

# A Theoretical Study of 5-methyl-2-isopropylphenol (Thymol) by DFT

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## ABSTRACT

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Gaussian 09, RevisionA.01, software package was used for the theoretical quantum chemical calculations of 5-methyl-2-isopropylphenol. DFT/B3LYP/6-311G (d, p) basis was used to perform geometric optimization and vibrational frequency determination of the molecule. The statistical thermochemical calculations of the molecule were done at DFT/B3LYP/6-311G (d, p) basis set to calculate the standard thermodynamic functions: heat capacity (CV), entropy (S) and Enthalpy (E). Various NLO properties like total dipole moment ( $\mu$ ), mean linear polarizability ( $\alpha$ ), anisotropic polarizability ( $\Delta\alpha$ ), first order polarizability ( $\beta$ ), and second order hyperpolarizability ( $\gamma$ ) in terms of x, y, z components were calculated at DFT/B3LYP/6-311G (d, p) basis set for 5-methyl-2-isopropylphenol. Mulliken population analysis was also done using the same basis set. Time Dependent DFT (TD-DFT) method using the same basis set was used to compute UV-Visible absorption spectra, ECD spectra, electronic transitions, vertical excitation energies and oscillator strengths of 5-methyl-2-isopropylphenol. FMO analysis, ESP study were also done using the same basis set.

**Keywords** : DFT, FMO, Mulliken population analysis, TD-DFT, NLO properties, ECD, Global reactive descriptors

## I. INTRODUCTION

Thymol, a natural monoterpene phenol, also known by the chemical names 2-isopropyl-5-methylphenol and 5-methyl-2-isopropylphenol in accordance with International Union of Pure and Applied Chemistry (IUPAC), is crystalline and colourless with a characteristic odour. The structural formula of this compound is shown in Fig. 1.

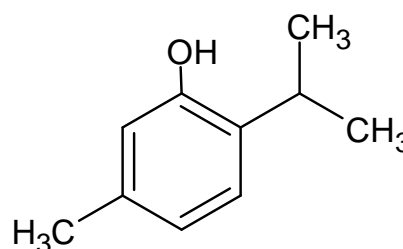


Figure 1: Structural formula of 5-methyl-2-isopropylphenol

Thymol isomeric with carvacrol is abundantly found in certain plants such as *Thymus vulgaris* [1], *Ocimum gratissimum* [2], *Thymus ciliates* [3], *Satureja thymbra* [4], *Thymus zygis* [5], *Trachyspermum ammi* [6], *Carum* [7], *Thymbra capitata* [8] etc.

Thymol, a white crystalline solid has density 0.96 g/cm<sup>3</sup> at 25°C with a melting point ranging from 49°C to 51°C [9]. It is highly soluble in alcohol, alkaline solutions and other organic solvents due to deprotonation of phenol but is slightly soluble in water at neutral pH and it absorbs maximum UV radiation at 274nm[10-11].

Thymol has been known to possess biological activities like antiseptic, antibacterial, antifungal, anthelmintic, antiviral, antioxidant, expectorant, antispasmodic, carminative, diaphoretic, sedative, anti-rheumatic, and even anti-cancer, antihyperlipidemic and anti-hyperglycaemic action [12-19]. Thymol and its derivatives have been evaluated for quantitative structure -activity relationship to predict the biological activity [20]. Thymol is an important agent of natural origin and has generated interest in scientific community throughout the world for its new biological and pharmacology activities. This motivated us to carry out computational study of this compound. The computation of the geometry and electronic properties presented here are very helpful in understanding the structure-activity relationship of this compound.

## II. MATERIALS AND METHODS

All theoretical calculations of 5-methyl-2-isopropylphenol as depicted by graphical abstract in Fig. 2 have been performed using personal laptop using Gaussian 09, Revision A. 01 software package [21] and Gauss View 6.0 programme. DFT (Density Functional Theory), and the Becke three-parameter exchange functions in combination with the LYP

correlation function of the Lee, Yang and Parr (B3LYP) method were used for the theoretical study of 5-methyl-2-isopropylphenol. DFT/B3LYP/6-311G (d,p) basis set was used for determining geometrical optimizations and vibrational frequency of the molecule. Time Dependent DFT (TD-DFT) method using the same basis sets was used to compute the Simulated UV-Visible absorption spectra, oscillator strengths, vertical excitation energies and electronic transitions of the same molecule.



Figure 2: Graphical Abstract of 5-methyl-2-isopropylphenol

## III. RESULTS AND DISCUSSION

### Geometrical analysis

5-methyl-2-isopropylphenol commonly called Thymol having empirical formula C<sub>10</sub>H<sub>14</sub>O, Molecular mass:150.10447 amu, is an asymmetric top type of molecule with 69 degrees of freedom. The optimised molecular structure of the molecule under consideration i.e., 5-methyl-2-isopropylphenol is obtained from Gaussian 09, Revision A. 01, and Gauss view 6.0 programme with the numbering scheme of atoms as shown in Fig. 3. The optimised geometrical parameters (bond length, bond angle and dihedral angle) calculated by B3LYP/6-311G (d, p) level basis set are listed in Table 1.

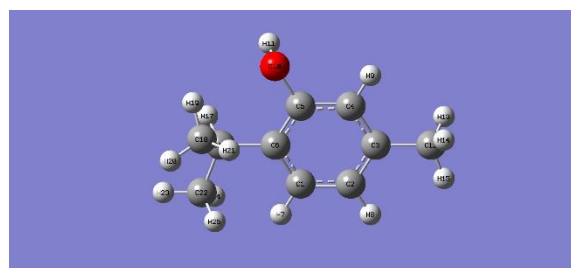


Figure 3: Optimised Molecular structure of 5-methyl-2-isopropylphenol

Table 1: The optimised geometrical parameters (bond length, bond angle and dihedral angle) of 5-methyl-2-isopropyl phenol as calculated by B3LYP/6-311G (d, p) level basis set

