Gaussian-03(W) program package without any constraint on the geometry [58]. The geometry of the CFPCP molecule is optimized by DFT method using a 6-311G++(d,p) basis set. The FMO analysis and quantum chemical study have been performed using the same basis set. Molecular electrostatic surface potential (MESP) was computed using the same method. All the calculations were carried out for the optimized structure in the gas phase.

Spectral data: FT-IR (KBr, ν_{max}, cm^{-1}): 3062.96, 2916.37, 1666.50, 1581.63, 1489.05, 1350.17, 1234.44, 1087.85, 823.25, 763.81, 694.37; ^{1}H NMR (500 MHz, $CDCl_3$, δ ppm): 7.23 (t, *J* = 8.1 Hz, 1H), 7.30 (d, *J* = 16.5 Hz, 1H), 7.37 (m, 3H), 7.54 (d, *J* = 6.3 Hz, 1H), 7.67 (d, *J* = 16.5 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$, δ ppm): 117.53, 117.72, 124.54, 124.69, 127.16, 127.19, 128.98, 130.46, 131.67, 132.16, 132.84, 135.31, 138.09, 138.13, 140.14, 155.80, 157.81, 190.74.

RESULTS AND DISCUSSION

The title compound (CFPCP) is synthesized by ultrasound method and characterized by FT-IR, ^{1}H NMR and ^{13}C NMR spectro-scopic methods. The presence of the IR absorption peak at 1666.50 cm^{-1} affirms the presence of a conjugated ketone carbonyl group. The other two important IR signals at 1581.63 cm^{-1} and 1489.05 cm^{-1} are acquired due to double bond stret-ching vibrations. Other signals are also in good agreement with the structure of the title compound. In ^{1}H NMR and ^{13}C NMR spectroscopic methods also, the signals have appeared as expected. The very important coupling constant value, *J* = 16.5 Hz suggests *trans*-stereochemistry around the olefinic double bond.

Molecular structure, bond length, bond angle study: The optimized molecular structure of the CFPCP molecule is shown in Fig. 1 while the optimized molecular structure of the title molecule along x, y, and z Cartesian axes is depicted in Fig. 2. The optimized structural arrangement indicates the structure has overall non-planarity of the rings. However, individual rings are planar. The dipole moment of the title molecule is 4.48 Debye which indicates a molecule is highly polar. This is ascribed to the presence of the halogen substituents in the molecule. The geometrical parameters of the title molecule obtained using the DFT method at 6-311++G(d,p) basis set are presented in Tables 1 and 2. The carbonyl bond is 1.2173 Å and the alkene double bond is 1.3419 Å long. These values are ideally matching with the structural framework. The C10-C12-C14 has a bond angle value of 118.7508° whereas C8-C10-C12 is 118.9965°. The important dihedral bond angle is H9-C8-C10-H11 and it



Scheme-I: Synthetic route of (E)-1-(2,4-dichloro-5-fluorophenyl)-3-(2,6-dichlorophenyl)prop-2-en-1-one (CFPCP)

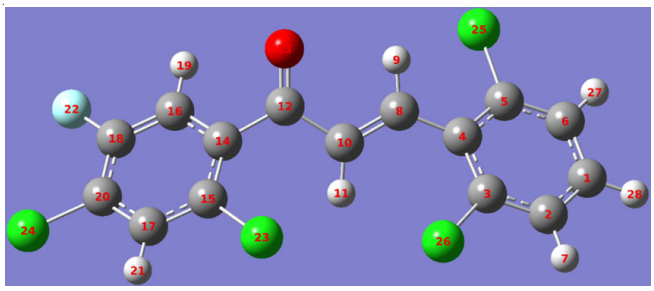


Fig. 1. Optimized molecular structure of the title molecule at B3LYP/6-311++G(d,p) basis set

TABLE-1
OPTIMIZED BOND LENGTHS OF THE TITLE MOLECULE AT B3LYP/6-311++G(d,p) BASIS

Bond lengths (Å)			
C1-C2	1.3889	C10-C12	1.4860
C1-C6	1.3895	C12-O13	1.2173
C1-H28	1.0833	C12-C14	1.5126
C2-C3	1.3901	C14-C15	1.4002
C2-H7	1.0816	C14-C16	1.4001
C3-C4	1.4113	C15-C17	1.3918
C3-Cl	1.7569	C15-Cl23	1.7577
C4-C5	1.4134	C16-C18	1.3804
C4-C8	1.4672	C16-H19	1.0823
C5-C6	1.3874	C17-C20	1.3889
C5-Cl25	1.7583	C17-H21	1.0810
C6-H27	1.0816	C18-C20	1.3941
C8-H9	1.0855	C18-F22	1.3396
C8-C10	1.3419	C20-Cl24	1.7406
C10-H11	1.0798	–	–

