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Quantum Chemical Studies on 2-chloro-N-(p-tolyl)propanamide using Density Functional Theory

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Abstract: *In the study of compound '2-chloro-N-(p-tolyl)propanamide', which has been analyzed and studied with Density function method in combination of DFT/B3LYP method with basis set 6-311++G(d, p). This compound of propanamide family exhibits many biological activities and hence it is relevant to study. The Electronic properties related to molecule calculated by 'frontier molecular orbitals'. The vibrational analysis for the compound performed at [B3LYP/6-311++G(d, p)] standard to study the various prominent vibrational modes for different atomic groups at respective frequencies. The DFT calculations provide optimized parameters which are helpful for information like bond length, dihedral angle, bond angel etc. The calculated reactivity parameters (global & local reactivity descriptors) of compound such as chemical potential, global softness, global hardness, Fukui function, local softness & electrophilicity indices etc. suggested about to electrophilic and nucleophilic sites. This holistic approach provides further details of compound for several utilities and pharmacological study and use.*

***Keywords**: Density function method, Molecular vibrational analysis, HOMO & LUMO, Reactivity descriptors*

I. Introduction

2-chloro-N-(p-tolyl)propanamide a component of naturally active organic molecules, which contain interesting characteristics[1]. Our major focus for the study of this organic molecule is to calculate, observe and analyze the reactivity descriptors, electronic & thermodynamic parameters and optimization of the molecule for the relevant result. The chemical formula of this propanamide family molecule is $C_{10}H_{12}ClNO$, which contains oxygen atom in a double bond with a carbon atom and a Cl atom in a single bond with the carbon atom and which could be referred as amide of propanoic-acid. This propanamide molecule contains a single-ring system and 2 methyl groups. The molecules of amide group could make reaction through many organic processes to synthesis or develop useful compound. This compound belongs to the family of organic compounds which is primarily known as carboxylic acid amides. Carboxylic acid amides are compounds which belong to primary carboxylic acid amide functional group; so the density function theory method is used to study and discuss various characteristics and properties of the molecule 2-chloro-N-(4-methylphenyl)propanamide. We have arranged optimized parameters for lengths & angles of bonds and dihedral angles for the atoms understand deep structural arrangement of this organic molecule. The title compound has many similar vibrational and other parameter characteristics with the same propanamide family molecules with some variation in deformed mode of vibrations and energy band gap so the reactivity is the considerable point of discussion. Due to varied properties of the molecule it could be further studied or used for specific pharma or artificial application[2] on the basis of this study.

II. Computational Details and Methodology

For the computational study Gauss View (version 5.0) program has been used to obtain molecular information, Vibrational (spectroscopic) analysis, Highest Occupied & lowest unoccupied Orbit observations for molecule, optimized parameters, electronic and thermodynamic studies, reactivity descriptors (both global and local) and also some other observations for which study based on [B3LYP/DFT] combination and the basis set employed [6-311G++ (d,p)]; as density function theory[3,4] offers good compromise for computational calculation and result with accuracy for molecules that's why is has been applied for previous studies[5-7]. These calculations and observations helped to do a better analysis and observation of molecular properties for this molecule. Here the basis set combination which is already quoted, employed with polarization functions on heavy and hydrogen atoms are used for advanced description regarding the polar-bonds for the compound[8, 9]. The Gaussian 09 coded platform is very popular for this kind of study[10]. Optimized geometry operations used for vibrational Infrared frequency calculations and the scaling factor for the frequencies is 0.9682[11,12] to prevent basis set deficiencies. No symmetry constrains have been used for the Geometry optimization for the compound. The operation for reactivity descriptor for example local electrophilicity indices ($\omega_k^{\pm}$) Fukui function ($f_k^{\pm}$), local softness ($s_k^{\pm}$) performed to understand the most electrophilic or nucleophilic sites.