S. No.	Bond between atoms	Bond length(Å)	Bond angle between atoms	Bond angle (°)	Dihedral angle between atoms	Dihedral angle(°)
1	R(1,2)	1.3944	A(2,1,6)	122.222	D(6,1,2,3)	-0.2158
2	R(1,6)	1.3973	A(2,1,7)	118.5813	D(6,1,2,8)	179.8521
3	R(1,7)	1.0835	A(6,1,7)	119.1966	D(7,1,2,3)	179.8447
4	R(2,3)	1.3969	A(1,2,3)	120.5507	D(7,1,2,8)	-0.0874
5	R(2,8)	1.0847	A(1,2,8)	119.6073	D(2,1,6,5)	0.0805
6	R(3,4)	1.3965	A(3,2,8)	119.842	D(2,1,6,16)	-177.803
7	R(3,12)	1.5101	A(2,3,4)	118.0216	D(7,1,6,5)	-179.9804
8	R(4,5)	1.3939	A(2,3,12)	121.5052	D(7,1,6,16)	2.1361
9	R(4,9)	1.0851	A(4,3,12)	120.468	D(1,2,3,4)	0.0899
10	R(5,6)	1.409	A(3,4,5)	121.1895	D(1,2,3,12)	-179.0809
11	R(5,10)	1.3724	A(3,4,9)	120.7266	D(8,2,3,4)	-179.9782
12	R(6,16)	1.5248	A(5,4,9)	118.0838	D(8,2,3,12)	0.851
13	R(10,11)	0.9634	A(4,5,6)	121.3213	D(2,3,4,5)	0.1642
14	R(12,13)	1.095	A(4,5,10)	116.0158	D(2,3,4,9)	-179.8879
15	R(12,14)	1.0936	A(6,5,10)	122.6604	D(12,3,4,5)	179.3439
16	R(12,15)	1.0916	A(1,6,5)	116.6941	D(12,3,4,9)	-0.7081
17	R(16,17)	1.0999	A(1,6,16)	122.7654	D(2,3,12,13)	109.4264
18	R(16,18)	1.5439	A(5,6,16)	120.5064	D(2,3,12,14)	-131.3191
19	R(16,22)	1.5349	A(5,10,11)	110.0982	D(2,3,12,15)	-10.6066
20	R(18,19)	1.093	A(3,12,13)	111.0946	D(4,3,12,13)	-69.7243
21	R(18,20)	1.0937	A(3,12,14)	111.3282	D(4,3,12,14)	49.5302
22	R(18,21)	1.0938	A(3,12,15)	111.2481	D(4,3,12,15)	170.2426
23	R(22,23)	1.0929	A(13,12,14)	107.0864	D(3,4,5,6)	-0.3036
24	R(22,24)	1.0928	A(13,12,15)	107.7451	D(3,4,5,10)	179.1331
25	R(22,25)	1.0934	A(14,12,15)	108.1556	D(9,4,5,6)	179.7471
26			A(6,16,17)	107.8209	D(9,4,5,10)	-0.8161
27			A(6,16,18)	110.9679	D(4,5,6,1)	0.1759
28			A(6,16,22)	113.9318	D(4,5,6,16)	178.1102
29			A(17,16,18)	107.5539	D(10,5,6,1)	-179.2229
30			A(17,16,22)	105.6424	D(10,5,6,16)	-1.2885
31			A(18,16,22)	110.5516	D(4,5,10,11)	173.573
32			A(16,18,19)	111.7492	D(6,5,10,11)	-6.9986
33			A(16,18,20)	110.7198	D(1,6,16,17)	-143.5051
34			A(16,18,21)	110.2091	D(1,6,16,18)	98.9487
35			A(19,18,20)	108.0161	D(1,6,16,22)	-26.5991
36			A(19,18,21)	107.8006	D(5,6,16,17)	38.6896
37			A(20,18,21)	108.2209	D(5,6,16,18)	-78.8566
38			A(16,22,23)	109.7996	D(5,6,16,22)	155.5957
39			A(16,22,24)	111.5833	D(6,16,18,19)	55.5012
40			A(16,22,25)	111.6222	D(6,16,18,20)	175.9601
41			A(23,22,24)	108.1172	D(6,16,18,21)	-64.3388
42			A(23,22,25)	107.3555	D(17,16,18,19)	-62.2077
43			A(24,22,25)	108.2055	D(17,16,18,20)	58.2512
44					D(17,16,18,21)	177.9524

45					D(22,16,18,19)	-177.0814
46					D(22,16,18,20)	-56.6225
47					D(22,16,18,21)	63.0786
48					D(6,16,22,23)	-173.1717
49					D(6,16,22,24)	-53.3145
50					D(6,16,22,25)	67.8983
51					D(17,16,22,23)	-55.0092
52					D(17,16,22,24)	64.8479
53					D(17,16,22,25)	-173.9392
54					D(18,16,22,23)	61.0606
55					D(18,16,22,24)	-179.0822
56					D(18,16,22,25)	-57.8694

### Vibrational analysis

The fundamental vibration of a non-linear molecule which contains N atoms is equal to  $(3N-6)$ , apart from three translational and three rotational degrees of freedom [22-24]. 5-methyl-2-isopropylphenol, molecule being studied belongs to asymmetric top group symmetry and has 25 atoms; hence normal modes of vibrations possible are 69. As mentioned above, IR and Raman vibrational properties of the molecule has been studied using B3LYP by DFT at 6-311G (d, p) basis level set and the theoretical IR and Raman spectra are as shown in Fig. 4 and Fig. 5 respectively while the frequencies, intensities and their corresponding assignments for the theoretical spectra are tabulated in Table 2. Animations generated for various vibrational modes by Gauss view 6.0 program were inspected visually and the standard values [22,24] reported were used for

vibrational assignment. A comprehensive account of characteristic group absorptions and their relationship to molecular structure is discussed below.

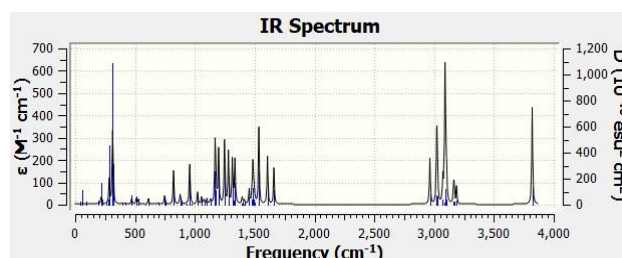


Figure 4: Theoretical IR spectra of 5-methyl-2-isopropylphenol

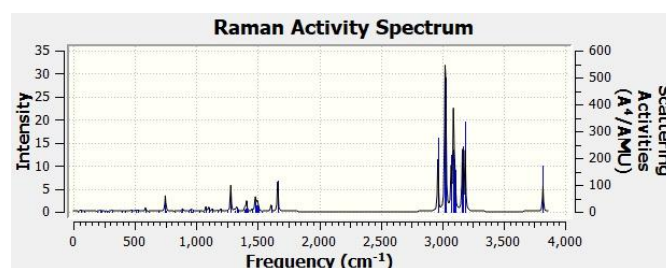


Figure 5: Theoretical Raman spectra of 5-methyl-2-isopropylphenol

Table 2 : The frequencies, intensities, and their corresponding assignments for the theoretical IR and Raman spectra of 5-methyl-2-isopropylphenol

Mode	Frequency	Infrared	Raman	Depolar-p	Depolar-u	Vibrational assignment
1	38.90	0.2085	0.8584	0.7492	0.8567	
2	61.43	1.7192	5.4622	0.7481	0.8559	
3	91.54	0.5501	2.6675	0.7500	0.8571	
4	189.39	1.4255	0.5472	0.7500	0.8571	
5	216.28	8.9079	4.1968	0.7460	0.8545	
6	223.79	2.2296	3.9680	0.7317	0.8450	
7	256.34	1.3721	0.2963	0.7095	0.8301	
8	274.81	2.6993	0.5131	0.2617	0.4149	