TABLE-2
OPTIMIZED BOND ANGLES OF THE TITLE MOLECULE AT B3LYP/6-311++G(d,p) BASIS

Bond angles (°)			
C2-C1-C6	120.0764	H11-C10-C12	118.4636
C2-C1-H28	119.9321	C10-C12-O13	122.3955
C6-C1-H28	119.9907	C10-C12-C14	118.7508
C1-C2-C3	119.8497	O13-C12-C14	118.6141
C1-C2-H7	120.8845	C12-C14-C15	126.6034
C3-C2-H7	119.2639	C12-C14-C16	115.6180
C2-C3-C4	122.3980	C15-C14-C16	117.7583
C2-C3-Cl26	116.2359	C14-C15-C17	121.3406
C4-C3-C2	121.3198	C14-C15-Cl23	121.7384
C3-C4-C5	115.3571	C17-C15-Cl23	116.8131
C3-C4-C8	125.4558	C14-C16-C18	121.0705
C5-C4-C8	119.1576	C14-C16-H19	119.4272
C4-C5-C6	123.0698	C18-C16-H19	119.5022
C4-C5-Cl25	119.7857	C15-C17-C20	119.8733
C6-C5-Cl25	117.1273	C15-C17-H21	120.2751
C1-C6-C5	119.2425	C20-C17-H21	119.8473
C1-C6-H27	121.1457	C16-C18-C20	120.5624
C5-C6-H27	119.6114	C16-C18-F22	119.5882
C4-C8-H9	115.5807	C20-C18,-F22	119.8491
C4-C8-C10	128.2938	C17-C20-C18	119.3498
H9-C8-C10	116.0382	C17-C20-Cl24	120.4812
C8-C10-H11	122.4118	C18-C20-Cl24	120.1655
C8-C10-C12	118.9965	–	–

is 176.4171°. The other important dihedral bond angles are O13-C12-C14-C16 (39.0386°), C8-C10-C12-O13 (1.6161°), C3-C4-C8-C10 (40.2228°) and C5-C4-C8-C10 (141.8489°). The other bond lengths, bond angles and dihedral bond angles

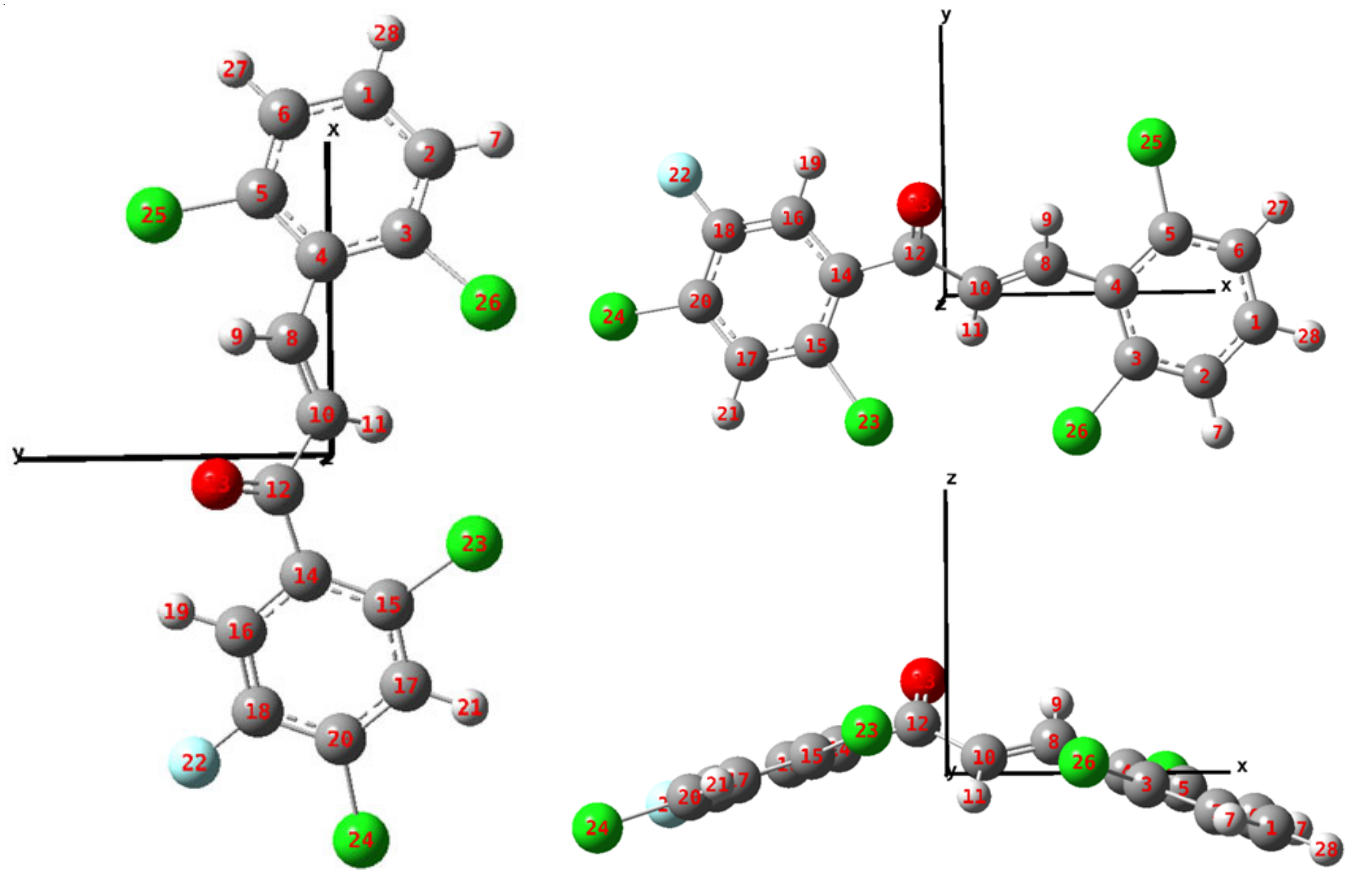


Fig. 2. Optimized molecular structure of the title molecule along x, y and z axes

are also in good agreement and matches with the optimized structure of the title compound.