III. Molecular Discussion and Result

Structure of Molecule

In this paper Fig.1 represents the optimized structure of molecule 2-chloro-N-(p-tolyl)propanamide, $C_{10}H_{12}ClNO$ which consists single ring system and single Oxygen(O), Nitrogen(N) and Chlorine(Cl) atoms. The bond length is normal between atoms with little variation also discussed in previous experimental study of this molecule[13, 14]. This propanamide molecule contains a single-ring system, 2 methyl groups and a nitrogen atom in double bond configuration with carbon and single bonded hydrogen shown in the figure1.

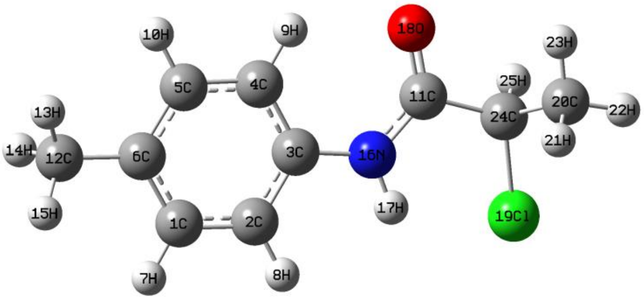

Fig. 1. Optimized geometry for the title molecule by using Chemcraft software

Optimized Parameters

The Optimized Parameters for molecule 2-chloro-N-(p-tolyl) propanamide have been compiled with lengths & angles of bonds and dihedral angles at [B3LYP/6-311++G(d,p)] standard which has been compiled in Table: 1. The molecule exhibits similar normal modes and angle with some variation as compared to previous study[15].

Table: 1. Optimized Parameters of "2-chloro-N-(p-tolyl)propanamide" at "B3LYP/6-311G(d,p)" level

Parameter		Parameter	
Bond-length(Å)		H23-C20-C24	108.58
C1-C2	1.39	C11-C24-Cl19	114.40
C1-C6	1.4	C11-C24-C20	111.26
C1-H7	1.08	C11-C24-H25	106.25
C2-C3	1.4	Cl19-C24-C20	109.61
C2-H8	1.08	Cl19-C24-H25	104.18
C3-C4	1.4	C20-C24-H25	110.86

