Vibrational assignments, Frontier Molecular orbitals and Natural Bonding Orbital Analysis of 2-methyl-1-phenylpropan-2-amine

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ABSTRACT

The geometric parameters and theoretical vibrational frequencies of 2-methyl-1-phenylpropan-2-amine calculated using Hartree-Fock method and Density functional theory (B3LYP) methods with 6-31G(d,p) basis sets. The scaled wave numbers are compared with the experimental values. The FT-IR and FT-Raman spectra were recorded in the region of 4000–400 cm^{-1} and 4000 –100 cm^{-1} respectively. Stability of the molecule arising from hyper-conjugative interactions, charge delocalization has been analyzed using Natural Bond Orbital (NBO) analysis. Mulliken analysis and thermodynamic parameters like entropy, Zero-point Vibrational energy, Specific heat, Rotational constant and Dipole moment have been calculated for the title molecule were performed by HF and DFT method.

Keywords: 2-methyl-1-phenylpropan-2-amine, HF, DFT, NBO

1. Introduction:

2-methyl-1-phenylpropan-2-amine is a central nervous system stimulant and it is more frequently used in the treatment of obesity. This is used for short period to promote weight loss in addition to exercise and calorie reduction.2-methyl-1-phenylpropan-2-amine, an anti-obesity medication reduces hunger sensation and helps to release norepinephrine, a neurotransmitter involved in stress responses and responsible for release of epinephrine outside the brain resulting in breakdown of stored fat. Thus, it is a sympathomimetic stimulant with appetite suppressant property[1-3]

2. Experimental details:

The Fourier Infrared spectra and Fourier Raman spectra of the molecule was taken from SDBS recorded in region 4,000–400 and 4,000–100 cm^{-1} respectively [4].

3. Computational details:

In the present work, the density functional method (DFT) has been employed using Becke's three parameter hybrid exchange functional with the Lee-Yang –Parr correlation functional to optimize the structure of the molecule and to calculate the electronic structure of the title molecule [5]. The entire calculations were performed at ab-initio Hartree -Fock(HF) and DFT method using B3LYP levels at 6-31 G(d,p) basis sets on a Pentium V/ 1.6 GHz personal computer using Gaussian 09W program package [6] and applying geometry optimization Initial geometry generated was minimized at the Hartree Fock level using 6-31 G (d,p) basis set. The vibrational modes are assigned using Gauss-View molecular visualization program package. The optimized structural parameters were used in the vibrational frequency calculations at the HF and DFT levels to characterize all stationary points as minima.

4. Molecular geometry

The optimize geometry structure of title molecule at DFT/B3LYP/6-31 G(d,p) level with atomic numbering shown in Fig.1. The global minimum energy obtained by DFT structure optimization is found to be -444.8767 Hartree. The optimized values of bond length and bond angles are shown in Table 1 and Table 2.

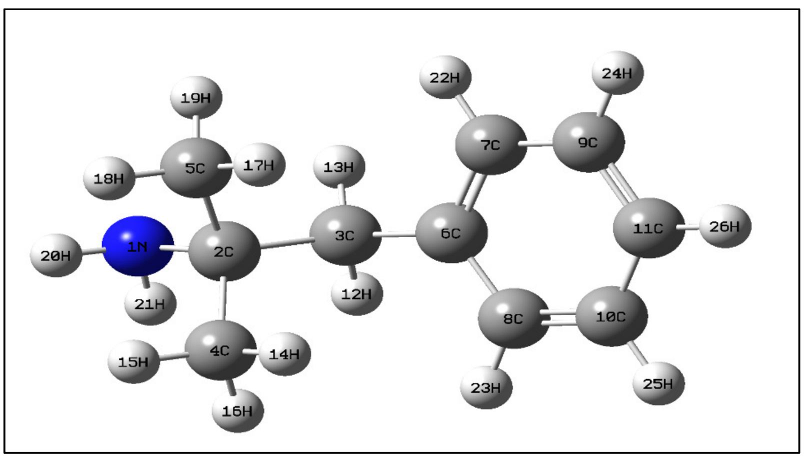


Fig.1 Optimized structure of 2-methyl-1-phenylpropan-2-amine

The most electronegative nitrogen atom is attached to the chain of carbon and hydrogen. Nitrogen is more electronegative than carbon which is more electronegative than hydrogen so, they electrons equally share in covalent bond. The bond length of N1-C2 is 1.4787 A°