9	285.16	32.3954	0.6556	0.3993	0.5707	
10	312.72	85.4998	4.8230	0.5138	0.6788	Aromatic ring vibration
11	317.43	25.0248	2.1408	0.4964	0.6634	Aromatic ring vibration
12	394.36	1.0524	2.1799	0.6146	0.7613	Aromatic ring vibration
13	421.26	1.7815	2.3755	0.1415	0.2479	Aromatic ring vibration
14	472.32	8.0745	5.3152	0.5624	0.7199	Aromatic ring vibration
15	510.58	7.7859	4.6722	0.4838	0.6521	Aromatic ring vibration
16	524.63	6.1153	5.4781	0.2328	0.3777	Aromatic ring vibration
17	584.56	0.4888	12.2919	0.5842	0.7375	Aromatic ring vibration
18	610.90	7.6024	0.5634	0.5796	0.7339	Aromatic ring vibration
19	692.95	2.4461	3.4089	0.1530	0.2654	Out-of-plane C-H vibrations(oops)
20	747.74	10.5073	49.3936	0.1060	0.1917	Out-of-plane C-H vibrations(oops)
21	752.11	2.8109	5.0422	0.1040	0.1884	Out-of-plane C-H vibrations(oops)
22	821.79	43.2679	0.5073	0.1229	0.2190	C-H out-of-plane wagging of -CH <sub>2</sub> group
23	877.17	12.9555	0.4383	0.7179	0.8358	C-H out-of-plane wagging of -CH <sub>3</sub> group
24	887.87	3.5630	10.7279	0.4186	0.5902	Out-of-plane rocking of -CH <sub>3</sub> of isopropyl group
25	933.28	2.0970	2.6849	0.7210	0.8379	Out-of-plane rocking of -CH <sub>3</sub> of isopropyl group
26	957.03	45.6497	7.8061	0.1668	0.2859	Aromatic ring vibrations (oops)
27	959.70	9.1272	1.8362	0.1578	0.2727	Aromatic ring vibrations (oops)
28	969.04	1.4070	6.5027	0.7497	0.8569	Out-of-plane rocking of -CH <sub>3</sub> of isopropyl substituent
29	1022.30	16.1965	3.5302	0.3729	0.5433	Aromatic ring vibrations
30	1056.71	9.2063	0.5030	0.5777	0.7323	In-plane C-H bending of -CH <sub>3</sub> group present at meta position
31	1077.92	6.4216	17.7909	0.2328	0.3776	In-plane C-H bending of -CH <sub>3</sub> group of isopropyl group substituent
32	1101.08	7.5154	15.8172	0.0877	0.1612	Out-of-plane C-H bending of -CH <sub>3</sub> group of isopropyl group present at meta position
33	1131.32	5.9663	10.3369	0.7466	0.8549	In-plane C-H bending of aromatic ring
34	1169.25	74.7816	4.5245	0.3516	0.5203	In-plane O-H bending of phenolic group
35	1175.25	33.3199	3.0005	0.7234	0.8395	Out -of--plane C-H bending of Aromatic ring
36	1198.46	71.3548	10.5743	0.2562	0.4079	In-of-plane C-H bending of Aromatic ring
37	1247.72	82.4735	2.9960	0.7409	0.8512	In-plane C-H bending of Aromatic ring
38	1280.19	68.3635	95.1323	0.0916	0.1678	Out-of-plane C-H bending of Aromatic ring
39	1313.24	57.7196	5.4522	0.7328	0.8458	Out-of-plane C-H bending of Aromatic ring
40	1327.38	9.6502	15.7383	0.4697	0.6391	In-plane C-H bending of Aromatic ring
41	1335.63	56.5284	9.1927	0.5668	0.7235	Out-of-plane C-H bending of Aromatic ring
42	1392.98	2.6977	6.7572	0.7345	0.8470	Out -of--plane C-H Bending of -CH <sub>2</sub> of isopropyl group
43	1396.31	7.8239	12.0548	0.6373	0.7785	In-plane C-H Bending of -CH <sub>2</sub> of isopropyl group
44	1408.32	0.9693	38.0529	0.4365	0.6077	-CH <sub>3</sub> group symmetric bending
45	1413.72	5.5573	2.9271	0.3384	0.5057	-CH <sub>3</sub> group symmetric bending
46	1454.28	19.2658	6.5210	0.3177	0.4822	Out -of--plane C-H bending of Aromatic ring
47	1477.49	13.6625	26.6209	0.7466	0.8549	Antisymmetric -CH <sub>3</sub> bending of methyl and isopropyl substituents
48	1481.42	1.5213	34.4875	0.7485	0.8562	Antisymmetric -CH <sub>3</sub> bending of methyl and isopropyl substituents
49	1485.14	48.3929	6.5994	0.3421	0.5098	Antisymmetric -CH <sub>3</sub> bending of methyl and

						isopropyl substituents
50	1491.82	16.1846	22.8425	0.6069	0.7554	Antisymmetric -CH <sub>3</sub> bending
51	1496.38	10.2599	25.2532	0.7408	0.8511	C-H wagging of -CH <sub>3</sub> of isopropyl substituent
52	1503.38	5.3641	18.3050	0.6327	0.7751	C-H wagging of -CH <sub>3</sub> of isopropyl substituent
53	1535.02	99.9613	1.0330	0.3454	0.5135	C=C stretching vibration of benzene ring
54	1607.00	62.4923	25.5243	0.6692	0.8018	C=C stretching vibration of benzene ring
55	1661.25	47.5561	117.8209	0.6009	0.7507	C=C stretching vibration of benzene ring
56	2964.72	59.7300	277.5760	0.2433	0.3914	C-H stretching of isopropyl group
57	3021.52	52.2467	118.9682	0.0245	0.0478	C-H symmetric stretching of -CH <sub>3</sub> group
58	3023.60	48.0440	518.0691	0.0501	0.0954	C-H asymmetrical stretching of -CH <sub>3</sub> groups
59	3028.85	32.9316	498.3556	0.0063	0.0125	C-H symmetrical stretching of -CH <sub>3</sub> groups
60	3073.20	31.9908	213.4689	0.7237	0.8397	C-H stretching of -CH <sub>3</sub> present at meta position
61	3086.83	9.7102	63.8336	0.6758	0.8066	C-H asymmetric stretching of -methyl group of isopropyl substituents
62	3090.60	64.6598	230.4451	0.7041	0.8264	Symmetrical C-H stretching of methyl groups of isopropyl substituent
63	3091.50	93.6901	227.9133	0.6282	0.7717	Asymmetrical C-H stretching of methyl groups of isopropyl substituent
64	3096.72	54.1333	195.6445	0.7410	0.8513	Symmetrical C-H stretching of methyl groups of isopropyl substituent
65	3104.43	33.9640	157.6080	0.7467	0.8550	Symmetrical C-H stretching of methyl group
66	3163.63	20.4860	182.5776	0.5804	0.7345	Symmetrical =C-H stretching of aromatic ring
67	3167.44	19.3639	242.8225	0.2610	0.4140	Asymmetrical =C-H stretching of aromatic ring
68	3187.51	22.9948	334.6880	0.2003	0.3338	Symmetrical =C-H stretching of aromatic ring
69	3819.89	126.2007	171.0489	0.1814	0.3071	O-H stretching vibration of non-hydrogen bonded hydroxyl group of phenol

### 1) C-H Stretching Vibrations

Absorption arising from C-H stretching in alkanes occur in the general region of 3000-2840 cm<sup>-1</sup>. In case of methyl group two distinct bands occur at 2962 cm<sup>-1</sup> & 2872 cm<sup>-1</sup>. Band at 2962cm<sup>-1</sup> results from the asymmetrical(as) stretching mode in which two C-H bonds of methyl group are extending while the third one is contracting ( $\nu_{as}$  CH<sub>3</sub>). Band at 2872 cm<sup>-1</sup> arises from symmetrical (s) stretching ( $\nu_s$  CH<sub>3</sub>) in which all three of C-H bonds extend and contract in phase. In case of methylene groups, the asymmetrical stretching ( $\nu_{as}$  CH<sub>2</sub>) and ( $\nu_s$  CH<sub>2</sub>) occur near 2926 and 2853 cm<sup>-1</sup> respectively. C-H stretching vibrations due to isopropyl group is very weak and usually lost in other aliphatic C-H absorption and is observed near 2890 cm<sup>-1</sup>.