C3-N16	1.41	**Dihedral-angle (degree)**	
C4-C5	1.39	C6-C1-C2-C3	0.08
C4-H9	1.08	C6-C1-C2-H8	179.82
C5-C6	1.4	H7-C1-C2-C3	179.79
C5-H10	1.08	H7-C1-C2-H8	0.06
C6-C12	1.51	C2-C1-C6-C5	0.28
C11-N16	1.36	C2-C1-C6-C12	178.51
C11-O18	1.22	H7-C1-C6-C5	179.6
C11-C24	1.54	H7-C1-C6-C12	1.61
C12-H13	1.09	C1-C2-C3-C4	0.08
C12-H14	1.09	C1-C2-C3-N16	179.76
C12-H15	1.09	H8-C2-C3-C4	179.65
N16-H17	1.01	H8-C2-C3-N16	0.02
Cl19-C24	1.84	C2-C3-C4-C5	0.05
C20-H21	1.09	C2-C3-C4-H9	179.83
C20-H22	1.09	N16-C3-C4-C5	179.70
C20-H23	1.09	N16-C3-C4-H9	0.18
C20-C24	1.52	C2-C3-N16-C11	178.94
C24-H25	1.09	C2-C3-N16-H17	1.08
Bond-Angle(in degree)		C4-C3-N16-C11	1.40
C2-C1-C6	121.23	C4-C3-N16-H17	179.26
C2-C1-H7	119.05	C3-C4-C5-C6	0.16
C6-C1-H7	119.72	C3-C4-C5-H10	179.78
C1-C2-C3	120.52	H9-C4-C5-C6	179.96
C1-C2-H8	119.70	H9-C4-C5-H10	0.09
C3-C2-H8	119.78	C4-C5-C6-C1	0.32
C2-C3-C4	119.14	C4-C5-C6-C12	178.47
C2-C3-N16	117.18	H10-C5-C6-C1	179.63
C4-C3-N16	123.68	H10-C5-C6-C12	1.585
C3-C4-C5	119.37	C1-C6-C12-H13	152.11
C3-C4-H9	119.86	C1-C6-C12-H14	88.25
C5-C4-H9	120.77	C1-C6-C12-H15	31.43
C4-C5-C6	122.26	C5-C6-C12-H13	29.15
C4-C5-H10	118.40	C5-C6-C12-H14	90.49
C6-C5-H10	119.33	C5-C6-C12-H15	149.83
C1-C6-C5	117.47	O18-C11-N16-C3	0.37
C1-C6-C12	121.19	O18-C11-N16-H17	178.24
C5-C6-C12	121.33	C24-C11-N16-C3	179.17
N16-C11-O18	125.85	C24-C11-N16-C17	2.97
N16-C11-C24	117.57	N16-C11-C24-Cl19	10.82
O18-C11-C24	116.57	N16-C11-C24-C20	114.07
C6-C12-H13	111.36	N16-C11-C24-H25	125.18
C6-C12-H14	111.11	O18-C11-C24-Cl19	170.27
C6-C12-H15	111.44	O18-C11-C24-C20	64.84
H13-C12-H14	107.37	O18-C11-C24-H25	55.91
H13-C12-H15	108.01	H21-C20-C24-C11	65.57
H14-C12-H15	107.35	H21-C20-C24-Cl19	61.96
C3-N16-C11	128.84	H21-C20-C24-H25	176.42
C3-N16-H17	115.70	H22-C20-C24-C11	173.64
C11-N16-H17	115.43	H22-C20-C24-Cl19	58.83
H21-C20-H22	108.79	H22-C20-C24-H25	55.63
H21-C20-H23	108.86	H23-C20-C24-C11	54.05
H21-C20-C24	111	H23-C20-C24-Cl19	178.42
H22-C20-C23	109.08	H23-C20-C24-H25	63.96

Vibrational Spectroscopic Analysis

For the analysis of Vibrational of the compound, some operations have been performed which combine the calculative result by Gauss view 09[16] and VEDA 4 program. Here the compound exhibit 25 atoms and that's why 69 normal-modes of vibrations (3n-6) have been observed. Regarding the simplicity and easy understanding of vibrational analysis Table: 2 has been arranged for selected vibration modes and respective frequencies. All the vibrational wavenumber used in discussion in this paper are scaled with scaling factor 0.9614[17, 18] to reduce anharmonicity. In table: 2 properties like asymmetric kind of stretching, symmetric stretching; scissoring of atoms (for example H-N-C), rocking of atoms such as H-N-C, bending at out of plane and torsion (for example N-C atoms) has been assigned for respective frequency band.

Table: 2 Analysis vibrations of prominent modes of 2-chloro-N-(p-tolyl)propanamide at [B3LYP/6-311G(d,p)] level

