

Physico-Chemical Properties and DFT Calculations of 2-Methoxy - 4 - (Prop-1-En-1-Yl) Phenol (ISOEUGENOL) Using Gaussian Basis Set

¹ Raksha Gupta, ². Sachin Kumar

¹Associate Professor, Department of Chemistry, A.S (P.G.) College, Mawana, Meerut, India

²Associate Professor, Department of Physics, A.S (P.G.) College, Mawana, Meerut, India

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ABSTRACT

Physico-chemical properties plays an important role in determining toxicity of a material hence were calculated using acclab/chemsketch and the data predicted is generated using ACD/Labs Percepta Platform - PhysChem Module. Gaussian 09, RevisionA.01, software package was used for the theoretical quantum chemical calculations of 2-methoxy -4-(prop-1-en-1-yl) phenol commonly called Isoeugenol. 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 (C_v), entropy (S) and Enthalpy (E). DFT/B3LYP/6-311G (d, p) basis set was used to calculate the various NLO properties like dipole moment (μ), mean linear polarizability (α), anisotropic polarizability ($\Delta\alpha$), first order hyperpolarizability (β), second order hyperpolarizability (γ) in terms of x, y, z components for Isoeugenol (2-methoxy -4-(prop-1-en-1-yl) phenol. Same basis set was used to carry out Mulliken population analysis. UV-Visible absorption spectra, ECD spectra, electronic transitions, vertical excitation energies and oscillator strengths of Isoeugenol (2-methoxy -4-(prop-1-en-1-yl) phenol) were computed by Time Dependent DFT (TD-DFT) method using the same basis set. FMO analysis, Molecular electrostatic potential study was also done using the same basis set.

Keywords: Physico-chemical property, acclab /chemsketch, DFT, FMO, Mulliken population analysis, TD-DFT, NLO properties, ECD, Global reactive descriptors.

I. INTRODUCTION

Isoeugenol also known as propenyl guaiacol, belongs to the class of organic compounds known as methoxyphenols. Methoxyphenols are compounds containing a methoxy group attached to the benzene ring of a phenol moiety. Chemical name of isoeugenol

is 2-methoxy -4-(prop-1-en-1-yl) phenol in accordance with International Union of Pure and Applied Chemistry (IUPAC), Other names by which Isoeugenol is known are 4-Hydroxy-3-methoxy-1-propenylbenzene, 2-methoxy-4-propenylphenol and 4-Propenylguaiacol. Isoeugenol can exist as either the cis (Z) or trans (E) isomer. Structural formula of both

cis (*Z*) and trans (*E*) the isomers of Isoeugenol are depicted in Figure -1(a) and 1 (b) respectively.

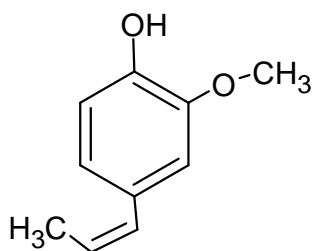


Figure-1a Structural formula of 2-methoxy-4-[(1*Z*)-prop-1-en-1-yl] phenol (Isoeugenol)

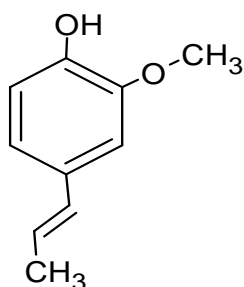


Figure-1b Structural formula of 2-methoxy-4-[(1*E*)-prop-1-en-1-yl] phenol (Isoeugenol)

Isoeugenol is a clear to pale yellow oily liquid with a spicy, sweet, carnation like odour [1] and taste of sweet spice and clove [2]. Isoeugenol has a molecular formula $C_{10}H_{12}O_2$, formula mass 164.2g/mol, $pK_a = 9.88$ at $25^\circ C$ i.e., weakly acidic, very slightly soluble in water and soluble in organic solvents [3]. Isoeugenol is a fragrant essential oil found in many different plants. It has been extracted, admixed with eugenol and other plant volatiles, from calamus, savory, basil, ylang-ylang, clove, tuberose, jonquil, nutmeg, tobacco, sandalwood, dill seed, mace, gardenia, petunia, and other flowers [4-7]. Due to sweet, floral fragrance isoeugenol is incorporated into various household cleaning agents and personal hygiene products, including perfumes, cream lotions, soaps and detergents [8]. Isoeugenol finds use in food products and in medicine as an antioxidant, local antiseptic, analgesic anti-inflammatory, potential anticancer, anti-fungal etc [9-17]. It is known to have anti-arthritic activity also [18]. Tasting like anise or licoricey isoeugenol is added to non-alcoholic drinks, baked foods, candy, and chewing gums. Moreover,

recent studies show that microbes readily convert isoeugenol to vanilla in up to 71% yield [19] by an epoxide/epoxide-diol pathway [20-22] hence it is also used in the manufacture of vanillin. Isoeugenol has found a wide range of uses in many areas of life due to its numerous properties and due to the growing interest in traditional and unconventional medicines that contain natural ingredients, Isoeugenol is an element of scientific research for its use as potential constituent for various medicinal and food products. Quantitative structure-activity relationship of a molecule has been studied to predict its biological activity [23]. Growing interest of researchers in this molecule motivated us to calculate physico-chemical properties and carry out quantum chemical calculations (computational study) of Isoeugenol. The computation of physico-chemical properties, geometry and electronic properties of this compound will clarify the structure – activity relationship of this compound.

II. METHODS AND MATERIAL

Calculation of the physico-chemical properties of 2-methoxy-4-[(1*E*)-prop-1-en-1-yl] phenol (Isoeugenol) is done using acclab/chemsketch [24] and the predicted data is generated using the ACD/Labs Percepta Platform - PhysChem Module. Quantum chemical calculation of 2-methoxy-4-[(1*E*)-prop-1-en-1-yl] phenol (Isoeugenol) has been performed using personal laptop using Gaussian 09, Revision A, 01 software package [25] and Gauss View 6.0.16 programme. Density Functional Density (DFT), and the Becke three -parameter exchange functions in combination with the LYP correlation function of the Lee, Yang and Parr (B3LYP) method was used to carry out theoretical study of 2-methoxy-4-[(1*Z*)-prop-1-en-1-yl] phenol (Isoeugenol). DFT/B3LYP/6-311G (d, p) basis set was used to optimise geometry, determine vibrational frequency, thermochemical calculations etc. UV-Visible spectra, electronic transitions, oscillator strengths, vertical excitation

energies, of 2-methoxy-4-[(1*Z*)-prop-1-en-1-yl] phenol (Isoeugenol) were computed using Time Dependent DFT (TD-DFT) method using the same basis set.

III. RESULTS AND DISCUSSION

Physical and chemical Properties of 2-Methoxy-4-(1-propen-1-yl)phenol (Isoeugenol)

Various physical and chemical properties of a substance determine the environmental behaviour. These include the solubility in water, vapour pressure, octanol/water partition coefficient etc. This compels the researchers to evaluate the role of these properties in determining associated environmental behaviour including toxicity. The physical and chemical properties of Isoeugenol were calculated using acdlab/chemsketch [24] and the predicted data is generated using the ACD/Labs Percepta Platform - PhysChem Module and are tabulated in Table-1.

