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Physico-Chemical Properties and Quantum Chemical Calculation of 2-methoxy-4-(prop-2-en-1-yl) phenol (EUGENOL)

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ABSTRACT

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Physico-chemical properties plays an important role in determining toxicity of a material hence were calculated using acdlab/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-2-en-1-yl) phenol commonly called Eugenol. 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). 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 (Δα), first order hyperpolarizability (β), second order hyperpolarizability (γ) in terms of x, y, z components for Eugenol (2-methoxy-4-(prop-2-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 Eugenol (2-methoxy-4-(prop-2-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, acdlab /chemsketch, DFT, FMO, Mulliken population analysis, TD-DFT, NLO properties, ECD, Global reactive descriptors

I. INTRODUCTION

Eugenol, a natural phenolic phytochemical, also known by the chemical name: 1-Hydroxy-2-methoxy-4-propenylbenzene, 4-Allyl-2-methoxyphenol or 2-methoxy-4-(prop-2-en-1-yl) phenol in accordance with International Union of Pure and Applied Chemistry (IUPAC). Structural formula of Eugenol is depicted in Figure 1.

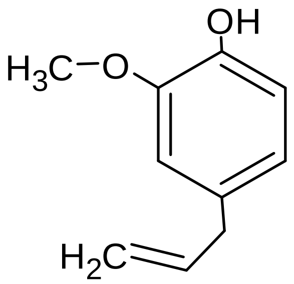


Figure 1: Structural formula of 2-methoxy-4-(prop-2-en-1-yl) phenol (Eugenol)

Eugenol appears as clear colourless pale yellow or amber -coloured liquid with odour of cloves and spicy pungent taste [1]. It has molecular formula $C_{10}H_{12}O_2$, formula mass 164.2g/mol, pKa = 10.19 at 25°C, partially soluble in water and soluble in organic solvent [2]. Eugenol is a volatile aromatic phenolic constitute of clove essential oil obtained from Eugenia caryophyllata tree (scientific name for clove tree). Clove tree has large leaves and flower buds which turns to red colour when ready for collection [3, 4]. Main extracted constituent (70-90%) of clove essential oil is Eugenol and it gives clove aroma [3] to clove essential oil. Eugenol got much attention by the researchers as Eugenol is a major component in the extracts of different medicinal herbs and this has opened research in its use as a medicine to cure different diseases. Eugenol is known to have several pharmacological properties like anaesthetic [5], antioxidant [6,10], antimicrobial [7,8], anthelmintic [9], anti-inflammatory [10], anticarcinogenic [11,12], anti-fumigant [13], anti-repellent [14] properties etc. From times Eugenol has been used as a traditional remedy to eliminate bad breath or ameliorate the pain of a bad tooth. Eugenol is a main component in cosmetics, perfumes, flavouring agents [15] etc. WHO (World Health Organization) and FAO (Food and Agriculture Organization) joint expert committee on food additives have allowed an acceptable daily intake of Eugenol of 2.5mg/Kg body weight for humans [16]

Eugenol has found a wide range of uses in many areas of life due to its numerous properties. Besides, due to the growing interest in traditional and unconventional medicines that contain natural ingredients, Eugenol is an element of scientific research for its use as potential constituent for various medicinal products. Quantitative structure-activity relationship of the molecule has been studied to predict its biological activity [17]. Growing interest of researchers in this molecule motivated us to calculate physico-chemical properties and carry out quantum chemical calculations (computational study) of Eugenol. The computation of physico-chemical properties, geometry and electronic properties of this compound will clarify the structure – activity relationship of this compound.

II. MATERIALS AND METHODS

Calculation of the physico-chemical properties of Eugenol (2-methoxy-4-(prop-2-en-1-yl) phenol) are done using acdlab/chemsketch [18] and the predicted data is generated using the ACD/Labs Percepta Platform - PhysChem Module. Quantum chemical calculation of Eugenol (2-methoxy-4-(prop-2-en-1-yl) phenol) have been performed using personal laptop using Gaussian 09, Revision A, 01 software package [19] 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 Eugenol. 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 Eugenol were computed using Time Dependent DFT (TD-DFT) method using the same basis set.

III. RESULTS AND DISCUSSIONS

Physico-chemical Properties of Eugenol

Various physico-chemical properties influence the toxic manifestations of a material. This compels the researchers to evaluate the role of these properties in determining associated toxicity issues. The physico-chemical properties of Eugenol were calculated using acdlab/chemsketch [18] and the predicted data is generated using the ACD/Labs Percepta Platform - PhysChem Module and are tabulated in Table-1.