### 2) C-H Bending Vibrations

Two bending vibrations can occur in methyl group-symmetrical bending vibration involving in-phase bending of C-H bonds and asymmetrical bending vibration involving out-of-phase bending of C-H bonds. The symmetrical bending vibration ( $\delta_s$ CH<sub>3</sub>) occurs near 1375 cm<sup>-1</sup>, the asymmetrical bending vibration ( $\delta_{as}$ CH<sub>3</sub>) near 1450 cm<sup>-1</sup>. The four bending vibrations are referred to as scissoring, rocking, wagging, and twisting. The band resulting from methylene rocking vibration ( $\rho$  CH<sub>2</sub>), appears near 720cm<sup>-1</sup>. Configuration in which two methyl groups are attached to the same carbon atoms exhibits distinctive absorption in the C-H bending region. A strong doublet with peaks of almost equal intensities at 1385-1380 and 1370-1365 cm<sup>-1</sup> are shown by isopropyl group. Weak bands result from methyl rocking vibrations in

isopropyl group and occur in the range 922-919 $\text{cm}^{-1}$ .

### 3) Mononuclear Aromatic Hydrocarbon

Spectra of aromatic compounds show prominent and informative bands in the low frequency range of 900-675 $\text{cm}^{-1}$ . Out-of-plane("oop") bending of C-H bonds of aromatic ring results in these strong absorption bands. In-plane bending bands appear in the 1300-1000 $\text{cm}^{-1}$  region. Absorptions in 1600-1585 and 1500-1400  $\text{cm}^{-1}$  regions are due to skeletal vibrations involving carbon-carbon stretching within the aromatic ring. As per the nature of ring constituents, skeletal bands appear as doublets frequently. 3100 and 3000  $\text{cm}^{-1}$  range contain aromatic C-H stretching bands. Weak combination and overtone bands appear in the 2000-1650  $\text{cm}^{-1}$  range.

The in-phase and out-of-plane bending of a ring hydrogen atom is strongly coupled to adjacent hydrogen atoms. The position of absorption of the out-of-plane bending bands is therefore characteristic of the number of adjacent hydrogen atoms on the ring. The bands are frequently intense and appear at 900-675  $\text{cm}^{-1}$ .

### 4) Phenol

The characteristic bands observed in the spectra of phenols result from O-H stretching and C-O stretching. These vibrations are sensitive to hydrogen bonding. Strong absorptions in 3700-3584  $\text{cm}^{-1}$  region are due to O-H stretching vibration of free hydroxyl group (non-hydrogen bonded hydroxyl group) present in phenol. Due to intermolecular hydrogen bonding additional bands appear at lower frequency, 3550-3200  $\text{cm}^{-1}$ . Strong bands in 1260-1000  $\text{cm}^{-1}$  region are due to C-O stretching vibrations in alcohols and phenols. Phenols absorb at 1390-1330 and 1260-1180  $\text{cm}^{-1}$ . These bands apparently result from interaction between O-H bending and C-O stretching.

### 5) O-H Bending vibrations

The O-H in-plane bending vibrations occurs in the general region of 1420-1330  $\text{cm}^{-1}$ . Out-of-plane bending of bonded O-H group in phenols show broad absorption spectra in 769-650  $\text{cm}^{-1}$  region.

### Thermochemical properties

The statistical thermo chemical analysis of 5-methyl-2-isopropylphenol is carried out considering the molecule to be at room temperature of 300 K and one atmospheric pressure. Thermodynamic properties help to understand energetic, structural and reactivity properties of a molecule. Zero-point energies, thermal correction to internal energy, enthalpy, entropy, and heat capacity for a molecular system are computed using frequency calculations and compiled in Table 3a. Thermodynamic stability of the system at given conditions of pressure and temperature are described by these functions. The standard thermodynamic functions: heat capacity ( $C_v$ ), entropy (S), and enthalpy (E) have been obtained at B3LYP/6-311G (d, p) level and are listed in Table 3b.

Table 3a : Thermodynamic Functions computed by frequency calculations of 5-methyl-2-isopropylphenol

Zero-point correction	0.215393 (Hartree/Particle)
Thermal correction to Energy	0.227042
Thermal correction to Enthalpy	0.227986
Thermal correction to Gibbs Free Energy	0.177884
Sum of electronic and zero-point Energies	-464.643431
Sum of electronic and thermal Energies	-464.631781
Sum of electronic and thermal Enthalpies	-464.630837
Sum of electronic and thermal Free Energies	-464.680939

Table 3b : Thermochemical properties of 5-methyl-2- isopropyl phenol as calculated at B3LYP/6-311G(d, p) level.

Type	E(Thermal) (kCal/Mol)	Cv (Cal/Mol- kelvin)	S (Cal/Mol- Kelvin)
Total	142.471	44.258	105.449
Electronic	0.000	0.000	0.000
Translational	0.889	2.981	40.929
Rotational	0.889	2.981	30.290
Vibrational	140.694	38.297	34.230
Vibration 1	0.594	1.981	5.314
Vibration 2	0.597	1.973	4.411
Vibration 3	0.602	1.955	3.627
Vibration 4	0.633	1.854	2.234
Vibration 5	0.645	1.816	1.990
Vibration 6	0.649	1.805	1.928
Vibration 7	0.666	1.752	1.687
Vibration 8	0.677	1.720	1.566
Vibration 9	0.683	1.701	1.503
Vibration 10	0.701	1.649	1.348
Vibration 11	0.704	1.640	1.323
Vibration 12	0.761	1.482	0.984
Vibration 13	0.784	1.424	0.888
Vibration 14	0.829	1.311	0.731
Vibration 15	0.866	1.227	0.632
Vibration 16	0.880	1.195	0.599
Vibration 17	0.942	1.065	0.477
Vibration 18	0.970	1.009	0.431

### Nonlinear optical properties

Quantum chemical calculations have been very useful for predicting the molecular NLO properties of optically active compounds [25-26]. The relationship between nonlinear optical properties and molecular structure can be better understood with the help of Hyperpolarizability [27]. DFT at B3LYP/-311G(d,p) level was useful in calculating various electric moments like components of electric dipole moment, total dipole moment ( $\mu$ ), mean linear polarizability ( $\alpha$ ), anisotropic polarizability ( $\Delta\alpha$ ), first-order hyperpolarizability ( $\beta$ ) and second-order hyperpolarizability ( $\gamma$ ) in terms of x,y,z components by Gaussian 09,