Mulliken atomic charges and molecular electrostatic surface potential analysis: The Mulliken atomic charges and molecular electrostatic surface potential analysis of CFPCP are given in Figs. 3 and 4, respectively. The Mulliken atomic charges are also given in Table-3. The H9 (0.164671) hydrogen atom is the most electropositive amongst all hydrogen atoms present in the title compound. This effect is due to the proximity of the carbonyl oxygen near the H9 hydrogen atom. On the other hand, the most electropositive carbon atom is C18 (0.374579). MESP analysis provides information regarding the chemical reactivity sites. The MESP suggests that the title compound is highly susceptible to nucleophilic attack and therefore will undergo attack nucleophile rather than electrophilic attacks. As per MESP, the positive potential is around hydrogen atoms. The enone system is prone to nucleophilic addition reactions.

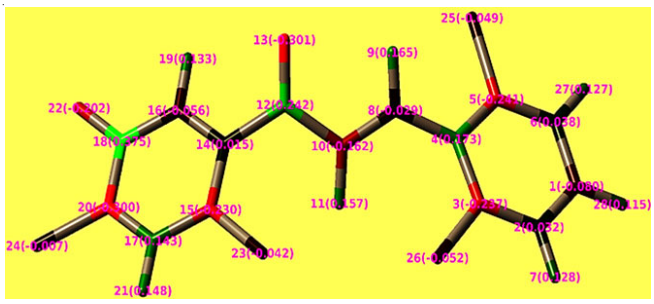


Fig. 3. Mulliken atomic charges of the title molecule at B3LYP/6-311++G (d,p) basis set

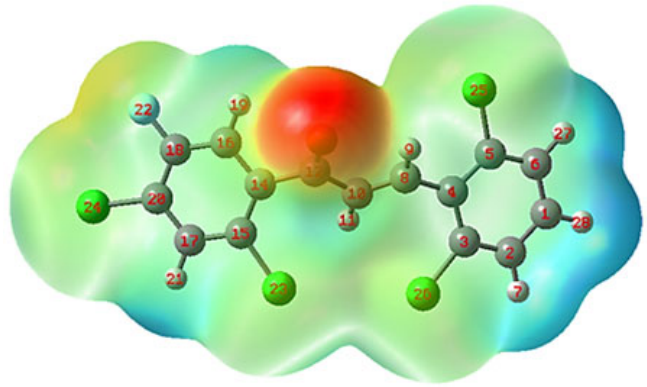


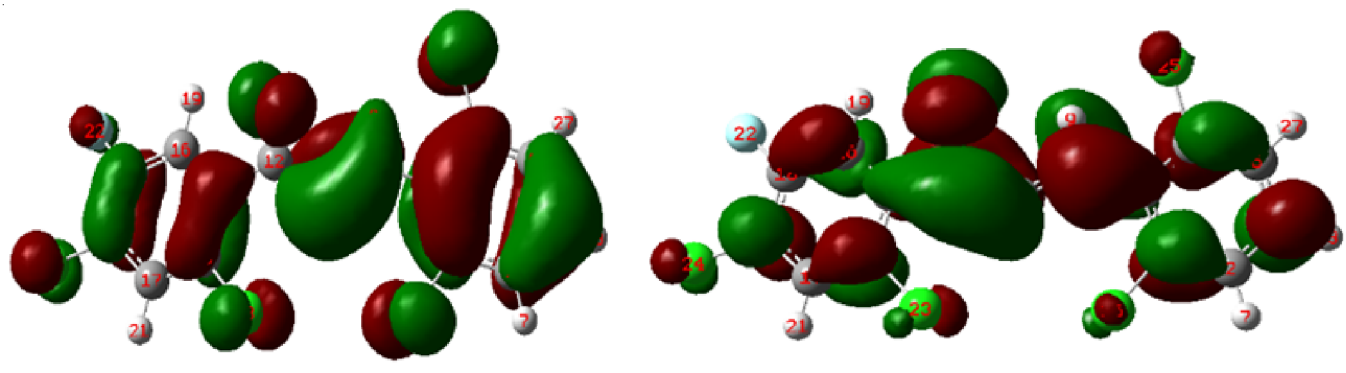
Fig. 4. MEP of the title molecule at B3LYP/6-311++G(d,p) basis set

TABLE-3
MULLIKEN ATOMIC CHARGES

Atom	Charge	Atom	Charge
1 C	-0.080315	15 C	-0.230456
2 C	0.032288	16 C	-0.056269
3 C	-0.236714	17 C	0.142599
4 C	0.173171	18 C	0.374579
5 C	-0.240704	19 H	0.132708
6 C	0.038263	20 C	-0.299967
7 H	0.127664	21 H	0.147716
8 C	-0.029308	22 F	-0.202221
9 H	0.164671	23 Cl	-0.042273
10 C	-0.161803	24 Cl	-0.007462
11 H	0.157486	25 Cl	-0.048797
12 C	0.241790	26 Cl	-0.051815
13 O	-0.301362	27 H	0.126877
14 C	0.015021	28 H	0.114631

Frontier molecular orbital investigation: The investigations of frontier molecular orbitals of CFPCP are discussed. The HOMO and LUMO orbitals of the title compound are presented in Fig. 5. The HOMO energy decides the nucleophilic power and the LUMO energy decides the electrophilic. The energy gap is a vital aspect to decide the chemical reactivity of the molecules. It also provides information about the charge transfer phenomenon. The HOMO-LUMO energies also provide the idea of various quantum chemical parameters. The HOMO-LUMO energy gap in the title compound is 4.28 eV. The absorption wavelength for the first singlet excitation of the electron is 371.10 nm with excitation energy 3.3410 eV and the oscillator strength, f = 0.0322. The maximum charge transfer value is 2.37. The absolute hardness value is 2.14 eV and the global softness 0.47 eV. The global electrophilicity index is 6.00 eV which indicates the molecule CFPCP is highly electrophilic.