Table 1: Physico-chemical properties of Eugenol (2-methoxy-4-(prop-2-en-1-yl) phenol)

Physico-chemical property	**Calculated values of the property**
Molecular Formula:	$C_{10}H_{12}O_2$
Formula Weight:	164.20108
Boiling Point	255.0±0.0 °C at 760 mmHg
Composition:	C(73.15%) H(7.37%) O(19.49%)
Molar Refractivity:	48.72 ± 0.3 cm^3
Molar Volume:	156.2 ± 3.0 cm^3
Parachor:	384.3 ± 4.0 cm^3
Index of Refraction:	1.535 ± 0.02
Vapour Pressure:	0.0±0.5 mmHg at 25°C
Enthalpy of Vaporization:	51.2±3.0 kJ/mol
Flash Point:	119.8±8.1 °C
Surface Tension:	36.5 ± 3.0 dyne/cm
Density:	1.050 ± 0.06 g/cm^3
Dielectric Constant:	Not available
Polarizability:	19.31 ± 0.5 $10^{-24}cm^3$
#H bond acceptors:	2
#H bond donors:	1
#Freely Rotating Bonds:	3
#Rule of 5 Violations:	0
RDBE:	5
Monoisotopic Mass:	164.08373 Da
Nominal Mass:	164 Da
Average Mass:	164.2011 Da
ACD/LogP:	2.20
ACD/LogD (pH 5.5):	2.48
ACD/BCF (pH 5.5):	45.18
ACD/KOC (pH 5.5):	532.35
ACD/LogD (pH 7.4):	2.48
ACD/BCF (pH 7.4):	45.12
ACD/KOC (pH 7.4):	531.68
Polar Surface Area:	29.5 $Å^2$

Geometrical Analysis

The molecular structure of Eugenol (2-methoxy-4-(prop-2-en-1-yl) phenol) having Molecular formula $C_{10}H_{12}O_2$ 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 was used for the optimisation of molecular structure of Eugenol and the obtained optimised molecular structure along with the atom numbering scheme is shown in Figure 2.

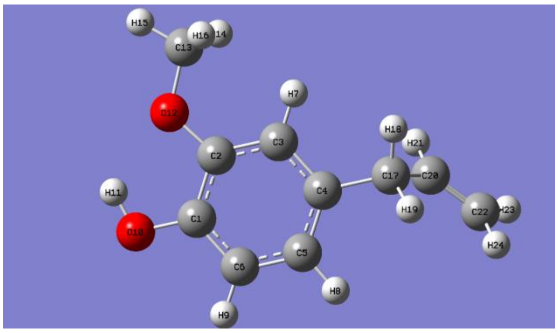


Figure 2: Optimised geometrical structure of Eugenol (2-methoxy-4-(prop-2-en-1-yl) phenol)

Geometrical parameters i.e., Bond Length, Bond Angle, Dihedral Angle of Eugenol after optimisation as calculated by DFT/ B3LYP/66-311G (d, p) level basis set are listed in Table 2.

Table 2: Optimised Geometrical parameters (bond length, bond angle, dihedral angle) of Eugenol (2-methoxy-4-(prop-2-en-1-yl) phenol) as calculated by DFT/B3LYP/6-311G (d, p) level basis set

S.No.	Bond between Atoms	Bond Length (A°)	Bond Angle between Atoms	Bond Angle (°)	Dihedral Angle between Atoms	Dihedral Angle (°)
1	R(1,2)	1.4082	A(2,1,6)	119.4645	D(6,1,2,3)	-0.0311
2	R(1,6)	1.3873	A(2,1,10)	120.1043	D(6,1,2,12)	-179.7709
3	R(1,10)	1.3654	A(6,1,10)	120.4308	D(10,1,2,3)	179.7394
4	R(2,3)	1.3909	A(1,2,3)	120.1104	D(10,1,2,12)	-0.0005
5	R(2,12)	1.369	A(1,2,12)	113.7316	D(2,1,6,5)	-0.1687
6	R(3,4)	1.4039	A(3,2,12)	126.1574	D(2,1,6,9)	179.7055
7	R(3,7)	1.0829	A(2,3,4)	120.5494	D(10,1,6,5)	-179.9384
8	R(4,5)	1.3943	A(2,3,7)	120.0534	D(10,1,6,9)	-0.0642
9	R(4,17)	1.5201	A(4,3,7)	119.3966	D(2,1,10,11)	0.1072
10	R(5,6)	1.3969	A(3,4,5)	118.7689	D(6,1,10,11)	179.8754
11	R(5,8)	1.0846	A(3,4,17)	120.4095	D(1,2,3,4)	0.1332
12	R(6,9)	1.084	A(5,4,17)	120.806	D(1,2,3,7)	-179.5908
13	R(10,11)	0.9679	A(4,5,6)	120.9413	D(12,2,3,4)	179.8382
14	R(12,13)	1.4286	A(4,5,8)	119.7889	D(12,2,3,7)	0.1143
15	R(13,14)	1.0938	A(6,5,8)	119.2697	D(1,2,12,13)	-179.6749
16	R(13,15)	1.0879	A(1,6,5)	120.165	D(3,2,12,13)	0.6038