Table-1 Physical and chemical properties of 2-Methoxy-4-(1-propen-1-yl) phenol (Isoeugenol)

1	Molecular Formula	C ₁₀ H ₁₂ O ₂
2	Formula Weight	164.20108
3	Composition	C (73.15%) H (7.37%) O (19.49%)
4	Molar Refractivity	50.70 ± 0.3 cm ³
5	Molar Volume	152.8 ± 3.0 cm ³
6	Parachor	381.9 ± 4.0 cm ³
7	Index of Refraction	1.577 ± 0.02
8	Surface Tension	38.9 ± 3.0 dyne/cm
9	Density	1.074 ± 0.06 g/cm ³
10	Boiling Point:	266.6±20.0°C at760 mmHg
11	Vapour Pressure:	0.0±0.6 mmHg at 25°C
12	Enthalpy of Vaporization:	52.5±3.0 kJ/mol
13	Flash Point:	122.9±6.7 °C
14	#H bond acceptors:	2
15	#H bond donors:	1
16	#Freely Rotating	2

	Bonds:	
17	#Rule of 5 Violations:	0
18	Dielectric Constant	Not available
19	Polar Surface Area:	29 Å ²
20	Polarizability	20.10 ± 0.5 10 ⁻²⁴ cm ³
21	RDBE	5
22	Monoisotopic Mass	164.08373 Da
23	Nominal Mass	164 Da
24	Average Mass	164.2011 Da
25	M+	164.083181 Da
26	M-	164.084278 Da
27	[M+H] ⁺	165.091006 Da
28	[M+H] ⁻	165.092103 Da
29	[M-H] ⁺	163.075356 Da
30	[M-H] ⁻	163.076453 Da
31	ACD/LogP:	2.45
32	ACD/LogD(pH 5.5):	2.55
33	ACD/BCF (pH 5.5):	51.21
34	ACD/KOC (pH 5.5):	582.31
35	ACD/LogD(pH 7.4):	2.55
36	ACD/BCF (pH 7.4):	51.11
37	ACD/KOC (pH 7.4):	581.18

High solubility in water and low partition coefficient of isoeugenol suggests low potential for bioaccumulation and moderate concerns for the environment i.e., is environmentally friendly and hence can be used to produce other aromatic flavourings and fragrances.

A. Geometrical Analysis

The molecular structure of 2-Methoxy-4-(1-propen-1-yl) phenol (Isoeugenol) having Molecular formula C₁₀H₁₂O₂ Molecular mass: 164.08373 amu, is an asymmetric top type of molecule with 66 degrees of freedom. Gaussian 09, Revision A.01, and Gauss View 6.0.16 programme [25] was used for the optimisation of molecular structure of Isoeugenol and the obtained optimised molecular structure along with the atom numbering scheme is shown in Figure 2.

Figure -2 Optimised Geometrical structure of 2-Methoxy-4-(1-propen-1-yl) phenol (Isoeugenol)



Geometrical parameters i.e., Bond Length, Bond Angle, Dihedral Angle of 2-Methoxy-4-(1-propen-1-yl) phenol (Isoeugenol) after optimisation as calculated by DFT/ B3LYP/6-311G (d, p) level basis set are listed in Table 2.

Table 2: Optimised geometrical parameters (bond length, bond angle, dihedral angle) of 2-Methoxy-4-(1-propen-1-yl) phenol (Isoeugenol) as calculated by DFT/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)	1.4058	A(2,1,6)	119.1283	D(6,1,2,3)	-0.0006
2	R(1,6)	1.3892	A(2,1,10)	120.4458	D(6,1,2,12)	179.9974
3	R(1,10)	1.3607	A(6,1,10)	120.4258	D(10,1,2,3)	-179.9985
4	R(2,3)	1.3874	A(1,2,3)	120.2778	D(10,1,2,12)	-0.0005
5	R(2,12)	1.3752	A(1,2,12)	113.6557	D(2,1,6,5)	0.0007
6	R(3,4)	1.4088	A(3,2,12)	126.0665	D(2,1,6,9)	-179.9985
7	R(3,7)	1.0829	A(2,3,4)	120.9913	D(10,1,6,5)	179.9986
8	R(4,5)	1.4007	A(2,3,7)	120.1537	D(10,1,6,9)	-0.0005
9	R(4,17)	1.4698	A(4,3,7)	118.855	D(2,1,10,11)	-0.0095
10	R(5,6)	1.391	A(3,4,5)	117.909	D(6,1,10,11)	-180.0074
11	R(5,8)	1.083	A(3,4,17)	118.3583	D(1,2,3,4)	-0.0015
12	R(6,9)	1.0835	A(5,4,17)	123.7327	D(1,2,3,7)	180.0026
13	R(10,11)	0.9666	A(4,5,6)	121.2149	D(12,2,3,4)	180.0007
14	R(12,13)	1.4208	A(4,5,8)	120.1124	D(12,2,3,7)	0.0048
15	R(13,14)	1.0953	A(6,5,8)	118.6727	D(1,2,12,13)	179.9602
16	R(13,15)	1.0888	A(1,6,5)	120.4787	D(3,2,12,13)	-0.0419
17	R(13,16)	1.0953	A(1,6,9)	118.3325	D(2,3,4,5)	0.0035
18	R(17,18)	1.0896	A(5,6,9)	121.1888	D(2,3,4,17)	-179.9991
19	R(17,19)	1.3378	A(1,10,11)	107.0896	D(7,3,4,5)	-180.0006
20	R(19,20)	1.0878	A(2,12,13)	118.4986	D(7,3,4,17)	-0.0031
21	R(19,21)	1.4992	A(12,13,14)	111.2334	D(3,4,5,6)	-0.0034
22	R(21,22)	1.0964	A(12,13,15)	106.0714	D(3,4,5,8)	179.9946
23	R(21,23)	1.0964	A(12,13,16)	111.2331	D(17,4,5,6)	179.9993
24	R(21,24)	1.0928	A(14,13,15)	109.3768	D(17,4,5,8)	-0.0027
25			A(14,13,16)	109.468	D(3,4,17,18)	-0.0222
26			A(15,13,16)	109.3828	D(3,4,17,19)	179.981

27			A(4,17,18)	114.5597	D(5,4,17,18)	179.9751
28			A(4,17,19)	128.0017	D(5,4,17,19)	-0.0218
29			A(18,17,19)	117.4386	D(4,5,6,1)	0.0014
30			A(17,19,20)	119.6909	D(4,5,6,9)	180.0005
31			A(17,19,21)	124.5645	D(8,5,6,1)	-179.9967
32			A(20,19,21)	115.7446	D(8,5,6,9)	0.0025
33			A(19,21,22)	111.2774	D(2,12,13,14)	61.1769
34			A(19,21,23)	111.2767	D(2,12,13,15)	-179.9836
35			A(19,21,24)	111.5813	D(2,12,13,16)	-61.1371
36			A(22,21,23)	106.4606	D(4,17,19,20)	-0.0024
37			A(22,21,24)	108.0137	D(4,17,19,21)	179.9951
38			A(23,21,24)	108.0109	D(18,17,19,20)	180.0008
39					D(18,17,19,21)	-0.0017
40					D(17,19,21,22)	120.7353
41					D(17,19,21,23)	-120.7114
42					D(17,19,21,24)	0.0099
43					D(20,19,21,22)	-59.267
44					D(20,19,21,23)	59.2862
45					D(20,19,21,24)	-179.9924