Vibrational assignments and thermochemical properties: The theoretical and experimental IR spectra are presented in Figs. 6, respectively. The title molecule CFPCP contains 28 atoms and therefore 78 fundamental modes of vibrations. The molecule is non-linear and thus 3N-6 formula is applied to deduce the total fundamental modes of vibrations. The selected vibrational assignments were made and presented in Table-4. The DFT computations overestimate the computed IR frequencies and therefore they are scaled by the 0.96 scaling factor [46]. In present study, a good agreement between the



HOMO LUMO

Fig. 5. HOMO-LUMO pictures of the title molecule at B3LYP/6-311++G (d,p) basis set

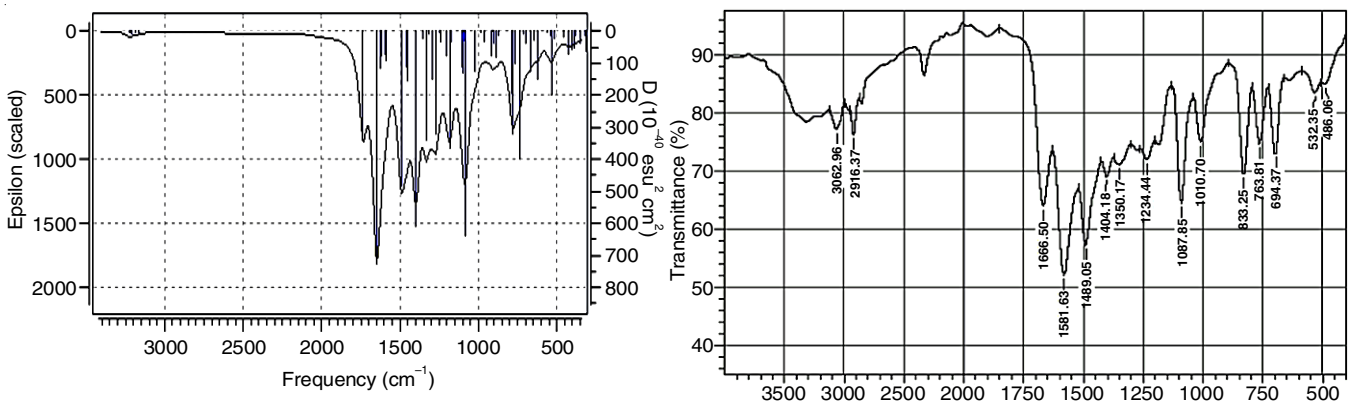


Fig. 6. Theoretical and the experimental IR spectra of (*E*)-1-(2,4-dichloro-5-fluorophenyl)-3-(2,6-dichlorophenyl)prop-2-en-1-one (CFPCP)

TABLE-4
SELECTED EXPERIMENTAL AND THEORETICAL VIBRATIONAL ASSIGNMENTS
OF THE TITLE MOLECULE CALCULATED AT 6-311++ G(d,p) LEVEL

Mode	Computed scaled frequencies (cm^{-1})	IR intensity (km) (mol^{-1})	Observed frequencies (cm^{-1})	Assignments
78	3098.10	1.16	–	ν C10-H
74	0	0.19	–	asym C2-H-C6-H
73	3058.95	2.59	3062.96	ν C1-H + sym C2-H-C6-H
71	1665.89	136.24	1666.50	ν C=O
70	1584.16	300.72	1581.63	ν C=C (alkene)
66	1525.01	35.85	1489.05	ν C=C (ring B)
62	1342.35	213.66	1350.17	ν C=C (ring A)
58	1240.63	47.94	1234.44	def (ring B)
51	1058.17	30.44	1087.85	β C2-H + β C6-H + β C16-H
47	978.70	31.66	–	γ C8-H + γ C10-H
40	838.57	3.01	823.25	β C17-H
39	755.63	37.87	763.81	def (ring A) + def (ring B)
35	704.95	73.65	694.37	def (ring A)

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

theoretical and experimental absorption frequencies is found. Thus, the correct assignment of vibrational frequencies has been made. The thermochemical data are given in Table-5. The impor-tant thermodynamic functions such as total energy ($E_{thermal}$), total heat capacity (Cv) and total entropy is discussed. The title molecule has 151.146 cal/mol-Kelvin entropy which indicates the total degree of freedom in the title compound. Based on the thermodynamic data, other important thermochemical data could be derived by using suitable thermodynamic relationships.

TABLE-5
THERMOCHEMICAL PROPERTIES

	E (thermal) (Kcal/mol)	Cv (cal/mol Kelvin)	S (cal/mol Kelvin)
Total	122.908	69.302	151.146
Translational	0.889	2.98	43.552
Rotational	0.889	2.981	35.777
Vibrational	121.131	63.340	71.817

Conclusions

In the present work, 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 (*E*)-1-(2,4-dichloro-5-fluorophenyl)-3-(2,6-dichlorophenyl)prop-2-en-1-one (CFPCP) molecule. The results are summarized below:

• The title compound was synthesized and its structure of was affirmed based on Fourier-transform infrared spectroscopy (FTIR), proton nuclear magnetic reso-nance (^{1}H NMR) and carbon nuclear magnetic resonance (^{13}C NMR) spectroscopic techniques.