and 1.4646A° at DFT/6-31G(d,p) and HF/6-31G(d,p) respectively. Also, bond length of N1-H20 and N1-H21 are 1.0193 A°, 1.0197 A° and 1.0016 A°, 1.0019 A° at DFT/6-31G(d,p) and HF/6-31G(d,p) respectively. The experimental and calculated FT-IR and FT-RAMAN Spectra at DFT/B3LYP/6-31(d,p) and HF/6-31+G (d,p)levels are shown in Fig. 2 & Fig. 3.

Table 1. Optimized parameters bond length of2-methyl-1-phenylpropan-2-amine.

S.NO	OPTIMIZED PARAMETERS	BOND LENGTH (A°)	
		B3LYP/6-31G(d,p)	HF/6-31G(d,p)
1	1N-2C	1.4787	1.4646
2	1N-20H	1.0193	1.0016
3	1N-21H	1.0197	1.0019
4	2C-3C	1.5591	1.5494
5	2C-4C	1.5413	1.5362
6	2C-5C	1.5351	1.5306
7	3C-6C	1.5139	1.5157
8	3C-12H	1.0983	1.088
9	3C-13H	1.0949	1.0844
10	4C-14H	1.0944	1.0841
11	4C-15H	1.0961	1.0869
12	4C-16H	1.0969	1.0876
13	5C-17H	1.093	1.0835
14	5C-18H	1.0965	1.0872
15	5C-19H	1.094	1.0846

Table 2. Optimized parameters bond angle of 2-methyl-1-phenylpropan-2-amine.

SI.NO	OPTIMIZED PARAMETERS	BOND ANGLE (A°)	
		B3LYP/6-31G(d,p)	HF/6-31G(d,p)
1	2C-1N-20H	109.0848	110.5789
2	2C-1N-21H	109.2871	110.8112
3	20H-1C-21H	105.6264	106.9028
4	1N-2C-3C	105.2806	105.3204
5	1N-2C-4C	112.1965	111.7481
6	1N-2C-5C	107.028	107.0445
7	3C-2C-4C	111.1416	111.5129
8	3C-2C-5C	111.1634	111.3792

9	4C-2C-5C	109.8928	109.693
10	2C-3C-6C	116.8832	117.393

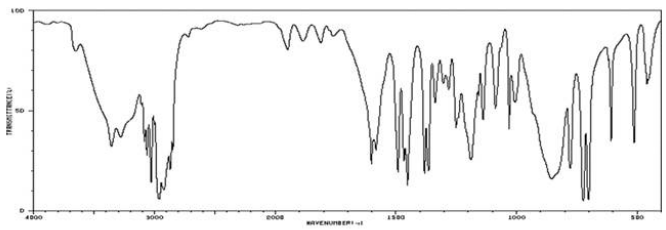


Fig.2. FT-IR spectrum of 2-methyl-1-phenylpropan-2-amine

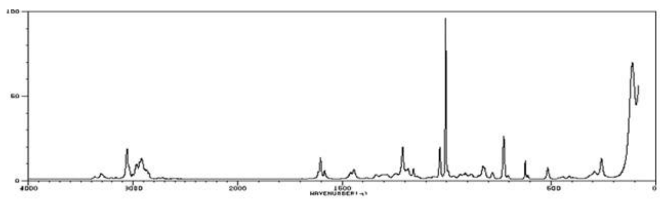


Fig..3: FT-RAMAN spectrum of 2-methyl-1-phenylpropan-1-amine

5. Vibrational analysis:

The title compound has 26 atoms with 72 normal modes of vibrations. All fundamental vibrations are active in both Infrared and Raman spectra. The harmonic-vibrational frequencies of studied molecule have been compared with the experimental frequencies and is given in Table.3. Obtain vibrational wave number slightly greater than the experimental data because of the combination of electron correlation effects and basis sets deficiencies. So, scale down the calculated harmonic wave number in order improve the agreement with the experimental data. Vibrational assignments are based on the observations of the animated modes in Gauss View 5.1 and reported in literature.