A. Vibrational Assignments

For a non-linear molecule with N atoms, the number of fundamental vibrations is equal to $(3N-6)$. This also includes three translational and three rotational degrees of freedom [26,27]. **2-Methoxy-4-(1-propen-1-yl) phenol** (Isoeugenol), the molecule under consideration, has an asymmetric top group symmetry and 24 atoms; hence 66 normal modes vibrations are possible. As already been stated DFT/B3LY/6-311 G (d, p) level basis set has been used to study the vibrational properties of **2-Methoxy-4-(1-propen-1-yl) phenol** (Isoeugenol) molecule and the theoretical IR spectra and Raman spectra so obtained are shown in Figure 3 and 4 respectively while frequencies (scaled and unscaled), Reduced mass, Force constant, Intensities, and corresponding vibrational assignment for the theoretical IR spectra of **2-Methoxy-4-(1-propen-1-yl) phenol** (Isoeugenol) are tabulated in Table 3. Vibrational frequencies have been assigned

by visual inspection of modes animated by using the Gauss View 6.0.16 programme and the standard values reported [26]. A comprehensive account of the characteristic group absorptions and their relationship to molecular structure is discussed below.

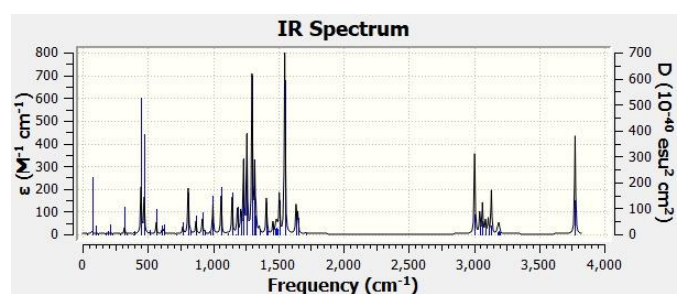


Figure 3: Theoretical IR spectra of **2-Methoxy-4-(1-propen-1-yl) phenol** (Isoeugenol)

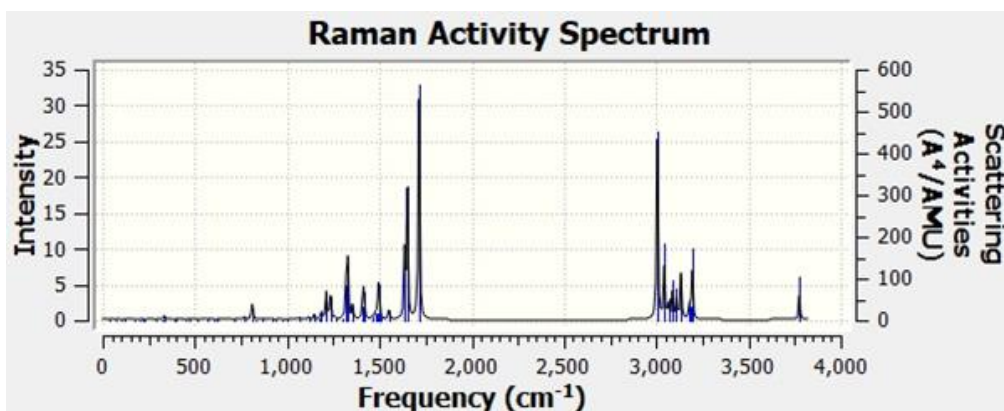


Figure 4: Theoretical Raman spectra of 2-Methoxy-4-(1-propen-1-yl) phenol (Isoeugenol)

Table 3: frequencies (scaled and unscaled), Reduced mass, Force constant, Intensities, and corresponding vibrational assignment for the theoretical IR spectra of 2-Methoxy-4-(1-propen-1-yl) phenol (Isoeugenol)

MODE	Frequency	Reduced Mass	Force Constant	Infrared	Raman Activity	Depolar-P	Depolar-U
1	35.10	2.3000	0.0017	0.0283	1.5209	0.7500	0.8571
2	71.98	3.0758	0.0094	3.9864	1.1281	0.7500	0.8571
3	103.48	2.3084	0.0146	0.8913	1.2103	0.7500	0.8571
4	119.34	3.4558	0.0290	0.0804	2.0702	0.7235	0.8396
5	175.28	2.7622	0.0500	0.1723	1.1601	0.7500	0.8571
6	196.16	1.2674	0.0287	0.6361	1.8693	0.7500	0.8571
7	214.79	3.4898	0.0949	2.0529	2.9016	0.3454	0.5134
8	228.76	1.4332	0.0442	0.0025	0.2080	0.7500	0.8571
9	288.75	2.5730	0.1264	0.3465	0.2695	0.7500	0.8571
10	321.93	4.3072	0.2630	8.5415	0.9972	0.2704	0.4257
11	335.33	4.7518	0.3148	0.2393	8.1201	0.1671	0.2863
12	385.49	4.2294	0.3703	0.1731	1.4495	0.7500	0.8571
13	397.00	3.7529	0.3485	1.0946	2.2526	0.7443	0.8534
14	448.18	1.6356	0.1936	59.1557	0.2917	0.7500	0.8571
15	472.13	1.5900	0.2088	45.4766	3.1363	0.7500	0.8571
16	515.50	5.3180	0.8326	1.9644	0.9504	0.7436	0.8529
17	565.16	4.9394	0.9295	13.9290	3.9650	0.3995	0.5709
18	608.97	3.3170	0.7247	5.1031	0.1569	0.7500	0.8571
19	622.01	5.2611	1.1993	6.1108	2.9431	0.3126	0.4763
20	713.09	4.7064	1.4100	0.0887	0.0297	0.7499	0.8571
21	769.22	4.6251	1.6124	9.3755	7.6186	0.6000	0.7500
22	808.50	1.4335	0.5521	29.2321	9.8007	0.7500	0.8571
23	810.63	4.7395	1.8349	32.8119	26.0650	0.1293	0.2290
24	828.65	1.5222	0.6158	3.2564	1.7247	0.7500	0.8571
25	869.37	1.6069	0.7156	16.1587	3.9740	0.7500	0.8571