Calculated freq	**Scaled freq**	**Intensity**	**Vibration assignments**
3579	3441	76.89	ν_s(N16-H17)(100)
3240	3115	3.85	R[ν_s(C4-H9)(99)]
3170	3048	12.22	R[ν_s(C1-H7)(94)]
3161	3039	16.70	R[ν_s(C5-H10)(86)]
3151	3029	13.71	R[ν_{as}(C1-H7)(51)+ν_{as}(C2-H8)(44)]
3128	3007	11.2	ν_s(C20-H22)(83)
3124	3003	6.4	ν_s(C20-H23)(89)
3108	2988	3.03	ν_s(C24-H25)(87)
3100	2980	15.91	ν_{as}(C12-H15)(96)
3073	2954	19.83	ν_{as}(C12-H14)(97)
3045	2927	10.60	ν_{as}(C20-H21)(76)
3019	2902	37.7	ν_s(C12-H14)(98)
1733	1666	289.94	ν_s(O18-C11)(79)
1655	1591	8.92	R[ν_s(C2-C1)(48)]
1632	1569	107.90	R[ν_s(C6-C5)(17)+ρ(H17-N16-C3)(21)]
1567	1506	450.42	R[σ(H17-N16-C3)(36)]
1544	1484	48.10	R[σ(H7-C1-C2)(47)]
1496	1438	1.86	ρ(H22-C20-C21)(64)+ ρ(H21-C20-C24)(16)
1493	1435	36.75	σ(H15-C12-H14)(62)
1490	1432	6.42	ρ(H21-C20-C23)(70)+τ(H21-C20-C24-C11)(20)
1489	1431	70.74	ρ(H13-C12-H15)(72)+ρ(H14-C12-C6)(21)
1437	1381	43.12	R[ν_s(C1-C2)(28)]
1415	1360	0.21	σ(H15-C12-H13)(91)
1407	1353	8.36	σ(H23-C20-H23)(90)
1345	1293	52.19	R[ρ(H10-C5-C4)(52)]
1336	1284	16.34	ν_s(C1-C6)(40)
1316	1265	1.16	ν_s(C20-C24)(18)+τ(C24-C11-C20-H25)(17)
1268	1219	34.70	ν_s(N16-C3)(15)
1264	1215	38.21	σ(H25-C24-Cl19)(35)+τ(C24-C11-C20-H25)(18)
1237	1189	0.27	ν_s(C12-C6)(17)
1227	1180	5.97	ν_s(C5-C4)(25)+ ν_s(C12-C6)(20)
1207	1160	0.56	ν_s(H8-C2-C3)(71)
1147	1103	11.26	ν_s(H10-C5-C4)(56)+ ν_s(C5-C4)(19)
1094	1052	9.23	ν_s(C20-C24)(21)+τ(H22-C20-C24-C11)(26)
1090	1048	25.66	τ(H21-C20-C24-C11)(27)
1060	1019	13.51	R[τ(H13-C12-C6-C5)(55)]
1035	995	0.86	R[ν_s(C1-C6-C5)(68)]
1009	970	2091	R[τ(H15-C12-C6-C5)(46)]

993	955	22.09	ν_s(C20-C24)(32)+τ(H23-C20-C24-C11)(15)
990	952	1.35	R[τ(H9-C4-C3-N16)(78)]
952	915	1.25	R[τ(H7-C1-C2-C3)(69)+ R[τ(C2-C1-C6-C5)(22)]
933	897	9.83	ν_s(C24-C11)(18)+ ν_s(O18-C11-N16)(19)
863	830	0.18	R[ν_s(C3-C4)(26)]
782	752	0.23	R[ν_s(C12-C6)(27)]
737	708	0.98	τ(O18-C24-C11-N16)(49)
721	693	1.9	R[τ(C2-C1-C6-C5)(41)+τ(N16-C2-C4-C3)(17)]
699	672	54.46	ν_s(Cl19-C24)(32)
653	628	1.57	R[ρ(C1-C6-C5)(63)]
523	503	17.40	τ(N16-C2-C4-C3)(45)
458	440	19.28	ρ(O18-C11-N16)(17)
419	403	0.14	R[τ(H7-C1-C2-C3)(22)+τ(C3-C4-C5-C6)(74)]
415	399	4.34	ν_s(Cl19-C24)(28)+R[ν_s(N16-C3-C4)(21)]

Frequency is shown in cm−1 and Intensity in a.u.; Abbreviations; ν_{as}: asymmetric stretching, ν_s: symmetric stretching, σ: scissoring, ρ: rocking, τ: out of plane torsion, R: ring systems.