C-H Vibrations:

The aromatic organic molecule shows the presence of the wave number region 3000-3100 cm^{-1} and it is the characteristics region for the identification of C-H stretching vibrations [7-8]. The aromatic C-H stretching modes assigned to 3119, 3084, 3062, 3028, 3002 and 2961 cm^{-1} in the FT-IR spectrum. C-H stretching modes assigned to 3058, 2998, 2956 and 2925 cm^{-1} in the FT-RAMAN spectrum. The band absorbed at 3107, 3097, 3090,3080, 3076, 3043, 3023, 3015, 3003, 2997, 2951, 2939 and 2936 cm^{-1}in DFT/B3LYP/6-31G(d,p) method. The band absorbed at 3335, 3323, 3315, 3303, 3298, 3245, 3230, 3214, 3211, 3196, 3154, 3148 and 3138 cm^{-1} in HF/6-31G(d,p) method.

N-H Vibrations:

In generally aromatic primary amines absorb the region 3420-3300 $cm^{-1}$and it's the characteristics region for the identification of N-H stretching vibrations [8]. NH stretching vibration occur in FT-IR spectrum at 3366 cm^{-1}. In FT-RAMAN spectrum at 3377 cm^{-1}. The stretching absorbed at 3439 and 3358 cm^{-1} in DFT/B3LYP/6-31G(d,p) method. In HF/6-31G(d,p) method absorbed at 3772 and 3687 cm^{-1}.

N-C Vibrations:

In generally primary amines containing carbon atoms absorbs region 1030–1200 cm^{-1} and its characteristics region for the identification N-C stretching vibrations [8-9].N-C stretching vibration absorbs at 1189 and 856 cm^{-1} in FT-IR spectrum. N-C stretching absorbs at 1180 cm^{-1} in FT-RAMAN spectrum. The band region absorbs in DFT/B3LYP/6-31G(d,p) at 1182, 952, 918 and 860 cm^{-1}. In HF/6-31G(d,p) at 1302, 1078, 1028 and 951 cm^{-1}.

C-C Vibrations:

The CC stretching vibrations for phenyl ring are generally observed between 1600 and 1400 cm^{-1} is assigned to C-C stretching. C-C stretching absorbs in FT-IR spectrum at 1602 and 1583 cm^{-1}. C-C stretching absorbs in FT-RAMAN at 1605 and 1569 cm^{-1} [10]. In DFT/B3LYP/6-31 G(d,p) band absorbs at 1612 and 1588 cm^{-1}. In HF/6-31G(d,p) band absorbs at 1786 and 1762 cm^{-1}.

6. HOMO and LUMO analysis:

HOMO and LUMO are acronyms for Highest occupied molecular orbital and Lowest unoccupied molecular orbital respectively. It's sometimes called as Frontier molecular orbital. The HOMO is the orbital that primarily acts as an electron donor and the LUMO is the orbital that largely acts as an electron acceptor [11]. The positive and negative phase is represented in red and green colour, respectively. From the plots we can see that the regions of HOMO and LUMO levels spread over the entire molecule and the calculated energy gap of HOMO- LUMO explains the ultimate charge transfer interface within the molecule. The energy gap E_{HOMO}–E_{LUMO}, E_{HOMO+1}–E_{LUMO-1}, E_{HOMO+2}–E_{LUMO-2} is found to be 6.3208eV, 6.5937eV, 8.7065eV respectively. The energy gap between HOMO-LUMO is shown in Fig.4.