26	917.50	2.6417	1.3102	19.1878	3.7830	0.0538	0.1021
27	935.90	1.2972	0.6694	3.4511	0.7870	0.7500	0.8571
28	978.94	2.1584	1.2187	1.7728	1.9722	0.4304	0.6018
29	999.31	1.0940	0.6437	37.0426	0.0773	0.7498	0.8570
30	1062.20	4.1973	2.7902	48.6484	4.4956	0.3030	0.4651
31	1063.57	1.5251	1.0164	0.0772	2.1081	0.7500	0.8571
32	1115.53	2.2839	1.6745	1.6067	7.5904	0.6029	0.7523
33	1146.55	1.6222	1.2564	46.1954	13.0620	0.1975	0.3298
34	1171.77	1.2699	1.0273	0.5562	2.8189	0.7500	0.8571
35	1186.28	1.7017	1.4110	31.3611	17.8181	0.3633	0.5330
36	1212.66	1.6330	1.4149	27.0608	64.0755	0.3158	0.4800
37	1234.60	1.3996	1.2569	90.0304	54.7331	0.2935	0.4538
38	1259.83	3.0105	2.8153	122.7136	6.3239	0.6730	0.8046
39	1298.96	3.0942	3.0760	199.5975	4.6139	0.6499	0.7878
40	1319.75	2.0378	2.0912	83.1938	85.6312	0.2469	0.3960
41	1328.96	1.5128	1.5742	24.5777	136.0845	0.2739	0.4300
42	1354.56	1.3847	1.4969	7.7477	30.7470	0.3593	0.5286
43	1409.48	2.1384	2.5030	43.0656	33.8548	0.1960	0.3278
44	1414.63	1.2659	1.4926	4.3700	67.1264	0.4121	0.5837
45	1459.12	2.6695	3.3485	14.6445	8.4889	0.2194	0.3599
46	1479.00	1.0445	1.3461	7.1810	14.7097	0.7500	0.8571
47	1484.65	1.2452	1.6171	9.5090	4.7440	0.6820	0.8109
48	1490.14	1.0452	1.3674	8.4302	17.1547	0.7500	0.8571
49	1495.80	1.1198	1.4761	4.9616	84.1192	0.4144	0.5860
50	1508.01	1.0656	1.4277	49.8771	8.2961	0.7043	0.8265
51	1549.87	3.2275	4.5677	230.5725	23.8384	0.6117	0.7591
52	1636.52	5.6196	8.8674	35.8611	163.6012	0.3803	0.5511
53	1650.28	6.3366	10.1675	26.3890	318.4674	0.4494	0.6201
54	1714.03	5.4909	9.5045	1.5377	562.6702	0.3139	0.4779
55	3005.36	1.0373	5.5200	58.1626	451.7891	0.1424	0.2493
56	3006.55	1.0341	5.5077	47.9687	194.2679	0.0140	0.0276
57	3044.38	1.0992	6.0022	26.7739	184.0977	0.7500	0.8571
58	3065.93	1.1066	6.1285	38.5587	52.0952	0.7500	0.8571
59	3088.52	1.0985	6.1736	16.1145	94.4199	0.7457	0.8543
60	3109.84	1.0881	6.1999	18.8693	74.3343	0.2392	0.3861
61	3134.13	1.0984	6.3569	27.8043	103.1793	0.5344	0.6966
62	3134.17	1.0890	6.3025	27.6319	63.4495	0.2901	0.4497
63	3180.15	1.0869	6.4765	6.7812	47.2364	0.7162	0.8346
64	3189.26	1.0892	6.5273	10.8547	33.3541	0.3538	0.5227
65	3195.75	1.0942	6.5842	7.5080	170.8143	0.2253	0.3677
66	3775.81	1.0648	8.9445	125.3302	105.1243	0.2322	0.3769

1) *Alkenes C=C stretching vibrations*

C=C stretching mode of unconjugated alkenes usually shows moderate to weak absorption at 1667-1640 cm^{-1} . Monosubstituted alkenes i.e. vinyl group absorbs near 1640 cm^{-1} with moderate intensity.

2) *Alkene C-H stretching vibrations*

In general, any C-H stretching bands above 3000 cm^{-1} result from aromatic, alkyne, or alkene C-H stretching. The frequency and intensity of alkene C-H stretching absorption are influenced by the pattern of substitution. Vinyl group produces three closely spaced C-H stretching bands, two of which results from symmetrical and asymmetrical stretching of the terminal C-H groups, and the third one from the stretching of the remaining single C-H group.

3) *Alkene C-H bending vibrations*

Alkene C-H bonds can undergo bending either in the same plane as the C=C bond or perpendicular to it; the bending vibrations can be either in phase or out of phase with respect to each other. The vinyl group absorbs near 1416 cm^{-1} because of a scissoring vibration of the terminal methylene. The most characteristic vibrational modes of alkene are the out-of-plane C-H bending vibrations between 1000 and 650 cm^{-1} . These bands are usually the strongest in the spectra of alkenes.

4) *Alkanes C-H Stretching Vibrations*

Absorption arising from C-H stretching in alkanes occur in the general region of 3000-2840 cm^{-1} . In case of methyl group two distinct bands occur at 2962 cm^{-1} & 2872 cm^{-1} . Band at 2962 cm^{-1} results from the asymmetrical (as) stretching mode in which two C-H bonds of methyl group are extending while the third one is contracting (CH_3). Band at 2872 cm^{-1} arises from symmetrical (s) stretching (CH_3) in which all three of C-H bonds extend and contract in phase. In case of methylene groups, the asymmetrical stretching (CH_2) and symmetrical stretching (CH_2) occur near 2926 and 2853 cm^{-1} 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^{-1} .

5) *Alkane C-H Bending Vibrations*

Two bending vibrations can occur in methyl group-symmetrical bending vibration involving in-phase bending and asymmetrical bending vibration involving out-of-phase bending of C-H bonds. The symmetrical bending vibration (CH_3) occurs near 1375 cm^{-1} , the asymmetrical bending vibration (CH_3) near 1450 cm^{-1} . The four bending vibrations are referred to as scissoring, rocking, wagging, and twisting. The band resulting from methylene rocking vibration (CH_2), appears near 720 cm^{-1} . Configuration in which two methyl groups are attached to the same carbon atoms exhibits distinctive absorption in the C-H bending region

6) *Mononuclear Aromatic Hydrocarbon*

In the spectra of aromatic compounds most prominent and informative bands occur in the frequency region between 900-675 cm^{-1} . These strong absorption bands are the result of out-of-plane ("oop") bending C-H bonds of the ring. In the 1300-1000 cm^{-1} region In-plane bending bands are observed. Skeletal vibrations, involving stretching of carbon-carbon bonds within the benzene ring, absorb in the 1600-1585 and 1500-1400 cm^{-1} regions. The skeletal bands frequently appear as doublets and depends on the nature of the ring substituents. Aromatic C-H stretching bands occur between 3100 and 3000 cm^{-1} . Weak combination and overtone bands appear in the 2000-1650 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 cm^{-1} .

7) *Phenol*

The characteristic bands due to O-H stretching and C-O stretching observed in the spectra of phenols are sensitive to hydrogen bonding-H stretching vibrations of non-hydrogen bonded or free hydroxyl group of phenol absorbs strongly in the 3700-3584

cm^{-1} region. Due to intermolecular hydrogen bonding additional bands appear at lower frequency, 3550-3200 cm^{-1} . C-O stretching vibrations in alcohols and phenols produce a strong band in the 1260-1000 cm^{-1} region of the spectrum. Phenols absorb at 1390-1330 and 1260-1180 cm^{-1} . These bands apparently result from interaction between O-H bending and C-O stretching.