• The geometry of the CFPCP molecule was optimized by DFT/B3LYP method at 6-311++G(d,p) basis set and established at the same level of theory. The various structural and quantum chemical parameters have been investigated for the title molecule at the 6-311G++(d,p) basis set.

• To explore the electron distribution, Mulliken atomic charges and molecular electrostatic potential surfaces are discussed. The study revealed that the title molecule is electrophilic and more prone to nucleophilic attacks.

• The vibrational assignments were made and the scaled frequencies have been compared with the experimental frequencies. A good agreement between the theoretical and experimental IR frequencies was found.

• Some significant thermochemical functions are explored using harmonic vibrational frequencies. This data is valuable for the further assessment of the thermodynamic functions.

ACKNOWLEDGEMENTS

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

spectral analysis. Authors also would like to thank Principals of Lokenete Vyankatrao Hiray Arts, Science and Commerce College Panchavati, Nashik and Arts, Science and Commerce College, Manmad 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 Prashant Hiray, Coordinator, MG Vidyamandir Institute, is gratefully acknowledged for the Gaussian package.

REFERENCES

1. M.J. Elarfi and H.A. Al-Difar, Synthesis of Some Heterocyclic Compounds Derived from Chalcones, *Sci. Rev. Chem. Commun.*, **2**, 103 (2012).
2. A.V. Velikorodov, V.A. Ionova, S.I. Temirbulatova, O.L. Titova and N.N. Stepkina, Synthesis and Application of Chalcones to the Preparation of Heterocyclic Structures, *Russ. J. Org. Chem.*, **49**, 1610 (2013); https://doi.org/10.1134/S1070428013110080
3. O. Mazimba, Antimicrobial activities of Heterocycles Derived from Thienylchalcones, *J. King Saud Univ. Sci.*, **27**, 42 (2015); https://doi.org/10.1016/j.jksus.2014.06.003
4. Z.N. Siddiqui, M. Asad and S. Praveen, Synthesis and Biological Activity of Heterocycles from Chalcone, *Med. Chem. Res.*, **17**, 318 (2008); https://doi.org/10.1007/s00044-007-9067-y
5. V.D. Joshi, M.D. Kshirsagar and S. Singhal, Synthesis and Antimicrobial Activities of Various Pyrazolines from Chalcones., *Int. J. ChemTech Res.*, **4**, 971 (2012).
6. C.A. Escobar, O. Donoso-Tauda, R. Araya-Maturana and D. Sicker, Synthesis of 1,5-Benzodiazepines with Unusual Substitution Pattern from Chalcones Under Solvent-Free Microwave Irradiation Conditions, *Synth. Commun.*, **39**, 166 (2008); https://doi.org/10.1080/00397910802372517
7. K.L. Ameta, N.S. Rathore and B. Kumar, Synthesis and *in vitro* Anti Breast Cancer Activity of Some Novel 1,5-Benzothiazepine Derivatives, *J. Serb. Chem. Soc.*, **77**, 725 (2012); https://doi.org/10.2298/JSC110715219A
8. S.S. Chobe, V.A. Adole, K.P. Deshmukh, T.B. Pawar and B.S. Jagdale, Poly (ethylene glycol)(PEG-400): A Green Approach Towards Synthesis of Novel Pyrazolo[3, 4-*d*]pyrimidin-6-amines Derivatives and their Antimicrobial Screening, *Arch. Appl. Sci. Res.*, **6**, 61 (2014).
9. Z. Rozmer and P. Perjési, Naturally Occurring Chalcones and their Biological Activities, *Phytochem. Rev.*, **15**, 87 (2016); https://doi.org/10.1007/s11101-014-9387-8
10. Y. Li, B. Sun, J. Zhai, L. Fu, S. Zhang, J. Zhang, H. Liu, W. Xie, H. Deng, Z. Chen and F. Sang, Synthesis and Antibacterial Activity of Four Natural Chalcones and their Derivatives, *Tetrahedron Lett.*, **60**, 151165 (2019); https://doi.org/10.1016/j.tetlet.2019.151165
11. H. Boulebd, The Role of Benzylic-Allylic Hydrogen Atoms on the Anti-radical Activity of Prenylated Natural Chalcones: A Thermodynamic and Kinetic Study, *J. Biomol. Struct. Dyn.*, (2020) (In press); https://doi.org/10.1080/07391102.2020.1740791
12. A. Rammohan, J.S. Reddy, G. Sravya, C.N. Rao and G.V. Zyryanov, Chalcone Synthesis, Properties and Medicinal Applications: A Review, *Environ. Chem. Lett.*, **18**, 433 (2020); https://doi.org/10.1007/s10311-019-00959-w
13. B. Ardiansah, Chalcones Bearing N, O, and S-Heterocycles: Recent Notes on their Biological Significances, *J. Appl. Pharm. Sci.*, **9**, 117 (2019); https://doi.org/10.7324/JAPS.2019.90816
14. K. Vongdeth, P. Han, W. Li and Q.A. Wang, Synthesis and Antiproliferative Activity of Natural and Non-Natural Polymethoxychalcones and Polymethoxyflavones, *Chem. Nat. Compd.*, **55**, 11 (2019); https://doi.org/10.1007/s10600-019-02605-x