Table 3. Vibrational assignments of 2-methyl-1-phenylpropan-2-amine

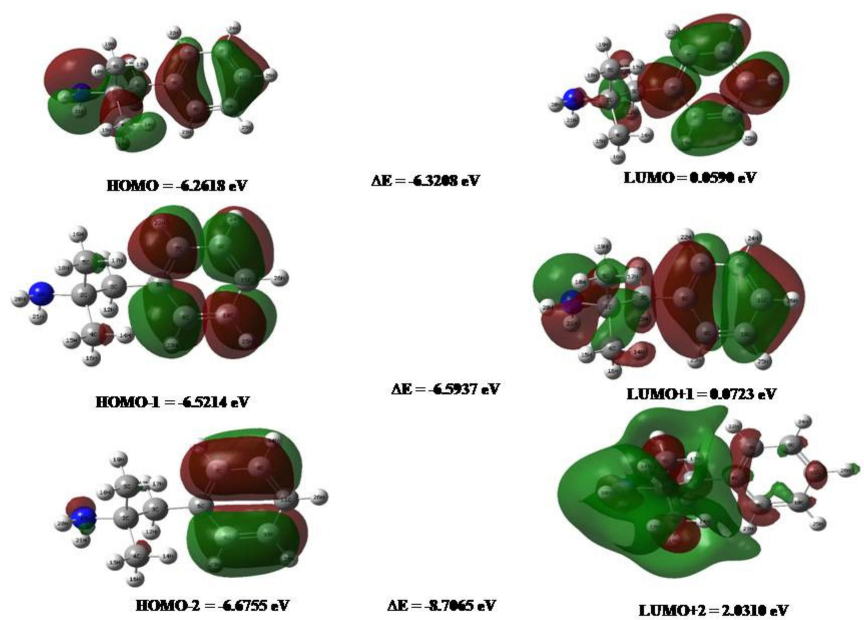
Observed Wave number		Calculated Wave number		Vibrational assignments	IR Intensity		Raman Activity	
FT-IR cm^{-1}	FT-RAMAN cm^{-1}	DFT	HF		DFT	HF	DFT	HF
-	-	3439.62	3772.89	ν(N-H)	1.78	80.75	0.03	73.15
3366	3377	3358.14	3687.75	ν(N-H)	4.18	139.34	0.4	111.59
3119	-	3107.88	3335.31	ν(C-H)	18.45	292.91	20.7	280.11
-	-	3097.21	3323.43	ν(C-H)	40.97	26.76	52.66	16.06
-	-	3090.42	3315.51	ν(C-H)	12.41	100.96	19.99	86.67
3084	-	3080.72	3303.63	ν (C-H)	1.15	91.2	0.43	99.66
3062	-	3076.84	3298.68	ν (C-H)	6.69	15.64	5.91	15.93
-	3058	3043.86	3245.22	ν (C-H)	24.43	43.96	43.64	53.69
3028	-	3023.49	3230.37	ν (C-H)	39.25	57.29	38.51	44.92
-	-	3015.73	3214.53	ν (C-H)	26.08	51.11	42.13	77.88
3002	-	3003.12	3211.56	ν (C-H)	34.48	72.14	23.35	40.79
-	2998	2997.3	3196.71	ν (C-H)	11.09	35.22	42.84	54.93
2961	2956	2951.71	3154.14	ν (C-H)	16.86	182.73	16.72	210.71
-	-	2939.1	3148.2	ν (C-H)	36.87	99.55	52.43	30.39
2920	2925	2936.19	3138.3	ν (C-H)	23.09	12.92	28.07	36.26
-	-	1614.08	1790.91	β(H-N-C), τ(H-N-C-C)	29.35	10.14	6.05	28.46
1602	1605	1612.14	1786.95	ν (C-C)	2.45	29.2	40.96	4.54
1583	1569	1588.86	1762.2	ν (C-C), β (C-C-C)	0.8	9.21	1.58	9.59
1492	-	1492.83	1648.35	β (H-C-C)	10.2	0.29	14.06	0.56
-	-	1477.31	1623.6	β (H-C-H)	4.65	1.54	3.69	1.43
1467	-	1475.37	1621.62	β (H-C-H)	8.72	14.7	8.99	9.71
-	-	1458.88	1605.78	β (H-C-H)	1.2	0.46	1.91	0.39