Revision A. 01 package for 5-methyl-2-isopropylphenol. The mentioned NLO properties have been calculated by using the Equation 1 to Equation 5 [28-29] and the results are summarized in Table 4.

$$\mu = (\mu_x^2 + \mu_y^2 + \mu_z^2)^{1/2} \quad \dots (1)$$

$$\alpha = \frac{1}{3}(\alpha_{xx} + \alpha_{yy} + \alpha_{zz}) \quad \dots (2)$$

$$\Delta\alpha = \frac{1}{\sqrt{2}}[(\alpha_{xx} - \alpha_{yy})^2 + (\alpha_{yy} - \alpha_{zz})^2 + (\alpha_{zz} - \alpha_{xx})^2 + 6(\alpha_{xy}^2 + \alpha_{yz}^2 + \alpha_{zx}^2)]^{1/2} \quad \dots (3)$$

$$\beta = [(\beta_{xxx} + \beta_{xyy} + \beta_{xzz})^2 + (\beta_{yyy} + \beta_{yzz} + \beta_{yxx})^2 + (\beta_{zzz} + \beta_{zxx} + \beta_{zyy})^2]^{1/2} \quad \dots (4)$$

$$\gamma = \frac{1}{5}[\gamma_{xxxx} + \gamma_{yyyy} + \gamma_{zzzz} + 2(\gamma_{xxyy} + \gamma_{xxzz} + \gamma_{yyzz})] \quad \dots (5)$$

The conversion factor of  $\alpha$ ,  $\beta$  and  $\gamma$  in atomic unit are:

1 atomic unit (a.u.) =  $0.1482 \times 10^{-24}$  electrostatic unit (esu) for  $\alpha$ ,

1 a.u. =  $8.6393 \times 10^{-33}$  esu for  $\beta$  and

1 a.u. =  $5.0367 \times 10^{-40}$  esu for  $\gamma$ .

The above function of the molecular system is calculated using B3LYP/6-311G (d, p) method, based on (field-independent basis). Urea is one of the prototype molecules and is used as threshold value for comparative study of NLO properties of other molecular systems. The computed electric dipole moment ( $\mu$ ) of 5-methyl-2-isopropylphenol molecule ( $\mu=1.8730D$ ) was calculated to be 0.79 times that of the standard reference material of prototypical molecule urea ( $\mu=2.3732D$ ) hyperpolarizability  $\beta$  is  $1.137671499 \times 10^{-31}$  esu and is about 0.31 times the hyperpolarizability of urea ( $\beta$  of urea =  $3.728 \times 10^{-31}$  esu). Thus, it is not recommended to 5-methyl-2-isopropylphenol as a prospective building block for nonlinear optical materials.



Table 4: Dipole moment ( $\mu$ ) in Debye, Mean Linear Polarizability ( $\alpha$ ) in a.u First order Hyperpolarizability ( $\beta$ ) in au Second order Hyperpolarizability( $\gamma$ ) in au as calculated by DFT/B3LYP/6-311G (d, p) for 5-methyl-2-isopropylphenol

Dipole moment( $\mu$ ) in Debye		Mean Linear Polarizability( $\alpha$ ) in au		First Order Hyperpolarizability( $\beta$ ) in au		Second Order Hyperpolarizability ( $\gamma$ ) in au	
$\mu_x$	-1.6769	$\alpha_{xx}$	-57.7106	$\beta_{xxx}$	1.4042	$\gamma_{xxxx}$	-1890.2341
$\mu_y$	-0.8096	$\alpha_{yy}$	-67.8773	$\beta_{yyy}$	-4.4913	$\gamma_{yyyy}$	-636.9377
$\mu_z$	-0.2022	$\alpha_{zz}$	-70.6487	$\beta_{zzz}$	-2.9932	$\gamma_{zzzz}$	-207.6154
Total $\mu$	1.8730	$\alpha_{xy}$	-2.5547	$\beta_{xyy}$	-4.3134	$\gamma_{xxxxy}$	-17.8675
		$\alpha_{xz}$	1.5121	$\beta_{xxy}$	10.1108	$\gamma_{xxxz}$	10.5098
		$\alpha_{yz}$	-1.0063	$\beta_{xxz}$	-2.7483	$\gamma_{yyyx}$	-24.4633
		Total $\alpha$	-65.4122	$\beta_{xzz}$	-3.9644	$\gamma_{yyyz}$	-9.4711
		$\Delta\alpha$	12.9883	$\beta_{yzz}$	4.5786	$\gamma_{zzzx}$	2.5585
		$\alpha$	$-9.69408804 \times 10^{-24}$ esu	$\beta_{yyz}$	1.0337	$\gamma_{zzzy}$	-3.4169
				$\beta_{xyz}$	1.8956	$\gamma_{xxyy}$	-408.6183
				Total $\beta$	13.1685611	$\gamma_{xxzz}$	-368.9466
				$\beta$	$1.137671499 \times 10^{-31}$ esu	$\gamma_{yyzz}$	-142.6969
						$\gamma_{xxyz}$	-8.9572
						$\gamma_{yyxz}$	7.4024
						$\gamma_{zzxy}$	-0.2498
						Total $\gamma$	-915.06216
						$\gamma$	$-4.60889 \times 10^{-37}$ esu

### Mulliken population analysis; Mulliken atomic charges

Quantum chemical calculations play an important role in calculating Mulliken atomic charges [30] of a molecular system. Atomic charges affect dipole moment, polarizability, electronic and other properties of a molecular system. B3LYP method with 6-311G (d, p) basis set was used to calculate Mulliken atomic charges and APT charges of 5-methyl-2-isopropylphenol. Calculated values of Mulliken atomic charges and APT charges are given In Table 5 and plotted in Fig. 6.

Table 5: Mulliken and APT charges on each of the constituent element of 5-methyl-2-isopropylphenol as calculated by B3LYP level with 6-311G (d, p) basis set

S. No.	Atom No.	Mulliken Charge	APT Charge
1	1 C	-0.086265	0.056059
2	2 C	-0.102532	-0.221343
3	3 C	-0.113402	0.196848
4	4 C	-0.087559	-0.204039
5	5 C	0.159260	0.677394
6	6 C	-0.081965	-0.147205

7	7 H	0.104373	0.049160
8	8 H	0.093818	0.023032
9	9 H	0.096450	0.041694
10	10 O	-0.387413	-0.920362
11	11 H	0.267701	0.381108
12	12 C	-0.258147	0.096463
13	13 H	0.128151	-0.041277
14	14 H	0.123893	-0.032897
15	15 H	0.114447	-0.021145
16	16 C	-0.232140	0.230320
17	17 H	0.116926	-0.109376
18	18 C	-0.242184	0.046750
19	19 H	0.103695	-0.020181
20	20 H	0.114720	-0.050454
21	21 H	0.110148	-0.018325
22	22 C	-0.288748	0.062434
23	23 H	0.116600	-0.031397
24	24 H	0.117293	-0.024155
25	25 H	0.112879	-0.019107