8) O-H Bending vibrations

The O-H in-plane bending vibrations occur in the general region of 1420-1330 cm^{-1} . Phenols show a broad absorption band in the 769-650 cm^{-1} region because of out-of-plane bending of the bonded O-H group.

9) C-O Stretching vibrations in ethers

The characteristic response of ethers in IR is associated with the stretching vibration of the C-O-C systems. Since vibrations involving oxygen atoms result in greater change in dipole moments than those involving carbon atoms, hence more intense bands are observed for ethers. The C-O-C stretching bands of ethers, as is the case of C-O stretching bands of alcohols, involve coupling with other vibrations within the molecule. The spectra of aryl-alkyl ethers display an asymmetrical C-O-C stretching band at 1275-1200 cm^{-1} with a symmetrical stretching band near 1075-1020 cm^{-1} . Resonance, which results in the strengthening of the C-O bond, is responsible for the shift in the asymmetrical absorption band of aryl-alkyl ethers.

B. Thermochemical properties

Thermodynamic properties help to understand energetics, structural and reactivity properties of a molecule. Frequency calculations were used to compute the zero-point energies, thermal correction to internal energy and entropy as well as heat capacity for Isoeugenol molecule and are compiled in Table 4. The statistical thermochemical analysis of Isoeugenol (2-methoxy-4-(1-propen-1-yl) phenol) is carried out by assuming the molecule under

consideration to be at room temperature of 300K and one atmospheric pressure. The standard thermodynamic functions: heat capacity (C_v), enthalpy (E), entropy (S) have been obtained at B3LYP/6-311G (d, p) level basis set and are tabulated in Table 5. These functions describe the thermodynamic stability of the system at the given conditions of temperature and pressure.

Table 4: thermodynamic functions of Isoeugenol as computed by frequency calculations

Thermodynamic Functions	Value
Zero-point correction	0.197547 (Hartree/Particle)
Thermal correction to Energy	0.209665
Thermal correction to Enthalpy	0.210609
Thermal correction to Gibbs Free Energy	0.158868
Sum of electronic and zero-point Energies	-538.657406
Sum of electronic and thermal Energies	-538.645289
Sum of electronic and thermal Enthalpies	-538.644344
Sum of electronic and thermal Free Energies	-538.696085

Table 5: Thermodynamic properties of Isoeugenol as calculated by DFT/B3LYP/6-311 G (d, p) level basis set

	E (Thermal) KCal/Mol	C_v Cal/Mol- Kelvin	S Cal/Mol- Kelvin
Total	131.567	45.197	108.898
Electronic	0.000	0.000	0.000
Translational	0.889	2.981	41.194
Rotational	0.889	2.981	31.226
Vibrational	129.789	39.236	36.477
Vibration 1	0.594	1.982	5.518
Vibration 2	0.598	1.967	4.099
Vibration 3	0.605	1.946	3.388

Vibration 4	0.609	1.933	3.111
Vibration 5	0.627	1.873	2.378
Vibration 6	0.636	1.845	2.169
Vibration 7	0.645	1.818	2.003
Vibration 8	0.651	1.797	1.889
Vibration 9	0.685	1.695	1.481
Vibration 10	0.707	1.632	1.300
Vibration 11	0.716	1.605	1.234
Vibration 12	0.754	1.501	1.018
Vibration 13	0.764	1.477	0.974
Vibration 14	0.807	1.365	0.801
Vibration 15	0.829	1.312	0.732
Vibration 16	0.871	1.216	0.620
Vibration 17	0.921	1.107	0.514
Vibration 18	0.968	1.013	0.434

A. Nonlinear optical properties of Isoeugenol

Molecular NLO properties of active compounds can be predicted with the help of quantum chemical calculations [28,29]. The relationship between the nonlinear optical properties and the molecular structure can be better understood with the help of Hyperpolarizability [30-31]. DFT/B3LYP/6-311 G (d, p) has been used to compute the electronic properties like total dipole moment (μ), mean linear polarizability (α), anisotropic polarizability ($\Delta\alpha$), first-order hyperpolarizability (β) and second order hyperpolarizability (γ) in terms of x, y, z components by Gaussian 09, Revision A.01 package and Gauss View 6.0.16 programme for Isoeugenol molecule. Calculation of above mentioned NLO properties have been executed using equation-1 to equation-5[32-33] and the results are summarised in Table 6.

$$\mu = (\mu_x^2 + \mu_y^2 + \mu_z^2) \quad (1)$$

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

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

$$\beta = (\beta_x^2 + \beta_y^2 + \beta_z^2)^{1/2} \quad (4)$$

where $\beta_x = \beta_{xxx} + \beta_{xyy} + \beta_{xzz}$, $\beta_y = \beta_{yyy} + \beta_{yxx} + \beta_{yzz}$ and $\beta_z = \beta_{zzz} + \beta_{zxy} + \beta_{zxx}$

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

The conversion factor of α , β and γ in atomic unit are
For α 1 atomic unit (a.u.) = 0.1482×10^{-24} electrostatic unit (esu),

For β 1 a.u. = 8.6393×10^{-33} esu and

For γ 1a.u. = 5.0367×10^{-40} esu.

As mentioned above DFT/B3LYP/6-311G (d, p) method, based on field-independent basis is used to compute the nonlinear optical components of Isoeugenol. Urea is one of the prototype molecule which is used as a threshold value for comparative purpose hence is used to study the NLO properties of a molecular system. The computed electric dipole moment (μ) of Isoeugenol molecule ($\mu = 2.6222$ D) was calculated to be 1.1049 times that of the standard reference material of prototypical molecule urea ($\mu = 2.3732$ D) and first-order hyperpolarizability (β) of Isoeugenol molecule ($\beta = 5.1851 \times 10^{-31}$ esu) is about 1.3909 times the first order hyperpolarizability of urea (β of urea = 3.728×10^{-31} esu) indicating that isoeugenol has considerable nonlinear optical property hence it is recommended to use Isoeugenol molecule as a prospective building block for nonlinear optical material.