1453	-	1452.09	1601.82	β (H-C-H)	0.91	23.06	0.95	25.89
-	-	1450.15	1596.87	β (H-C-H)	0.94	23.96	8.1	2.83
-	1434	1448.21	1595.88	β (H-C-C)	4.29	1.77	0.35	21.29
1382	1401	1388.07	1543.41	β (H-C-H)	7.34	3.62	7.69	1.61
1365	-	1370.61	1526.58	β (H-C-H)	10.42	2.07	11.46	0.75
1338	1339	1329.87	1474.11	β (H-N-C), β (H-C-C)	2.13	3.83	0.23	6.73
-	-	1321.14	1465.2	ν (C-C), β (H-C-C)	0.16	0.84	2.56	3.46
1304	1308	1311.44	1451.34	ν (C-C), (H-C-C-C)	0.5	5.15	10.43	4.55
1282	1284	1296.89	1386	β (H-N-C), τ(H-C-C-C)	15.12	16.66	17.9	5.26
1243	1262	1241.6	1329.57	ν (C-C), τ (H-C-C-C)	19.11	5.03	9.97	1.6
-	1212	1195.04	1319.67	ν (C-C)	2.18	22.98	21.48	10.7
1189	1180	1182.43	1302.84	ν (N-C)	16.02	4.29	1.86	7.23
1168	-	1172.73	1284.03	β (H-C-C)	0.29	6.31	0.22	4.35
-	-	1150.42	1253.34	β (H-C-C)	0.02	5.42	8.06	9.96
1139	1133	1131.02	1202.85	β (H-C-C)	11.85	8.13	1.79	1.41
1088	1096	1082.52	1170.18	ν (C-C), β (H-N-C)	5.86	1.09	5.37	0.27
-	1036	1051.48	1158.3	β (H-N-C)	3.87	2.48	5.08	2.74
1031	1033	1025.29	1118.7	ν (C-C), β (H-C-C)	2.36	12.34	1.94	9.33
1007	1006	1003.95	1110.78	τ (H-C-C-C)	6.18	2.47	1.01	0.58
-	984	986.49	1109.79	β (C-C-C)	0.29	24.07	5.39	2.41
-	-	967.09	1090.98	τ (H-C-C-C), τ (C-C-C-C)	0.42	0.54	0.01	0.04
-	-	952.54	1078.11	ν (N-C), ν (C-C), τ (H-C-C-C)	0.93	9.61	0.15	26.43
938	-	943.81	1057.32	τ (H-C-C-C)	0	0.1	4.92	8.01
-	-	918.59	1028.61	ν (N-C)	12.26	10.09	3.83	4.3
-	-	913.74	1007.82	ν (C-C),	1.71	3.34	0.45	2.3