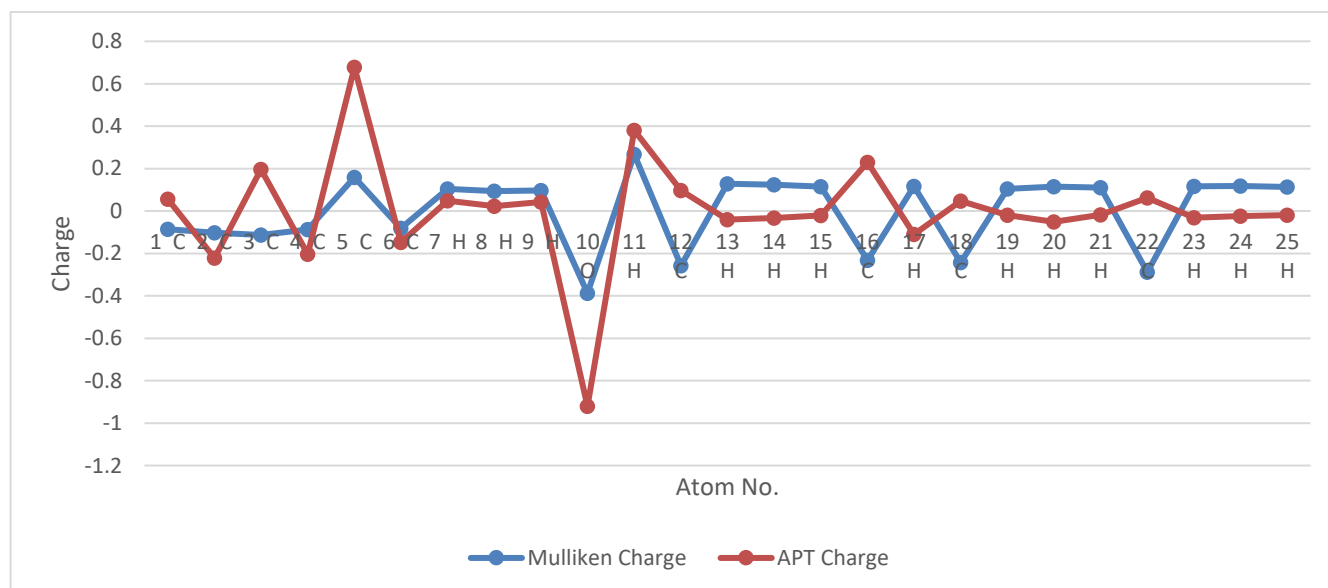


Figure 6: Mulliken and APT Charges on 5-methyl-2-isopropylphenol

For 5-methyl-2-isopropylphenol the Mulliken atomic charge of H-11 atom has the maximum positive value and becomes highly acidic while O-10 atom has maximum negative charge due to high electronegativity and hence is highly basic. Their

corresponding charges are 0.267701 and -0.387413 respectively.

## UV-VISIBLE Spectral Studies and Electronic Properties

TD-DFT calculations facilitates quantum chemists in better understanding of observed electronic absorption spectrum in terms of Excitation energies (E), absorption wavelength ( $\lambda$ ), oscillator strengths (f), molecular orbitals undergoing transitions, transition energy, electronic transitions etc. Molecular orbitals undergoing excitation transition, transition energy and assignments of electronic transitions have been calculated and gathered in Table 6 and the UV – Visible spectra of 5-methyl-2-isopropylphenol compound as obtained from TD-DFT calculations is shown in Fig. 7. The electronic transition from HOMO  $\rightarrow$  LUMO contribution is represented by absorption wavelength, which implies an electron density transfer as  $\pi - \pi^*$  transition. Electron excitation from HOMO  $\rightarrow$  LUMO describes these electronic absorptions mainly and corresponds to the transition from ground state to the first excited state. The  $\lambda_{\max}$ , absorption wavelength depends upon the nature of substitution, strong the electron donating

character of the substitution, more electrons are pushed into the benzene ring and hence,  $\lambda_{\max}$  becomes larger. The  $\pi - \pi^*$  transitions are expected to occur relatively at lower wavelength i.e., a hypsochromic shift, due to extended aromaticity of the benzene ring. Because of possible electronic transitions in a compound various bands appear in UV-Visible spectra of the molecule under consideration. In the UV-Visible spectra of 5-methyl-2-isopropylphenol B-band appears at 237.01 nm,  $\epsilon_{\max} < 100$  and it corresponds to  $\pi - \pi^*$  transition and is a forbidden band, R-band appears at 209.48 nm,  $\epsilon_{\max} < 1000$  which corresponds to  $n - \pi^*$  transition and is also a forbidden band, K-band appears at 193.07 nm,  $\epsilon_{\max} = 2500$  which corresponds to  $\pi - \pi^*$  transition and is also a forbidden band transition. All the bands are forbidden and that may be due to ISC. Applying the definition of  $t = 1.4999/(fE^2)$ , where E is the energy gap of different electronic states in unit of  $\text{cm}^{-1}$ , f is the oscillator strength of the electronic state and t is the life-span of this state in the unit of second, the life-span of a particular state can be figured out [31].

Table 6 : Theoretical absorption spectrum of 5-methyl-2-isopropylphenol | Excitation energies (E), Absorption wavelength( $\lambda$ ) and Oscillator strengths (f)

Excited State	Excitation Energy(E)	Absorption Wavelength( $\lambda$ )	Oscillator Strength(f)	Excitation Transition (MO)	Transition Energy (MO) Singlet A	Assignment of electronic Transitions
1	5.2311 eV	237.01 nm	0.0155	40 $\rightarrow$ 43	-0.39740	$\pi - \pi^*$
				41 $\rightarrow$ 42	0.58296	
2	5.9187 eV	209.48 nm	0.0259	40 $\rightarrow$ 42	0.45762	$n - \pi^*$
				41 $\rightarrow$ 43	0.53365	
3	6.4218 eV	193.07 nm	0.0541	40 $\rightarrow$ 43	-0.15433	$\pi - \pi^*$
				40 $\rightarrow$ 44	0.10236	
				41 $\rightarrow$ 42	-0.11525	
				41 $\rightarrow$ 44	0.66485	