N-H vibrations

The aromatic compound exhibits strong band association for the Nitrogen-Hydrogen atoms in symmetric stretching with intensity, which is observed at 3441 cm^{-1}. Other vibrations for Nitrogen observed for rocking mode at frequency at 1569, 440 cm^{-1} carbon and hydrogen molecules (H17-N16-C3). Scissoring vibration mode for H-N-C observed at frequency 1506 cm^{-1} with strong intensity.

C-H vibrations

Vibrations for C-H group observed at frequency range 3115 to 2902 cm^{-1}(scaled frequency) which exhibits the multiplicity from weak to moderate bonds. The C-H Stretching modes for the aromatic compounds are generally found in the extent 3100-300cm^{-1}. For this aromatic compound the normal C-H modes found during this frequency range and the deformed modes such as rocking, torsion, scissoring found below 1600cm^{-1}. Scissoring mode of vibrations for C-H-C group observed at frequencies 1484, 1432, 1360, 1353cm^{-1} for the entitled compound. The rocking mode of movement recorded for the nearby frequencies 1438, 1432, 1431cm^{-1} with low intensity. Other mode of vibration torsion for entitled compound observed at many frequencies below 1060cm^{-1}. Some out of plane modes of vibration observed at low frequencies for aromatic C-H group.

C=O vibrations

In the compound the carbonyl group (C=O) shows mixed vibration modes at scattered frequencies for the title compound. It is considerable that the frequencies of vibration depend on the bond length for carbonyl group. According to this study O=C vibration observed at scaled frequency 1666 cm^{-1}. In the previous study[18] C=O vibration modes stretching observed at frequencies 1678 and 1665cm^{-1} which is found in resemblance with current study. The O=C vibration mode calculated at wave number 1666 cm^{-1} which is identified for the symmetric kind of mode. O-C-N group found with symmetric and rocking mode of vibrations at frequencies 897 and 440cm^{-1} with low intensity. This identification assignment has been shown in table 2.

C-C vibrations

The calculation exhibits that the C-C symmetric vibration mode observed at frequency 1591, 1569 and 1381, 830, 752, 672cm^{-1} with low intensity in the aromatic ring and C-C vibrations for other modes observed at low frequency range. The “Carbon-Carbon” stretching for methyl group associated with the ring observed at 1431cm^{-1} with rocking mode of vibration. The torsion modes are observed at low frequencies. According to calculation torsion modes recorded at frequencies 1019, 955cm^{-1} for H-C-C-C group with low intensities. The mix modes for title compound observed below frequency 1590cm^{-1}. The considerable out of plane and torsion movement appear below 1020cm^{-1}.

Cl-C vibrations

The vibration for Cl-C bond with symmetric mode of vibration observed at frequencies 672 and 399cm^{-1}. A symmetric vibration mode for Cl-C-C observed at frequency 995cm^{-1} in the ring which exhibits vibration with low intensity. H-C-Cl group shows scissoring mode of vibration at frequency 1215cm^{-1} with low intensity.

N-C vibrations

Rocking vibration mode for H-N-C observed at 1569cm^{-1} with low intensity and Scissoring mode found at frequency 1506cm^{-1} with hydrogen and carbon atom associated in ring. Other C-N in symmetry vibration obtained at 1219, 399cm^{-1} with low intensities. Torsion for N-C bond group is obtained at many low frequencies. An O=C=N vibration in symmetry is also obtained at frequency 897cm^{-1}.