				τ (H-C-C-C)				
-	896	895.31	997.92	τ (H-C-C-C)	11.98	2.01	1.8	10.64
-	-	869.12	955.35	ν (C-C), τ (H-C-C-C)	0.15	4.37	14.64	4.69
856	-	860.39	951.39	ν (N-C), ν (C-C), τ (H-N-C-C)	110.6	5.6	133.12	6.21
-	839	837.11	948.42	τ (H-C-C-C)	0.02	4.71	7.63	0.71
-	828	814.8	893.97	ν (C-C), β (C-C-C)	14.86	5.28	11.15	6.66
776	-	761.45	845.46	ν(C-C), τ (H-C-C-C), τ (C-C-C-C)	13.89	2.8	26.43	1.36
702	708	707.13	781.11	ν (C-C), τ (H-C-C-C)	24.03	10.78	41.98	7.41
-	-	695.49	765.27	τ (C-C-C-C)	12.05	1.62	2.19	6.89
609	618	616.92	674.19	β (C-C-C)	0	4.24	0	4.49
-	-	598.49	658.35	β (C-C-C), τ (C-C-C-C)	5.81	0.79	6.5	0.94
514	-	505.37	557.37	β (N-C-C), ρ_O (C-C-C-C)	9.81	3.27	12	2.76
-	-	436.5	481.14	β (N-C-C), β (C-C-C), ρ_O (C-C-C-C)	0.25	0.83	0.18	0.68
-	-	430.68	473.22	β (N-C-C), τ (N-C-C-C), ρ_O (C-C-C-C)	7.69	0.52	8.1	0.52
-	-	407.4	453.42	τ (H-C-C-C), τ (C-C-C-C)	0	0.03	0	0.03
-	393	380.24	414.81	β (C-C-C), ρ_O (C-C-C-C)	1.68	0.69	1.46	0.85
-	360	369.57	405.9	β (C-C-C), τ (H-C-C-C)	1.03	0.26	1	0.3
-	-	312.34	339.57	β (N-C-C), β (C-C-C),	19.19	1.03	17.99	1.26

				τ (H-N-C-C)				
-	-	289.06	321.75	τ (H-N-C-C), τ (H-C-C-C)	16.2	0.86	19.74	0.85
-	-	276.45	303.93	β (C-C-C), τ (H-C-C-C)	0.25	0.29	0.22	0.5
-	250	258.99	287.1	β (C-C-C), τ (H-C-C-C)	5.28	1.19	7.99	1.06
-	-	244.44	267.3	β (C-C-C), τ (C-C-C-C)	1.13	3.83	1.08	3.6
-	-	236.68	261.36	τ (H-N-C-C), τ (H-C-C-C)	7.37	1.73	8.9	1
-	113	95.06	104.94	β (C-C-C), ρ_O(C-C-C-C)	0.23	5	0.31	4.67
-	-	89.24	95.04	τ (C-C-C-C)	0.17	3.02	0.16	2.15
-	-	47.53	46.53	τ (C-C-C-C)	0.32	4.01	0.36	4.08

Where, ν- Stretching, β- Bending, τ - Torsion, ρ_O - Out of plane.



. **Fig.5. Energy gap between HOMO-LUMO of 2-methyl-1-phenylpropen-2-amine**

7. NBO analysis

Natural bond orbital (NBO) analysis provides an efficient method for studying intra and intermolecular bonding and interaction among bonds and provides a convenient basis for investigating charge transfer or conjugative interaction in molecular systems. NBO theory also allows the assignment of the hybridization of atomic lone pairs and of the atoms involved in bond orbitals. Some electron donor orbital, acceptor orbital and the interacting stabilization energy resulted from the second-order micro-disturbance theory are reported. The second-order Fock matrix is carried out to evaluate the donor–acceptor interactions in NBO analysis [13]. The results of interactions are the loss of occupancy from the localized NBO of the idealized Lewis structure into an empty non-Lewis orbital. For each donor (i) and acceptor (j), the stabilization energy $E^{(2)}$ associated with the delocalization i→j is estimated as

$$E^{(2)} = E_{ij} = q_i \frac{F(i,j)^2}{(\varepsilon_i - \varepsilon_j)}$$

where q_i is the donor orbital occupancy, $\varepsilon_i$and $\varepsilon_j$the diagonal elements and F(i,j) is the off diagonal NBO Fock matrix element. The second order perturbation theory analysis of Fock matrix in NBO shows strong intermolecular hyper conjugative interactions, which are presented in Table. The larger the $E^{(2)}$ value, the more intensiveis the interaction between electron donors and electron acceptors, i.e. the more donating tendency from electron donors to electron acceptors and the greater the extent of conjugation ofthe whole system. Delocalization of electron density between occupied Lewis-type (bond or lone pair) NBO orbitals and formally unoccupied (anti-bond or Rydgberg) non-Lewis NBO orbitals correspond to a stabilizing donor–acceptor interaction [14-17].