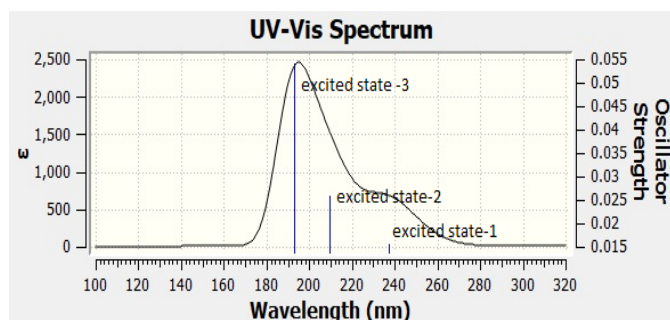


Figure 7: Theoretical UV spectra of 5-methyl-2-isopropylphenol

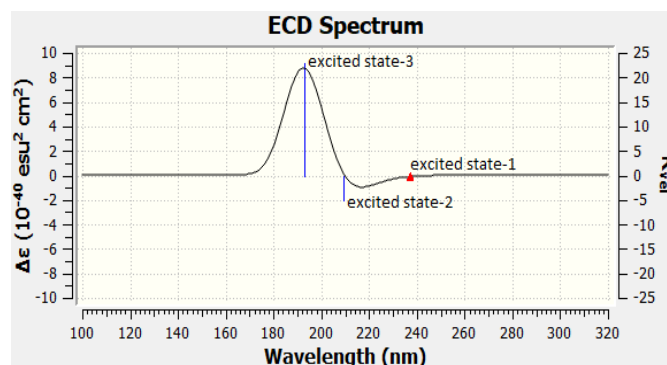


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### Electronic Circular Dichroism (ECD) spectroscopy

Electronic circular dichroism (ECD) has been found to be a powerful chiroptical tool for the assignment of absolute configuration of natural products with chromophores since 1960s [32-33]. CD is the phenomena of a chiral molecule that absorbs left and right circularly polarised light beams to different extent. The difference of the absorption is the measure of the magnitude of CD, which is expressed by the differential molar extinction coefficients as  $\Delta\epsilon = \epsilon_l - \epsilon_r$  ( $L \text{ mol}^{-1} \text{ cm}^{-1}$ ) [34]. TD-DFT method allows the simulation of the ECD spectrum of a medium size molecule on a desktop or PC in a reasonable time [35]. ECD spectra of 5-methyl-2-isopropylphenol was studied using B3LYP/TD-DFT/6-311G (d, p) level and the results are presented in Table-7 and spectra in Fig. 8. In 5-methyl-2-isopropylphenol molecule common chromophore and auxochrome groups are an aromatic ring and a phenolic group. The absorption bands are due to aromatic  $\pi - \pi^*$  and  $n - \pi^*$  transitions. A positive CE at 193.07nm,  $R_{\text{vel}}$  29.99 corresponds to R-configuration while a slightly negative CE at 209.48nm,  $R_{\text{vel}}$  -4.93 corresponds to S-configuration.

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				41 -> 44	0.66485	

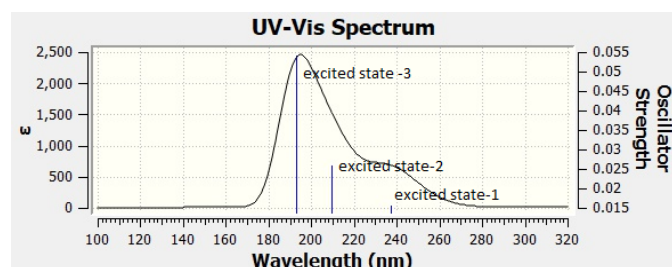


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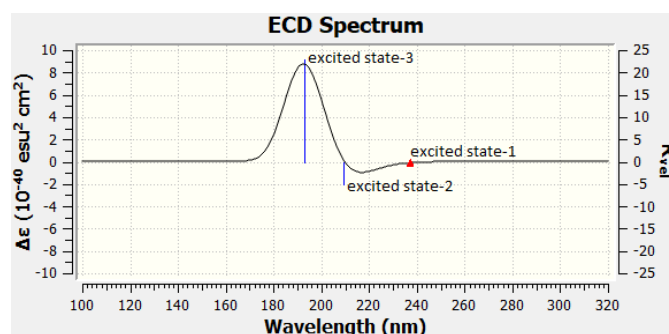


Figure 8 : Theoretical ECD spectra of 5-methyl-2-isopropylphenol

Table 7 : ECD spectral results of 5-methyl-2-isopropylphenol

Excited State	Wavelength (nm)	$R_{vel}$	$\Delta\epsilon$ ( $10^{-40} \text{ esu}^2 \text{ cm}^2$ )
1	237.01349	-0.159491593	$\approx 0$
2	209.4804273	-4.943140792	$\approx 0.2$
3	193.0679243	22.98588495	$\approx 9$

### Frontier Molecular Orbital (FMO) Analysis

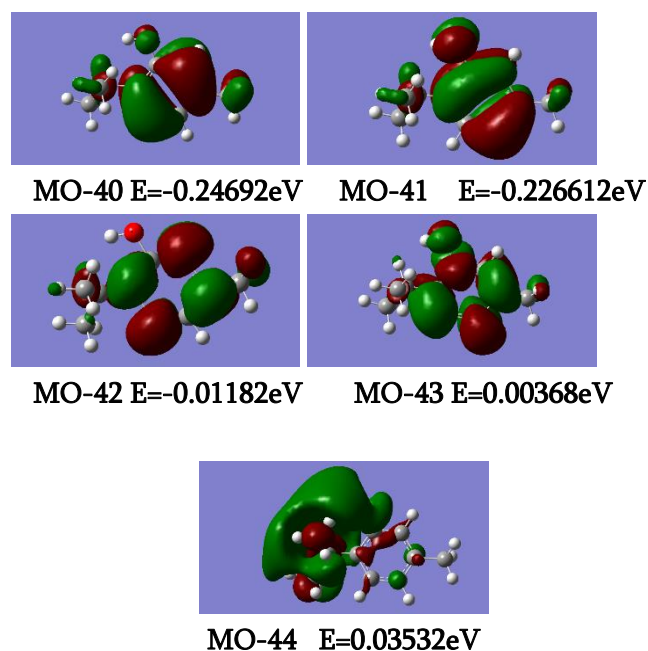


Figure 9: FMO analysis Result

Interaction of two atomic orbitals with each other produces two new orbitals called molecular orbitals – bonding molecular orbital and antibonding molecular orbitals. The bonding molecular orbital having lower energy and is occupied by a pair of electrons (a Lewis base) is called HOMO (Highest Occupied Molecular Orbital) while antibonding molecular orbital having lower energy remains and is unoccupied (a Lewis acid) is called LUMO (Lowest Unoccupied Molecular Orbital) of the compound. HOMO and LUMO are a pair of orbitals which interact most strongly. As they lie at the outermost boundaries of the electrons of a compound, they are together termed as Frontier Molecular Orbital (FMO). The FMO analysis for 5-methyl-2-isopropylphenol has been carried out using B3LYP/6-311G (d, p) basis set at DFT with structure of the molecule in singlet excited state and has been shown in Figure-9. In Table-8 energies of molecular orbitals undergoing major transitions and their energy gap ( $\Delta E$ ) have been presented.