Electronic and Thermodynamic property

The electrical characteristics of molecule studied through observation of "Frontier Molecular Orbitals" (FMO). FMO can be characterized by the study of LUMO and HOMO among many. These parameters are most useful quantum chemical parameters and these parameters provide idea about molecular interactions. FMOs are also useful to examine the behavior and reactivity of molecule and capability also to absorb light and kinetic stability as well as chemical reactivity characterized through band gap observation. The measurements for highly energized molecules from outermost orbit that is highest occupied orbit of molecule (HOMO) & lowest unoccupied orbital of molecule (LUMO) given below:

Energy - HOMO: 6.30eV

Energy - LUMO: 0.94eV

Energy gap of HOMO-LUMO: 5.36eV

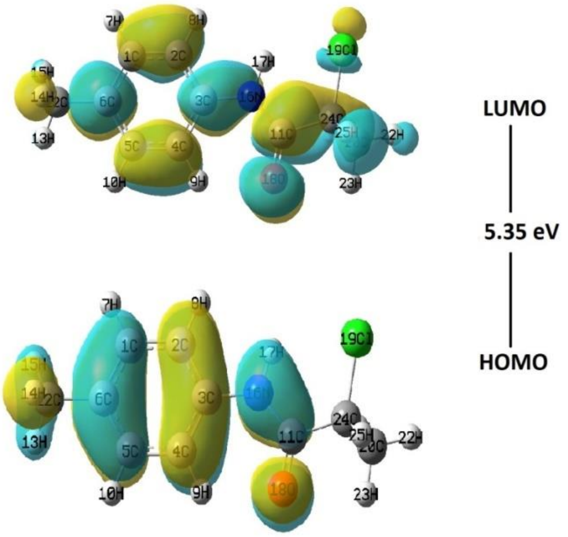

Fig. 2. HOMO & LUMO plots of title molecule

The frontier orbital gap for compound 2-chloro-N-(p-tolyl) propanamideis 5.35 eV which is shown in fig: 2. The electrostatic potential regions such as positive, negative and neutral alignment is shown through color grading for MESP representation. MESP provide useful detail to establish relationship between structure and physiochemical property. So the nucleophilic (blue region) which is electropositive and hence electron poor represents electron donating O-H bonds and the electrophilic (red region) is for electron rich region which could be studied through Molecular electrostatic potential graphic [11, 12]. For the title compound measurements for the electronic parameters and frontier orbital gap (ΔE=FLUMO-FHOMO) have been measured by using theoretical methods.

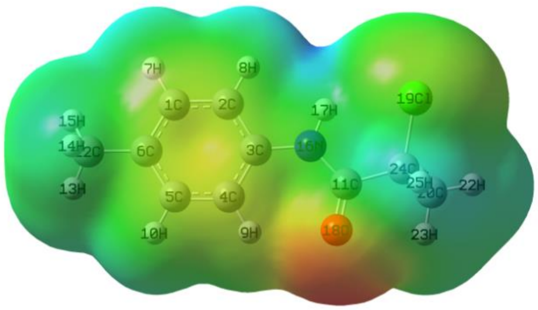

Fig. 3. MESP plot of title molecule

For the reactivity descriptors regarding above study and analysis like chemical-potential (μ), global-hardness (η) are obtained through following equations and chemical hardness (η), absolute electro negativity (χ), electron-affinity (A) and ionization-potential (I) studied and derived at [B3LYP/6-311++G(d, p)] standard.

$$\chi = \frac{1}{2}(I + A)$$

$$\eta = \frac{1}{2}(I - A)$$

$$s = 1/2\eta$$

For the thermodynamic study of entitled compound parameters such as heat capacity (Cv), 'E' represents thermal energy at room temperature, entropy (S) and (ZPE) as zero point energy has been arranged in the Table: 3.

Table: 3 Electronic & Thermodynamic parameters derived at [B3LYP/6-311++G (d,p(] level

Electronic Parameter	**Molecule**	**Thermodynamic Parameter**	**Molecule**
I (eV)	6.29	ZPE (kcal/mol)	126.37
A (eV)	0.94	E (kcal/mol)	134.12
E_g (eV)	5.35	C_v (cal/mol-K)	46.24
χ (eV)	3.61	S (cal/mol-K)	113.06
η(eV)	2.67		
μ (au)	1.62		