Table 6: nonlinear optical components of Isoeugenol as calculated by DFT/B3LYP/6-311 G (d, p) level basis set

Dipole moment (μ) In Debye		Mean Linear Polarizability (α) in a.u		First-order Hyperpolarizability (β) in a.u.		Second order Hyperpolarizability (γ) in a.u	
μ_x	-0.0380	α_{xx}	-64.6560	β_{xxx}	-27.5035	γ_{xxxx}	-2618.7766
μ_y	2.6219	α_{yy}	-64.8757	β_{yyy}	15.7507	γ_{yyyy}	-783.7295
μ_z	0.0008	α_{zz}	-75.7584	β_{zzz}	0.0011	γ_{zzzz}	-94.3136
Total μ	2.6222	α_{xy}	-8.2013	β_{xyy}	-8.6368	γ_{xxxxy}	-69.9238
		α_{xz}	-0.0026	β_{xxy}	18.3993	γ_{xxxz}	-0.0139
		α_{yz}	-0.0002	β_{xxz}	0.0098	γ_{yyyx}	-57.8955
		α	-68.43003 a.u	β_{xzz}	-11.3589	γ_{yyyz}	-0.0069
			$-10.14133 \times 10^{-24}$ esu	β_{yzz}	2.5362	γ_{zzzx}	0.0017
		$\Delta\alpha$	12.42992 a.u	β_{yyz}	0.0013	γ_{zzzy}	0.0024
				β_{xyz}	-0.0074	γ_{xxyy}	-596.2700
				β	60.0171 au	γ_{xxzz}	-495.8275
					5.1851×10^{-31} esu	γ_{yyzz}	-163.5812
						γ_{xxyz}	0.0023
						γ_{yyxz}	-0.0087
						γ_{zzxy}	-2.4027
						γ	-1201.6542 au
							-6.0524×10^{-37} esu

A. Mulliken population Analysis: Mulliken Atomic Charges.

Atomic charges, an important concept in chemistry which gives a simple picture of distribution of electron density within a molecule. Many properties of a molecule like dipole moments, electric potentials, NMR chemical shifts, reactivities, and electromagnetic spectra can be correlated to atomic charges in a molecule, and many structure-property theories of molecule are based on the idea of atomic charges [34]. Atomic Polar tensor (APT) charge is derived using quantum mechanically calculated dipole moment. DFT/B3LYP/6-311 G (d, p) level basis

set was used to calculate the Mulliken atomic charges, APT atomic charges, and Natural atomic charges. Calculated values of Mulliken, APT, Natural atomic charges are given in Table 7 and plotted in Figure 5. Atomic charge distribution is different due to the presence of polar -OH group on Carbon atom -1 and -OCH₃ group on carbon atom-2. Oxygen atom -12 has more negative charge than Oxygen atom-10 due to the presence of methyl group which has +I effect. Carbon atoms 1, 2 and 13 have positive charge as they are directly attached to electronegative oxygen atom hydrogen atom -11 has more positive charge because it is attached to oxygen atom of phenolic group.

Table 7: Mulliken, APT and Natural Atomic Charges on each of the constituent atom of Isoeugenol molecule as calculated by DFT/B3LYP/6-311 G (d, p) level basis set.

Atom No.	Natural Charge	Apt charge	Mulliken charge
C 1	0.30244	0.517260	0.151631
C 2	0.26080	0.450485	0.146602
C 3	-0.26558	-0.077965	-0.092515
C 4	-0.07262	-0.028416	-0.074996
C 5	-0.19020	-0.048879	-0.055026
C 6	-0.24007	-0.081379	-0.090106
H 7	0.20544	0.054056	0.095767
H 8	0.19904	0.038561	0.082918
H 9	0.21395	0.044186	0.099747
O 10	-0.66885	-0.820055	-0.359342
H 11	0.47626	0.339929	0.254512
O 12	-0.55928	-0.886803	-0.406252
C 13	-0.19056	0.523966	-0.122324
H 14	0.16683	-0.033234	0.116122
H 15	0.18452	-0.004064	0.128619
H 16	0.16685	-0.033211	0.116134
C 17	-0.20739	0.083523	-0.073277
H 18	0.18250	-0.001592	0.074043
C 19	-0.15263	-0.008135	-0.141841
H 20	0.17862	0.009584	0.089854
C 21	-0.58912	0.076911	-0.272021
H 22	0.20203	-0.047596	0.114474
H 23	0.20203	-0.047618	0.114478
H 24	0.19499	-0.019514	0.102798

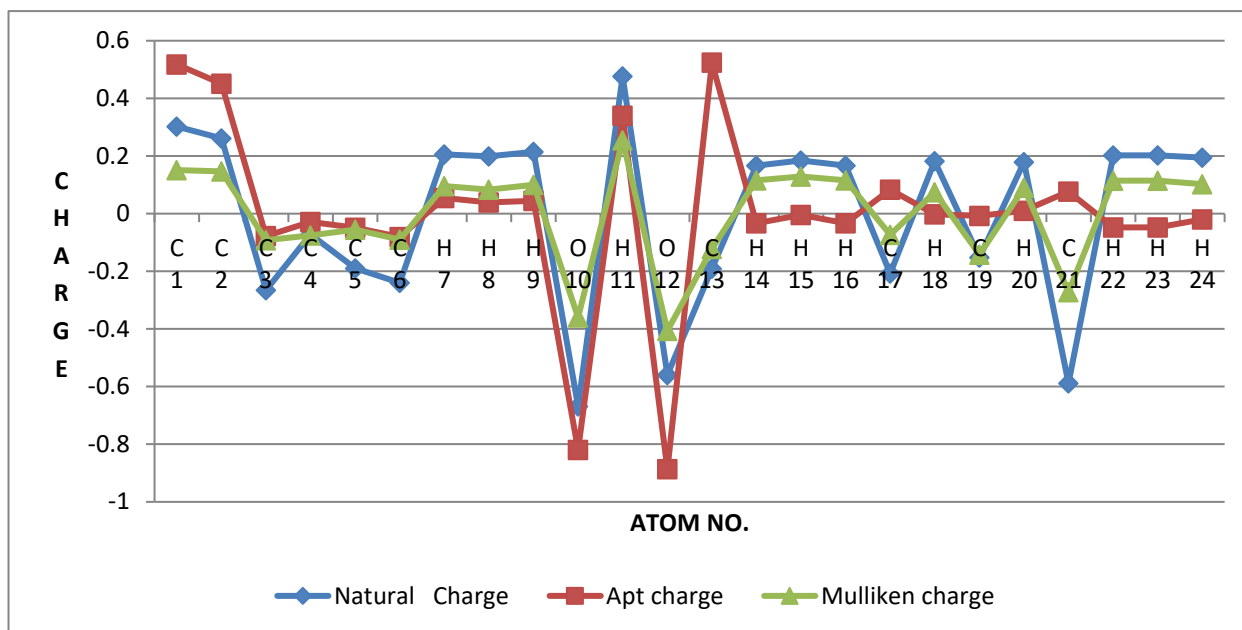


Figure 5: Mulliken, Apt, and Natural Charges on each of the constituent atom of Isoeugenol.

A. 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 (λ), oscillator strengths (f), molecular orbitals undergoing transitions, transition energy, electronic transitions etc [35-36]. Molecular orbitals undergoing excitation transition, transition energy and excitation energy, absorption wavelength etc have been gathered in Table 8 and the UV –Visible spectra of Isoeugenol compound as obtained from TD-DFT calculations is shown in Figure 6.

Table 8: UV-Visible spectral results (excitation energy, absorption wavelength, oscillator strength, transition energy) of Isoeugenol molecule as calculated by TD-DFT/ B3LYP/6-311g (d, p) basis set.