15. V.A. Adole, T.B. Pawar and B.S. Jagdale, Aqua-Mediated Rapid and Benign Synthesis of 1,2,6,7-Tetrahydro-8*H*-indeno[5,4-*b*]furan-8-one-Appended Novel 2-Arylidene Indanones of Pharmacological Interest at Ambient Temperature, *J. Chin. Chem. Soc. (Taipei)*, **67**, 306 (2020); https://doi.org/10.1002/jccs.201900015
16. V. Patil, S.A. Patil, R. Patil, A. Bugarin, K. Beaman and S.A. Patil, Exploration of (Hetero)aryl Derived Thienylchalcones for Antiviral and Anticancer Activities, *Med. Chem.*, **15**, 150 (2019); https://doi.org/10.2174/1573406414666180524074648
17. A. Singh, A. Viljoen, L. Kremer and V. Kumar, Synthesis and Anti-mycobacterial Evaluation of Piperazyl-alkyl-Ether Linked 7-Chloro-quinoline-Chalcone/Ferrocenyl Chalcone Conjugates, *ChemistrySelect*, **3**, 8511 (2018); https://doi.org/10.1002/slct.201801453
18. W.C. Chu, P.Y. Bai, Z.Q. Yang, D.Y. Cui, Y.G. Hua, Y. Yang, Q.Q. Yang, E. Zhang and S. Qin, Synthesis and Antibacterial Evaluation of Novel Cationic Chalcone Derivatives Possessing Broad Spectrum Antibacterial Activity, *Eur. J. Med. Chem.*, **143**, 905 (2018); https://doi.org/10.1016/j.ejmech.2017.12.009
19. Y.H. Wang, H.H. Dong, F. Zhao, J. Wang, F. Yan, Y.Y. Jiang and Y.S. Jin, Synthesis and Synergistic Antifungal Effects of Chalcones against Drug Resistant *Candida albicans*, *Bioorg. Med. Chem. Lett.*, **26**, 3098 (2016); https://doi.org/10.1016/j.bmcl.2016.05.013
20. N. Mateeva, S.V. Eyunni, K.K. Redda, U. Ononuju, T.D. Hansberry II, I.I.C. Aikens and A. Nag, Functional Evaluation of Synthetic Flavonoids and Chalcones for Potential Antiviral and Anticancer Properties, *Bioorg. Med. Chem. Lett.*, **27**, 2350 (2017); https://doi.org/10.1016/j.bmcl.2017.04.034
21. D.K. Mahapatra, S.K. Bharti and V. Asati, Chalcone Derivatives: Anti-Inflammatory Potential and Molecular Targets Perspectives, *Curr. Top. Med. Chem.*, **17**, 3146 (2017); https://doi.org/10.2174/1568026617666170914160446
22. A.M. AbuDief, I.F. Nassar and W.H. Elsayed, Magnetic $NiFe_2O_4$ Nanoparticles: Efficient, Heterogeneous and Reusable Catalyst for Synthesis of Acetylferrocene Chalcones and their Anti-tumour Activity, *Appl. Organomet. Chem.*, **30**, 917 (2016); https://doi.org/10.1002/aoc.3521
23. V.A. Adole, B.S. Jagdale, T.B. Pawar and A.A. Sagane, Ultrasound Promoted Stereoselective Synthesis of 2,3-Dihydrobenzofuran Appended Chalcones at Ambient Temperature, *S. Afr. J. Chem.*, **73**, 35 (2020); https://doi.org/10.17159/0379-4350/2020/v73a6
24. H. Kumar, V. Devaraji, R. Joshi, M. Jadhao, P. Ahirkar, R. Prasath, P. Bhavana and S.K. Ghosh, Antihypertensive Activity of a Quinoline Appended Chalcone Derivative and its Site Specific Binding Interaction with a Relevant Target Carrier Protein, *RSC Adv.*, **5**, 65496 (2015); https://doi.org/10.1039/C5RA08778C
25. M. Mellado, C.O. Salas, E. Uriarte, D. Viña, C. JaraGutiérrez, M.J. Matos and M. Cuellar, Design, Synthesis and Docking Calculations of Prenylated Chalcones as Selective Monoamine Oxidase B Inhibitors with Antioxidant Activity, *ChemistrySelect*, **4**, 7698 (2019); https://doi.org/10.1002/slct.201901282
26. Y. Xue, Y. Liu, L. Zhang, H. Wang, Q. Luo, R. Chen, Y. Liu and Y. Li, Antioxidant and Spectral Properties of Chalcones and Analogous Aurones: Theoretical Insights, *Int. J. Quantum Chem.*, **119**, e25808 (2019); https://doi.org/10.1002/qua.25808
27. C.A. Calliste, J.B. Le, P. Trouillas, C. Pouget, G. Habrioux, A.J. Chulia and J.L. Duroux, Chalcones: Structural Requirements for Antioxidant, Estrogenic and Antiproliferative Activities, *Anticancer Res.*, **21**, 3949 (2001).
28. C.S. Sharma, K.S. Shekhawat, C.S. Chauhan and N. Kumar, Synthesis and Anticonvulsant Activity of Some Chalcone Derivatives, *J. Chem. Pharm. Res.*, **5**, 450 (2013).
29. U. Berar, Chalcones: Compounds Possessing a Diversity in Applications, *Orbital Elec. J. Chem.*, **4**, 209 (2012).
30. S.L. Gaonkar and U.N. Vignesh, Synthesis and Pharmacological Properties of Chalcones: a Review, *Res. Chem. Intermed.*, **43**, 6043 (2017); https://doi.org/10.1007/s11164-017-2977-5
31. F. Bois, C. Beney, A. Boumendjel, A.M. Mariotte, G. Conseil and A. Di Pietro, Halogenated Chalcones with High-Affinity Binding to P-Glycoprotein: Potential Modulators of Multidrug Resistance, *J. Med. Chem.*, **41**, 4161 (1998); https://doi.org/10.1021/jm9810194
32. C. Yamali, H.I. Gul, H. Sakagami and C.T. Supuran, Synthesis and Bioactivities of Halogen Bearing Phenolic Chalcones and their Corresponding *bis*-Mannich Bases, *J. Enzyme Inhib. Med. Chem.*, **31(sup4)**, 125 (2016); https://doi.org/10.1080/14756366.2016.1221825