Reactivity Descriptors

For the study of reactivity descriptors; Global reactivity descriptors use some parameters where 'μ' represents chemical potential, [$\eta = \frac{1}{2}(I - A)$] global hardness and [$s = 1/2\eta$] global softness, which have been calculated and tabled to explain global reactivity means for the title compound. These descriptors of global-reactivity forecast regarding reactivity of compound but these descriptors don't tell about the sites of reactivity of molecule. So, we have used DFT to extract relevant local reactivity information i.e. information about reactivity sites of the molecule; these parameters known as ‘local-reactivity descriptors’. Descriptors of local reactivity observe the relative reactivity for various atoms for the title compound. In this section we are discussing about three descriptors of local reactivity such as Fukui function, local-softness and local-electrophilicity. These descriptors have been derived by using the following equations:

$f_k^+ = \{q(N+I)-q(N)\}$; for nucleophilic attack

$f_k^- = \{q(N)-q(N-I)\}$; for electrophilic attack

$s_k^\pm = s.f_k^\pm$

$\omega_k^\pm = \omega.f_k^\pm$

In the above equation:

total electrons at neutral state represented by q(N),

total electrons at anion state by q(N+1),

total electrons at cation state by q(N-1).

In table: 4 we have used (f_k, f_k^+,f_k^-), (s_k, s_k^+, s_k^-) and (ω_k, ω_k^+, ω_k^-) to represent neutral, nucleophilic and electrophilic attack respectively. It is observed from previous studies that the site in molecule, where the maximum value of (ω_k^+, ω_k^-) and (s_k^+, s_k^-) observed most electrophilic or nucleophilic positions also observed. In this study the site ‘C5’ is express the max value of all 3 descriptors of local reactivity for the title compound; it means that the site ‘C5’ is mostly in favor for the nucleophilic and electrophilic attacks. In addition at the site C5 the Fukui function f_k^- is greater than f_k^+ this means this site is favorable to electrophilic than nucleophilic substitution.

Table: 4 Local-reactivity descriptors for 2-chloro-N-(p-tolyl)propanamide at [B3LYP/6-311G(d,p)] level

Atom no.	f_k^+	f_k^-	s_k^+	s_k^-	ω_k^+	ω_k^-
1C	-0.0001	-0.5553	-0.00001	-0.1039	-0.0002	-1.3551
2C	0.0097	-0.3695	0.0018	-0.0691	0.0236	-0.9017
3C	-0.1435	0.1982	-0.0268	0.0371	-0.3501	0.4836
4C	0.0644	0.3237	0.0120	0.0605	0.1571	0.7899
5C	0.1367	0.5935	0.0255	0.1111	0.3336	1.4483
6C	0.0072	-0.1494	0.0013	-0.0279	0.0175	-0.3645
11C	0.0298	0.1011	0.0055	0.0189	0.0727	0.2467
12C	0.0755	0.0175	0.0141	0.0032	0.1842	0.0427
20C	0.0286	0.0505	0.0053	0.0094	0.0697	0.1232
24C	-0.0306	-0.4420	-0.0057	-0.0827	-0.0746	-1.0786

IV. Conclusion

The propanamide family molecule 2-chloro-N-(4-methylphenyl) propanamide has been studied and analyzed with DFT program for thermodynamic & electronic parameters, descriptors of reactivity, optimized parameters, analysis of vibrations has been studied. The study of this organic substance at [B3LYP/6-311G++(d,p)] standard derive useful details of vibration spectra at simplified way. The parameters HOMO, LUMO calculated which provide energy band gap 5.35 eV which exhibits very low reactivity. The graphical representation of HOMO & LUMO and energy gap explains the chemical reactivity of the title substance. For local reactivity descriptors, the site ‘C5’ is observed as the max value of reactivity descriptors for the title compound; it means that this site ‘C5’ is most favorable for both nucleophilic & electrophilic attack.

The characteristics and properties observed through this study envision for the specific and artificial application of this molecule after further study.

Conflict of interest

There is no conflict of interest.

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