Excited state	Excitation Energy (E)	Absorption Wavelength (λ)	Oscillator Strength (f)	Excitation Transition (MO)	Transition Energy (MO) Singlet A
1	4.7958 eV	258.52 nm	f=0.1113	43 -> 45 43 -> 46 44 -> 45 44 -> 46	0.29607 -0.14431 0.50973 0.34256
2	5.1129 eV	242.49 nm	f=0.2672	43 -> 45 44 -> 45 44 -> 46	-0.28254 0.46586 -0.43657
3	5.5365 eV	223.94 nm	f=0.1613	42 -> 45 42 -> 46 43 -> 45 44 -> 46 44 -> 47	0.15346 0.13338 0.53112 -0.36484 -0.16985

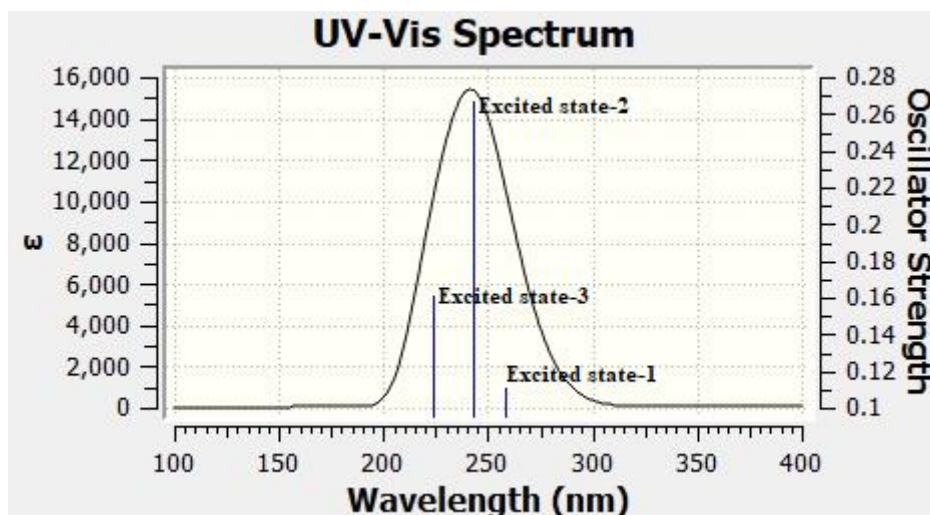


Figure 6: Theoretical UV-Visible spectra of Isoeugenol

G. Electronic Circular Dichroism (ECD) spectroscopy ECD (Electronic circular dichroism) has been found to be a powerful chiroptical tool for the determination of absolute configuration (AC) or conformation of natural products containing chromophores since 1960s [37-38]. CD is defined as the differential absorption of left and right circularly polarised electromagnetic radiation by a sample. The difference of the absorption is the measure of the magnitude of CD, which is expressed by the differential molar extinction coefficients as $\Delta\epsilon = \epsilon_l - \epsilon_r$ ($L \text{ mol}^{-1} \text{ cm}^{-1}$) [39]. TD-DFT method allows the simulation of the ECD spectrum of a medium size molecule on a desktop or PC in a reasonable time [40-41]. ECD spectra of Isoeugenol was studied using B3LYP/TD-DFT/6-311G (d, p) level and the results are presented in Table-9 and spectra in Fig. 7. In Isoeugenol molecule common chromophore and auxochrome groups are an aromatic ring, a phenolic, a methoxy group and an alkene group. The absorption bands are due to aromatic $\pi - \pi^*$ and $n - \pi^*$ transitions. A negative CE at 258.52 nm and 223.94 nm $R_{vel} < 100$ corresponds to S-configuration while slightly positive CE at 242.49 nm corresponds to R-configuration.

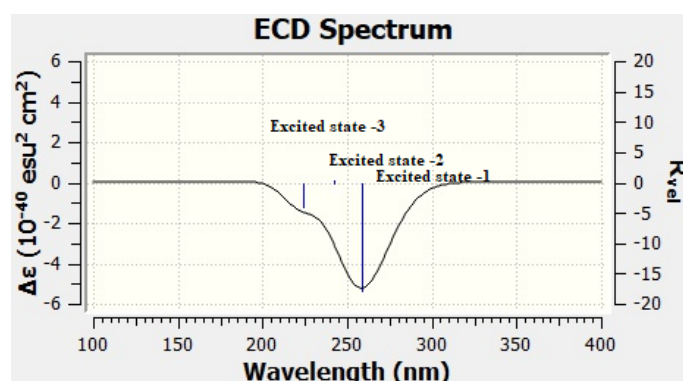


Figure -7- Theoretical ECD spectra of Isoeugenol

Table 9: ECD spectral results of Isoeugenol

Excited State	Wavelength (nm)	R_{vel}	$\Delta\epsilon$ ($10^{-40} \text{ esu}^2 \text{ cm}^2$)
1	258.524392	-17.89126734	≈ -5.2
2	242.4912143	0.3740610138	$\approx +1.3$
3	223.9415427	-4.002235682	≈ -1.3

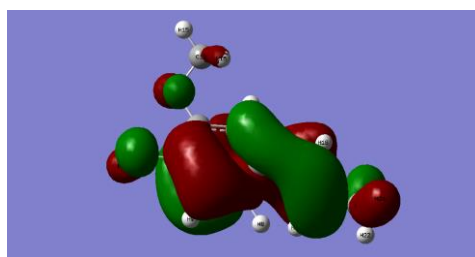
A. Frontier Molecular orbital analysis (FMO analysis)

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 has lower energy and is occupied by a pair of electrons (a Lewis

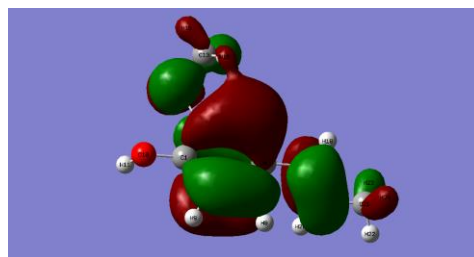
base) and is called Highest Occupied Molecular Orbital (HOMO) while antibonding molecular orbital has lower energy and does not contain electrons (a Lewis acid) and is called Lowest Unoccupied Molecular Orbital (LUMO) of the compound. HOMO and LUMO are a pair of orbitals which interact most strongly. They together are called Frontier Molecular Orbital (FMO) because they are present at the outermost boundaries of the electrons of a compound. The FMO analysis for Isoeugenol 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 8. In Table 10 energies of molecular orbitals undergoing major transitions and their energy gap (ΔE) have been presented.