33. K.L. Amole, I.A. Bello and A.O. Oyewale, Synthesis, Characterization and Antibacterial Activities of New Fluorinated Chalcones, *Chemistry Africa*, **2**, 47 (2019); https://doi.org/10.1007/s42250-019-00043-4
34. K.R. Abdellatif, H.A. Elshemy, S.A. Salama and H.A. Omar, Synthesis, Characterization and Biological Evaluation of Novel 4′-Fluoro-2′-hydroxychalcone Derivatives as Antioxidant, Anti-inflammatory and Analgesic Agents, *J. Enzyme Inhib. Med. Chem.*, **30**, 484 (2015); https://doi.org/10.3109/14756366.2014.949255
35. S. Burmaoglu, O. Algul, D.A. Anýl, A. Gobek, G.G. Duran, R.H. Ersan and N. Duran, Synthesis and Anti-Proliferative Activity of Fluoro-Substituted Chalcones, *Bioorg. Med. Chem. Lett.*, **26**, 3172 (2016); https://doi.org/10.1016/j.bmcl.2016.04.096
36. C.T. Hsieh, T.J. Hsieh, M. El-Shazly, D.W. Chuang, Y.H. Tsai, C.T. Yen, S.F. Wu, Y.C. Wu and F.R. Chang, Synthesis of Chalcone Derivatives as Potential Anti-Diabetic Agents, *Bioorg. Med. Chem. Lett.*, **22**, 3912 (2012); https://doi.org/10.1016/j.bmcl.2012.04.108
37. S. Burmaoglu, O. Algul, A. Gobek, D. Aktas Anil, M. Ulger, B.G. Erturk, E. Kaplan, A. Dogen and G. Aslan, Design of Potent Fluoro-Substituted Chalcones as Antimicrobial Agents, *J. Enzyme Inhib. Med. Chem.*, **32**, 490 (2017); https://doi.org/10.1080/14756366.2016.1265517
38. V.A. Adole, Synthetic Approaches for the Synthesis of Dihydropyrimidinones/Thiones (Biginelli Adducts): A Concise Review, *World J. Pharm. Res.*, **9**, 1067 (2020); https://doi.org/10.20959/wjpr20206-17660
39. V.A. Adole, T.B. Pawar, P.B. Koli and B.S. Jagdale, Exploration of Catalytic Performance of Nano-La_2O_3 as An Efficient Catalyst for Dihydropyrimidinone/thione Synthesis and Gas Sensing, *J. Nanostruct. Chem.*, **9**, 61 (2019); https://doi.org/10.1007/s40097-019-0298-5
40. V.A. Adole, R.A. More, B.S. Jagdale, T.B. Pawar and S.S. Chobe, Efficient Synthesis, Antibacterial, Antifungal, Antioxidant and Cytotoxicity Study of 2-(2-Hydrazineyl)thiazole Derivatives, *ChemistrySelect*, **5**, 2778 (2020); https://doi.org/10.1002/slct.201904609
41. L. Mammino, Intramolecular Hydrogen Bonding Patterns, Conformational Preferences and Molecular Properties of Dimeric Acylphloroglucinols: An *ab initio* and DFT Study, *J. Mol. Struct.*, **1176**, 488 (2019); https://doi.org/10.1016/j.molstruc.2018.07.013
42. G.T. Huang and J.S. Yu, Analyses on Molecular Properties of the Diamidinate CrI–CrI Complex by Multireference and DFT Approaches, *J. Phys. Chem. A*, **123**, 7803 (2019); https://doi.org/10.1021/acs.jpca.9b04423
43. M.F. Hassan and A.N. Ayyash, Study of Spectral and Molecular Properties of Polyatomic Molecule by Semiempirical and DFT Methods, *Asian J. Res. Chem*, **12**, 330 (2019); https://doi.org/10.5958/0974-4150.2019.00061.0
44. V.A. Adole, R.H. Waghchaure, B.S. Jagdale, T.B. Pawar and S.S. Pathade, Molecular Structure, Frontier Molecular Orbital and Spectroscopic Examination in Dihydropyrimidinones: A Comparative Computational Approach, *Int. J. Adv. Sci. Res.*, **11**, 64 (2020).
45. M. Bourass, A. Touimi Benjelloun, M. Benzakour, M. Mcharfi, F. Jhilal, F. Serein-Spirau, J. Marc Sotiropoulos and M. Bouachrine, DFT/TD-DFT Characterization of Conjugational Electronic Structures and Spectral Properties of Materials Based on Thieno[3,2-*b*][1]benzothiophene for Organic Photovoltaic and Solar Cell Applications, *J. Saudi Chem. Soc.*, **21**, 563 (2017); https://doi.org/10.1016/j.jscs.2017.01.001
46. N.B. Azaza, S. Elleuch, S. Khemakhem, Y. Abid and H. Ammar, Synthesis and Spectral Properties of Coumarins Derivatives Fluorescence Emitters: Experiment and DFT/TDDFT Calculations, *Opt. Mater.*, **83**, 138 (2018); https://doi.org/10.1016/j.optmat.2018.05.082