NBO analysis has been calculated on the title molecule by DFT/B3LYP using 6-31G(d,p)basis set. The NBO analysis has been performed to elucidate the intramolecular interaction, rehybridization and delocalization of electron density within the molecule, which are presented in Table 4.

In the molecule, a strong intramolecular hyper conjugative interaction of π-electrons with the large energy contributions from π(C8-C10) toπ*(C6-C7) have energy value 22.65 kcal/mol. Second large energy contributions π(C6-C7) → π*(C9-C11) and π(C9-C11) → π*(C8-C10) have energy value 21.43 kcal/mol and 21.1 kcal/mol respectively. Energy contributions π(C6-C7) → π*(C8-C10) and π(C8-C10) → π*(C9-C11) have energy value 19.84 and 19.79. Energy contributions π(C9-C11) → π*(C6-C7) have energy value18.69 kcal/mol.

The lone pair interactions were prominent in the title compound as expected due to the charge transfer that taking place from lone pair atom to the atom attached to it. The lone pair contribution energy from LP(N1) → σ*(C2-C4) have energy value 6.21 kcal/mol.

Table 4. Natural Bond Orbital of 2-methyl-1-phenylpropan-2-amine

Donor	ED/e	Acceptor	ED/e	$E^{(2)}$	Ej-Ei	F(i,j)
σ(C6-C7)	1.97376	σ*(C6-C8)	0.02385	4.19	1.3	0.066
π(C6-C7)	1.65287	π*(C8-C10)	0.33403	19.84	0.28	0.067
π(C6-C7)	1.65287	π*(C9-C11)	0.33492	21.43	0.28	0.069
σ(C6-C8)	1.97389	σ*(C6-C7)	0.02373	4.18	1.3	0.066
σ(C7-H22)	1.98157	σ*(C6-C8)	0.02385	4.38	1.12	0.063
π(C8-C10)	1.66697	π*(C6-C7)	0.34337	22.65	0.29	0.073
π(C8-C10)	1.66697	π*(C9-C11)	0.33492	19.79	0.28	0.067
σ(C8-H23)	1.98167	σ*(C6-C7)	0.02373	4.36	1.12	0.063
π(C9-C11)	1.66677	π*(C6-C7)	0.34337	18.69	0.29	0.066
π(C9-C11)	1.66677	π*(C8-C10)	0.33403	21.1	0.28	0.069
LP(N1)	1.96168	σ*(C2-C4)	0.03196	6.21	0.67	0.058

a $E^{(2)}$ means energy of hyper conjugative interaction (stabilization energy).

b Energy difference between donor and acceptor i and j NBO orbitals.

c F(i,j) is the Fock matrix element between i and j NBO orbitals.

8. Mulliken analysis

The total atomic charges of the molecule obtained by Mulliken using HF and B3LYP with basis set was listed in Table and the graphical representation of the atomic charges is shown in Fig.6. Mulliken charges arise from the Mulliken population analysis and provide a means of atomic charge distribution in the molecule from carried out computational methods. In the application of Quantum mechanical calculations to molecular system, the atomic charges calculations play in important role. The nitrogen atom (N1) carries negative charge. Carbon atom (C6) present in the ring is carries positive charge and carbon atom (C2) attached to nitrogen atom is also carries positive charge at DFT level. But other carbon atoms are carries negative charge. At HF level, C2 have negative charge. All hydrogen atoms present in the molecule have positive charge.