17	R(13,16)	1.0939	A(1,6,9)	118.7231	D(2,3,4,5)	-0.0343
18	R(17,18)	1.0961	A(5,6,9)	121.1118	D(2,3,4,17)	178.5391
19	R(17,19)	1.094	A(1,10,11)	107.281	D(7,3,4,5)	179.6914
20	R(17,20)	1.5092	A(2,12,13)	118.7074	D(7,3,4,17)	-1.7351
21	R(20,21)	1.0888	A(12,13,14)	111.0107	D(3,4,5,6)	-0.1675
22	R(20,22)	1.3308	A(12,13,15)	105.8897	D(3,4,5,8)	179.9689
23	R(22,23)	1.0846	A(12,13,16)	111.0478	D(17,4,5,6)	-178.7351
24	R(22,24)	1.0863	A(14,13,15)	109.5739	D(17,4,5,8)	1.4013
25			A(14,13,16)	109.6958	D(3,4,17,18)	25.4018
26			A(15,13,16)	109.5459	D(3,4,17,19)	142.2645
27			A(4,17,18)	108.8261	D(3,4,17,20)	-95.6131
28			A(4,17,19)	109.918	D(5,4,17,18)	-156.054
29			A(4,17,20)	112.6416	D(5,4,17,19)	-39.1913
30			A(18,17,19)	106.9875	D(5,4,17,20)	82.931
31			A(18,17,20)	109.0191	D(4,5,6,1)	0.271
32			A(19,17,20)	109.2837	D(4,5,6,9)	-179.6001
33			A(17,20,21)	115.5749	D(8,5,6,1)	-179.8647
34			A(17,20,22)	125.0534	D(8,5,6,9)	0.2642
35			A(21,20,22)	119.3708	D(2,12,13,14)	60.6582
36			A(20,22,23)	121.5947	D(2,12,13,15)	179.5052
37			A(20,22,24)	121.5642	D(2,12,13,16)	-61.6614
38			A(23,22,24)	116.841	D(4,17,20,21)	58.1742
39					D(4,17,20,22)	-121.4769
40					D(18,17,20,21)	-62.7305
41					D(18,17,20,22)	117.6185
42					D(19,17,20,21)	-179.3461
43					D(19,17,20,22)	1.0028
44					D(17,20,22,23)	179.9568
45					D(17,20,22,24)	-0.1766
46					D(21,20,22,23)	0.318
47					D(21,20,22,24)	-179.8154

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 [20, 21]. Eugenol, 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 Eugenol . molecule and the theoretical spectra so obtained is shown in Figure 3 while frequencies, intensities and their corresponding assignments for the theoretical spectra are tabulated in Table 3. Vibrational frequencies have been assigned by visual inspection of modes animated by using the Gauss View 6.0 programme and the standard values reported [20]. A comprehensive account of the characteristic group absorptions and their relationship to molecular structure is discussed below