47. T.B. Pawar, B.S. Jagdale, A.B. Sawant and V.A. Adole, DFT Studies of 2-[(2-Substituted phenyl)carbamoyl]benzoic Acids, *J. Chem. Biol. Phys. Sci.*, **7**, 167 (2017).
48. P. Gasiorski, M. Matusiewicz, E. Gondek, T. Uchacz, K. Wojtasik, A. Danel, Y. Shchur and A.V. Kityk, Synthesis and Spectral Properties of Halogen Methyl-phenyl-pyrazoloquinoxaline Fluorescence Dyes: Experiment and DFT/TDDFT Calculations, *J. Lumin.*, **198**, 370 (2018); https://doi.org/10.1016/j.jlumin.2018.02.037
49. H. Tezcan, H. Senöz and N. Tokay, Experimental and Quantum Chemical Studies of the Structural and Spectral Properties of Novel Diazenyl Formazans, *J. Mol. Struct.*, **1190**, 171 (2019); https://doi.org/10.1016/j.molstruc.2019.04.055
50. V.A. Adole, R.H. Waghchaure, B.S. Jagdale and 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. Interf.*, **10**, 22 (2020).
51. J. Kausteklis, V. Aleksa, M.A. Iramain and S.A. Brandán, DFT and Vibrational Spectroscopy Study of 1-butyl-3-methylimidazolium Trifluoromethanesulfonate Ionic Liquid, *J. Mol. Struct.*, **1175**, 663 (2019); https://doi.org/10.1016/j.molstruc.2018.08.014
52. B. Amul, S. Muthu, M. Raja and S. Sevvanthi, Spectral, DFT and Molecular Docking Investigations on Etodolac, *J. Mol. Struct.*, **1195**, 747 (2019); https://doi.org/10.1016/j.molstruc.2019.06.047
53. V.S. Kumar, Y.S. Mary, K. Pradhan, D. Brahman, Y.S. Mary, R. Thomas, M.S. Roxy and C.V. Alsenoy, Synthesis, Spectral Properties, Chemical Descriptors and Light Harvesting Studies of a New Bioactive Azo Imidazole Compound, *J. Mol. Struct.*, **1199**, 127035 (2020); https://doi.org/10.1016/j.molstruc.2019.127035
54. V.A. Adole, B.S. Jagdale, T.B. Pawar and A.B. Sawant, Experimental and Theoretical Exploration on Single Crystal, Structural and Quantum Chemical Parameters of (*E*)-7-arylidene-1,2,6,7-tetrahydro-8*H*-indeno-[5,4-*b*]furan8-one Derivatives: A Comparative Study, *J. Chin. Chem. Soc.*, (2020) (In press); https://doi.org/10.1002/jccs.202000006
55. M. Drozd, The Equilibrium Structures, Vibrational Spectra, NLO and Directional Properties of Transition Dipole Moments of Diguanidinium Arsenate Monohydrate and Diguanidinium Phosphate Monohydrate: The Theoretical DFT Calculations, *Spectrochim. Acta A Mol. Biomol. Spectrosc.*, **65**, 1069 (2006); https://doi.org/10.1016/j.saa.2006.02.007
56. J.S.P.P. Leela, R. Hemamalini, S. Muthu and A.A. Al-Saadi, Spectroscopic Investigation (FTIR spectrum), NBO, HOMO-LUMO Energies, NLO and Thermodynamic Properties of 8-methyl-N-vanillyl-6-nonenamide by DFT Methods, *Spectrochim. Acta A Mol. Biomol. Spectrosc.*, **146**, 177 (2015); https://doi.org/10.1016/j.saa.2015.03.027
57. J. Lorenc, I. Bryndal, M. Marchewka, E. Kucharska, T. Lis and J. Hanuza, Crystal and Molecular Structure of 2-Amino-5-chloro-pyridinium Hydrogen Selenate-Its IR and Raman Spectra, DFT Calculations and Physicochemical Properties, *J. Raman Spectrosc.*, **39**, 863 (2008); https://doi.org/10.1002/jrs.1925
58. M.J. Frisch, G.W. Trucks, H.B. Schlegel, G.E. Scuseria, M.A. Robb, J.R. Cheeseman, J.A. Montgomery, Jr., T. Vreven, K.N. Kudin, J.C. Burant, J.M. Millam, S.S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J.E. Knox, H.P. Hratchian, J.B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R.E. Stratmann, O. Yazyev, A.J. Austin, R. Cammi, C. Pomelli, J.W. Ochterski, P.Y. Ayala, K. Morokuma, G.A. Voth, P. Salvador, J.J. Dannenberg, V.G. Zakrzewski, S. Dapprich, A.D. Daniels, M.C. Strain, O. Farkas, D.K. Malick, A.D. Rabuck, K. Raghavachari, J.B. Foresman, J.V. Ortiz, Q. Cui, A.G. Baboul, S. Clifford, J. Cioslowski, B.B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R.L. Martin, D.J. Fox, T. Keith, M.A. Al-Laham, C.Y. Peng, A. Nanayakkara, M. Challacombe, P.M.W. Gill, B. Johnson, W. Chen, M.W. Wong, C. Gonzalez and J.A. Pople, Gaussian 03, Revision C.02, Gaussian, Inc., Wallingford CT (2004).