Table 8 : Energy Gap ( $\Delta E$ ) of major Electronic Transitions

LUMO (Energy $E_{LUMO}$ )	HOMO (Energy $E_{HOMO}$ )	Energy Gap ( $\Delta E$ ) ( $E_{LUMO} - E_{HOMO}$ )
43(0.00368eV)	40(-0.24692eV)	0.25060 eV
42 (-0.01182eV)	41(-0.22612eV)	0.21430 eV
42(-0.01182eV)	40 (-0.24692eV)	0.23510 eV
43(0.00368eV)	41(-0.22612eV)	0.22980 eV
44(0.03532eV)	40(-0.24692eV)	0.28224 eV
44(0.03532eV)	41(-0.22612eV)	0.26144 eV

### Global and Local Reactivity Descriptors

Global chemical reactivity descriptors of a compound like hardness, chemical potential, softness, electronegativity, electrophilicity index as well as local reactivity descriptors have been defined [36-40]. Robert Parr and others [36] proposed that a specific property of a chemical species, the square of its electronegativity divided by its chemical hardness, be taken as defining its electrophilicity index. Electronegativity, an atomic parameter, has long been known to be of great use in chemistry. Electronegativity has been defined as average of electron affinity and ionization potential by Pauling and Mulliken [41]. Robert G Parr and others [38] scrutinized the concept of electronegativity by applying Density Functional Theory (DFT) of Hohenberg and Kohn [42]. In the Hohenberg and Kohn density functional theory of the ground state negative of electronegativity is chemical potential. They observed that electronegativity is the same for all orbitals in an atom or molecule in its ground state. They also demonstrated how electronegativity differences between valence states drive electron transfers between atoms on molecule formation. Hardness refers to resistance to deformation or change and mathematically is half the difference of ionization potential and electron affinity. The minimum value of hardness is zero. Softness is the reciprocal of hardness thus zero hardness constitutes maximum softness [39-40]. Hence, we can say that different global reactive descriptors and energy gap of

major electronic transitions are helpful to describe the stability and reactivity of a molecule. The calculated values of various reactive descriptors are presented in Table -9. A low value of hardness indicates that 5-methyl-2-isopropylphenol is soft and can be easily

deformed but a negative value of chemical potential shows that it is quite stable and does not undergo decomposition.

Table 9: Reactive Descriptors of 5-methyl-2-isopropylphenol -values calculated from  $E_{LUMO}$  and  $E_{HOMO}$

Parameter	Relation	Calculated Value
Ionization Energy(I)	$-E_{HOMO}$	0.22612eV
Electron Affinity(A)	$-E_{LUMO}$	0.01182eV
Chemical Potential( $\Phi$ )	$\frac{-(I + A)}{2}$	-0.11897
Absolute Hardness( $\eta$ )	$\frac{(I - A)}{2}$	0.10715
Softness(S)	$\frac{1}{\eta}$	9.33271
Electronegativity( $\chi$ )	$\frac{(I + A)}{2}$	0.11897
Electrophilicity Index( $\omega$ )	$\frac{\Phi^2}{2\eta}$	0.066047
Electron Donating Capability( $\omega^-$ )	$\frac{(3I + A)^2}{16(I - A)}$	0.138925697
Electron Accepting Capability( $\omega^+$ )	$\frac{(I + 3A)^2}{16(I - A)}$	0.019955697

### Electrostatic Potential and Electron Density Surfaces

Molecular Electrostatic Potential (ESP) at a point in space around a molecule gives information about the net electrostatic effect produced at that point by the total charge distribution (electron + nuclei) of the molecule. ESP helps to correlates electrostatic potential with the dipole moment, electronegativity, partial charge, and chemical reactivity of a molecular system i.e., relative.

Shape, size, charge density, and site of chemical reactivity of a molecule is shown by an electron density isosurface mapped with electrostatic potential. Different colours represent different values of electrostatic potential - region of most negative electrostatic potential is represented by red region, region of most positive electrostatic potential is

represented by blue colour and region of zero potential is represented by green colour. Electrostatic potential decreases in the order blue > green > yellow > orange > red. The electron density surfaces and electrostatic potential for 5-methyl-2-isopropylphenol was computed using B3LYP/6-311G (d, p) basis set at DFT and are shown in Fig. 10 and Fig. 11, respectively. ESP for molecular orbital - 41(HOMO) and molecular orbital-42 ( LUMO) are shown in Fig. 12 and Fig. 13.

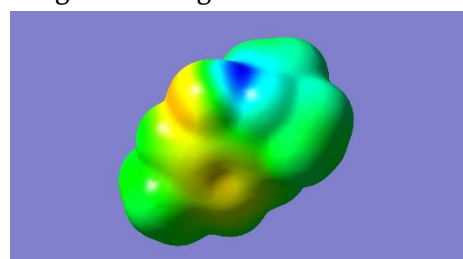


Figure 10: Electron Density of 5-methyl-2-isopropylphenol from Total SCF Density (isovalue =0.0004;mapped with ESP)

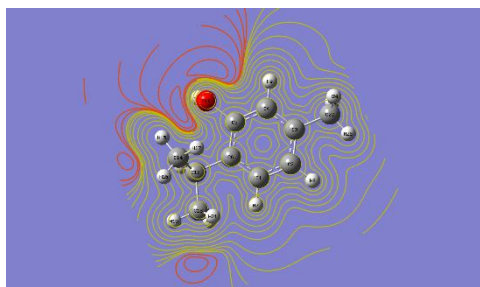


Figure 11: Electrostatic Potential from Total SCF Density (Red- negative charge -yellow-green -blue- Positive charge)

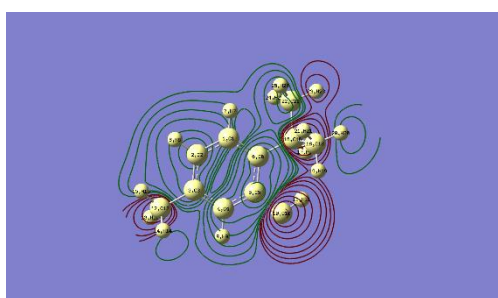


Figure 12: Electrostatic Potential from Total SCF Density (MO-41) HOMO

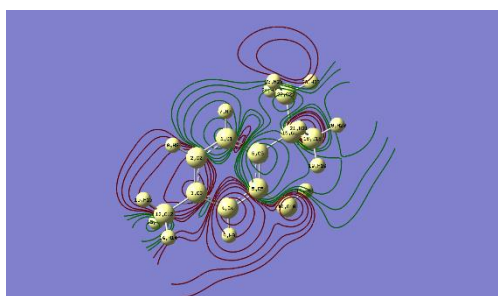


Figure 13: Electrostatic Potential from Total SCF Density (MO-42) LUMO

#### IV. CONCLUSION

To study the structure and reactivity of 5-methyl-2-isopropylphenol we carried out an extensive study of optimized geometry, dipole moment, electrostatic potential (ESP), atomic charge distribution, polarizability, hyperpolarizability, chemical potential,

electrophilicity, chemical hardness, chemical softness etc. using B3LYP,6-311G (d, p) level of theory. The Electrostatic potential (ESP) and Mulliken population analysis reveals the most possible site for nucleophilic attack is C-5 and for electrophilic attack is O-10. The magnitude of electric dipole ( $\mu$ ) molecular hyperpolarizability( $\beta$ ) shows that the 5-methyl-2-isopropylphenol studied has much lesser than that of urea which is used as a standard reference material of prototype molecule hence this molecule is not recommended to be used as a perspective building block for NLO material. A low value of hardness show that this molecule is soft and can be easily deformed but a negative value of chemical potential shows that it is quite stable and does not undergo decomposition.

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