Table.5. Mulliken charge analysis of 2-methyl-1-phenylpropan-2-amine

ATOMS	B3LYP/6-31G(d,p)	HF/6-31G(d,p)
N1	-0.58335	-0.68295
C2	0.139031	0.097854
C3	-0.22576	-0.20427
C4	-0.30649	-0.31169
C5	-0.30152	-0.30983
C6	0.123024	-0.00887
C7	-0.12246	-0.15594
C8	-0.12189	-0.15534
C9	-0.08615	-0.14472
C10	-0.08595	-0.14457
C11	-0.08781	-0.1557
H12	0.085043	0.111551
H13	0.112763	0.142652
H14	0.112031	0.124423
H15	0.09002	0.10238
H16	0.085468	0.096447
H17	0.111194	0.12312
H18	0.08903	0.101196
H19	0.109593	0.122759
H20	0.227537	0.26063
H21	0.227028	0.258645
H22	0.082485	0.147784
H23	0.077568	0.142928
H24	0.083728	0.147684
H25	0.083042	0.147047
H26	0.082791	0.146773

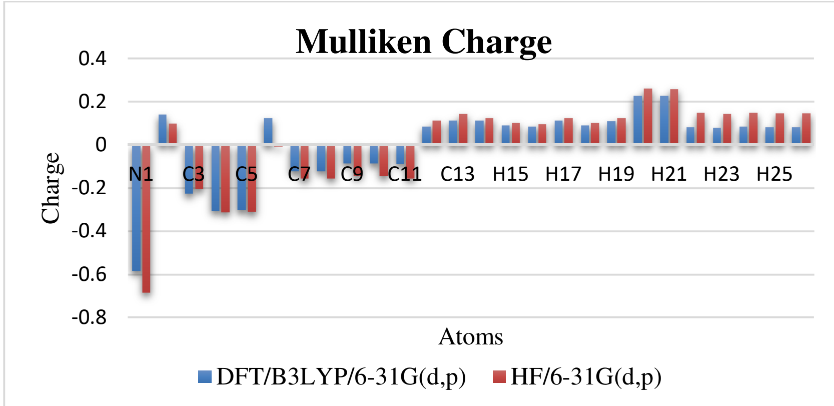


Fig.6. Muliken's atomic charges of 2-methyl-1phenylpropan-2-amine

9. Thermodynamic properties

Thermo dynamical parameter calculated at HF and B3LYP with basis set 6-31G(d,p) of the title compound is presented in Table 5. It is found that the SCF energy minimum at DFT levels than HF levels. The thermodynamic data provides useful information for further study on the title compound. These standard thermodynamic functions can be used as reference thermodynamic values to calculate changes of entropies ΔST, changes of enthalpies ΔHT and changes of Gibbs free energies ΔGT of the reaction. The dipole moment and its principal inertial axes are strongly depending upon the conformation of the molecule.

Table.5. Thermodynamic parameters of 2-methyl-1-phenlypropan-2-amine

THERMODYNAMIC PARAMETERS	DFT/B3LYP/ 6-31 G (d, p)	HF-B3LYP/ 6-31 G (d, p)
SCF energy (au)	-444.8767	-441.8933
Total energy (thermal) E_{total}(Kcal/mol)	151.641	160.932
Vibrational energy E_{vib}(kcal/mol)	149.864	159.154
Zero-point Vibrational energy (kcal/mol)	144.77904	154.50775
Specific heat, C_v (cal/mol K)	43.439	40.168
Entropy, S (cal/mol K)	101.232	98.756
Rotational constant (GHz)		
X	2.38753	2.42304
Y	0.64975	0.6512
Z	0.59095	0.59278
Dipole moment μ (Debye)		
μx	-0.2301	-0.1944
μy	-0.9505	-0.982
μz	0.7133	0.7455
Total	1.2104	1.2482

9. Conclusion

Density functional calculations have been successfully performed for the title compound of 2-methyl-1-phenlypropan-2-amine and the calculated results show that B3LYP/6-31 G(d,p) method can reproduce the title compound very well. Complete vibration assignments were made, and harmonic vibration frequencies calculated have been compared with experimental FT-IR and FT-Raman spectra. The observed and calculated frequencies are found be in good agreement. NBO analysis shows that charge transfer takes place in the molecule. Mulliken and Thermodynamic properties were tabulated. The results presented in this work indicate that DFT method of quantum mechanical calculation is reliable for analysis of vibrational frequency of the title compound.

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