Table 10 : Energy Gap (ΔE) of major electronic transitions

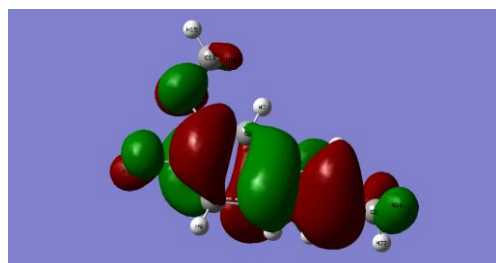
LUMO Energy (E_{LUMO})	HOMO Energy (E_{HOMO})	Energy gap (ΔE) ($E_{\text{LUMO}} - E_{\text{HOMO}}$)
45 (-0.02970)	44 (-0.22865)	0.19895
46 (-0.01422)	44 (-0.22865)	0.21443
47 (0.02160)	44 (-0.22865)	0.25025
45 (-0.02970)	43 (-0.24869)	0.21899
46 (-0.01422)	43 (-0.24869)	0.23447
45 (-0.02970)	42 (-0.27919)	0.24949
46 (-0.01422)	42 (-0.27919)	0.26497



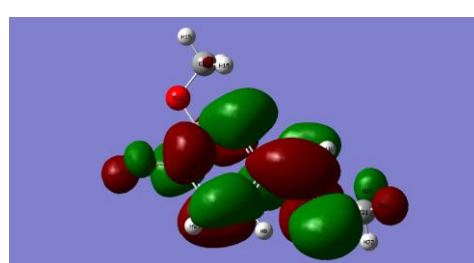
MO-42 E = -0.27919



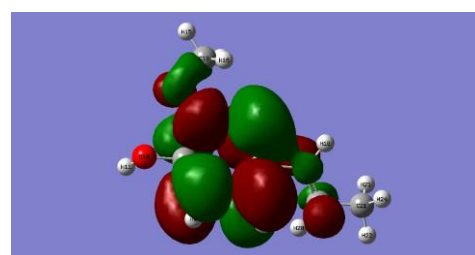
MO-43 E = -0.24869



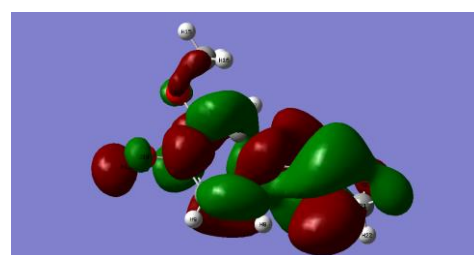
MO - 44 E = -0.22865



MO - 45 E = -0.02970



MO -46 E = -0.01422



MO - 47 E = 0.02160

Figure -8 – Frontier Molecular orbitals with Molecular Orbital No. and its energy indicated below each Molecular Orbital

I. Global and Local Reactivity Descriptors

Global chemical reactivity descriptors of a compound like absolute hardness, softness, chemical potential, electronegativity, electrophilicity index as well as local reactivity descriptors have been defined [42-46]. Robert Parr and others [42] defined Electrophilicity index and suggested that it can be calculated using chemical potential and absolute hardness. According to this definition electrophilicity index measures the susceptibility of chemical species to accept electrons. Thus, low value of it suggests a good nucleophile while higher value indicates the presences of good electrophile. Electronegativity, an atomic parameter, has long been known to be of great use in chemistry. Electronegativity has been defined by Pauling and Mulliken [48] as the average value of the ionization potential and electron affinity. Robert G Parr and others [45] scrutinized the concept of electronegativity from the point of view of Density Functional Theory of Hohenberg and Kohn [48]. 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 defined as the reciprocal of hardness thus zero hardness constitutes maximum softness [45-46]. 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 11. A low value of hardness indicates that Isoeugenol 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 11 : Calculated values of Global and Local Reactivity Descriptors of Isoeugenol

Parameter	Relation	Calculated Value
Ionization Energy(I)	$-E_{\text{HOMO}}$	0.22865
Electron Affinity (A)	$-E_{\text{LUMO}}$	0.02970
Chemical Potential(ϕ)	$-\frac{(I + A)}{2}$	-0.129175
Absolute hardness(η)	$\frac{(I - A)}{2}$	0.099475
Softness(S)	$\frac{1}{\eta}$	10.052778
Electronegativity (χ)	$\frac{(I + A)}{2}$	0.129175
Electrophilicity index (ω)	$\frac{\phi^2}{2\eta}$	0.083871
Electron donating capability(ω^-)	$\frac{(3I + A)2}{16(I - A)}$	0.160893
Electron accepting capability (ω^+)	$\frac{(I + 3A)2}{16(I - A)}$	0.031718

C. Electrostatic potential and electron density surfaces

Molecular Electrostatic Potential (ESP) is the potential that a unit positive charge would experience at any point surrounding the molecule due to the electron density distribution in a molecule and is correlated with dipole moment, electronegativity, partial charge, and chemical reactivity of the molecule. With the help of electrostatic potential chemical reactivity of a molecule can be predicted because regions of negative potential are expected to be sites of protonation i.e. site of nucleophilic attack, while regions of positive potential may indicate electrophilic sites. The different values of electrostatic potential are represented by different colours-red represents region of most negative electrostatic potential, blue represents the region of the most positive electrostatic potential and green represents the region of zero potential. Potential increases in the order red < orange < yellow < green < blue.

The electron density surfaces and electrostatic potential for Isoeugenol was computed using B3LYP/6-311G (d, p) basis set at DFT and are shown in Figure 9 and Figure 10 respectively.

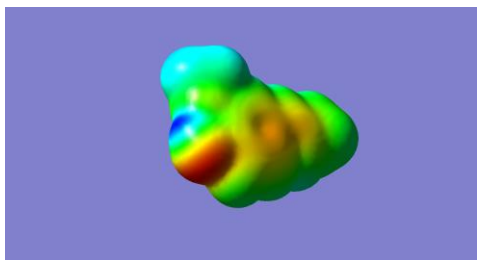


Figure 9: electron density of Isoeugenol from total scf density (isoval = 0.0004; mapped with esp)

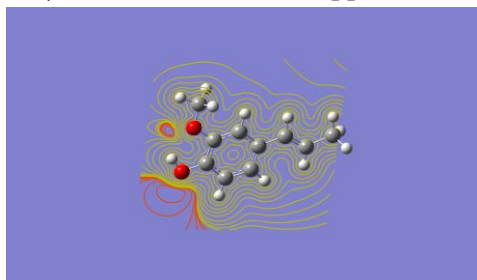


Figure-10: electrostatic potential from total scf density (red- negative charge -yellow-green -blue positive charge)

IV. CONCLUSIONS

An attempt was made to calculate various physico-chemical properties of Isoeugenol using acdlab/chemsketch as these properties influence the toxic manifestations of a material. Further efforts were made to study the geometry, dipole moment, molecular electrostatic potential (ESP), atomic charge distribution, polarizability, hyperpolarizability etc. Reactivity descriptors like chemical reactivity, electrophilicity, chemical potential, absolute hardness, chemical softness etc for Isoeugenol were discussed by analysing HOMO and LUMO calculated using B3LYP/6-311 G (d, p) basis set. The values of dipole moment (μ), hyperpolarizability (β) of Isoeugenol were calculated and were observed to be comparable to the values of standard reference material of prototype molecule urea hence this molecule is recommended for its use as a perspective building block for NLO material and a negative value of chemical potential indicates that Isoeugenol is quite stable and does not undergo decomposition readily. High solubility in water and low partition coefficient of isoeugenol suggests low potential for

bioaccumulation and moderate concerns for the environment i.e., is environmentally friendly.

V. REFERENCES

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