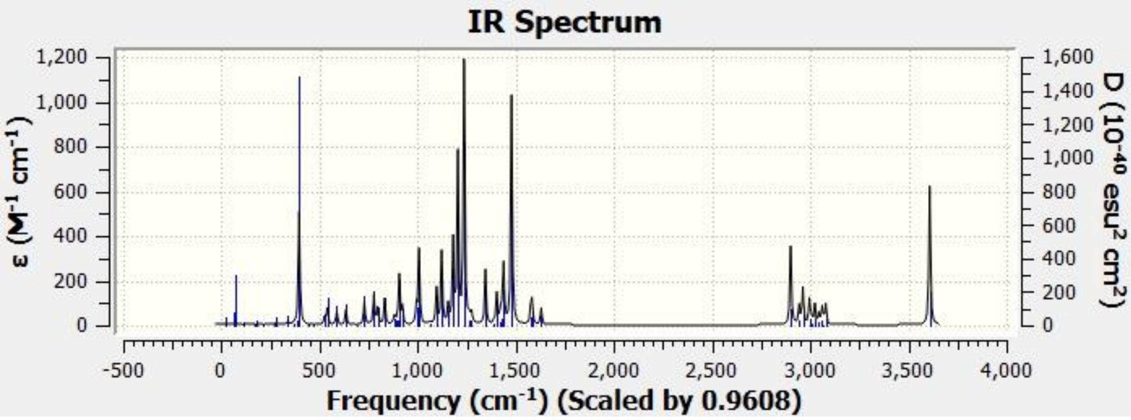


Figure 3: Theoretical IR spectra of Eugenol (2-methoxy-4-(prop-2-en-1-yl) phenol)

Table 3 : Frequencies (scaled and unscaled), intensities and corresponding vibrational assignment for the theoretical IR spectra of Eugenol (2-methoxy-4-(prop-2-en-1-yl) phenol)

Mode	Frequency unscaled (cm^{-1})	Frequency scaled (cm^{-1})	Intensity Epsilon ($M^{-1}cm^{-1}$)	Vibrational Assignment
1	24.34	23.38	0.3011	
2	68.39	65.71	1.3055	
3	73.94	71.04	5.6543	
4	114.13	109.65	0.6509	
5	177.56	170.60	0.3155	
6	188.06	180.69	1.2603	
7	222.75	214.02	0.6575	
8	281.84	270.79	0.3723	
9	289.66	278.31	3.6921	
10	352.96	339.12	5.4633	
11	381.08	366.14	1.2823	
12	396.85	381.29	3.3602	
13	412.03	395.88	153.2722	

14	463.47	445.30	0.8285	
15	489.68	470.48	0.8783	
16	547.95	526.47	9.0057	
17	560.77	538.79	23.2160	
18	611.71	587.74	18.3649	
19	661.00	635.09	20.9659	Out- of -plane ring C=C bending vibration
20	717.56	689.43	0.3077	Out-of-plane C-H bending vibration
21	757.83	728.12	32.5325	Out-of-plane C-H bending vibration
22	808.66	776.96	41.0686	Aromatic ring vibration
23	828.05	795.59	23.0770	Aromatic ring vibration
24	865.45	831.53	35.6129	Out-of-plane C-H vibrations(oops)
25	916.69	880.76	9.6594	Out-of-plane C-H vibrations(oops)
26	921.88	885.75	6.0960	Out-of-plane C-H vibrations(oops)
27	937.25	900.51	7.4591	Bending vibration of-CH_2 group
28	942.85	905.89	65.3154	In-plane C-H bending vibrations
29	958.77	921.19	24.1928	Aromatic ring vibrations (oops)
30	1034.10	993.57	26.8815	Out-of-plane C-H bending vibrations
31	1047.97	1006.89	101.9191	Symmetric C-O-C stretch
32	1106.02	1062.66	3.9143	Out-of-plane C-H bending vibrations of alkene.
33	1140.59	1095.88	49.4718	In-plane C-H bending of aromatic ring
34	1167.70	1121.93	95.6508	Aromatic ring vibrations
35	1169.43	1123.59	3.6744	In-plane C-H bending of -CH_3 group of methoxy
36	1202.44	1155.30	26.2305	In-plane C-H bending of aromatic ring
37	1225.65	1177.60	14.1228	In-plane C-O bending of phenolic group
38	1228.80	1180.63	104.4785	In-plane O-H bending of phenolic group
39	1253.87	1204.72	227.9839	Asymmetric C-O-C stretching vibration in ether
40	1286.40	1235.97	353.8247	C-O stretching vibration in phenol
41	1312.54	1261.09	10.8456	C-H bending vibration of allyl group
42	1325.19	1273.24	5.8546	Out-of-plane C-H bending of aromatic ring
43	1326.22	1274.23	9.8938	In-plane C-H bending of aromatic ring
44	1400.13	1345.25	74.5051	In-plane C-H bending of aromatic ring
45	1445.49	1388.82	4.6113	C-H bending of alkene of allyl group
46	1460.26	1403.02	40.8924	In-plane C-H bending of Aromatic ring
47	1475.42	1417.58	6.9605	Scissoring vibration of the terminal methylene group of alkene.
48	1481.67	1423.59	12.8902	In-plane C-H bending of -CH_3 group of methoxy group
49	1484.72	1426.52	9.4917	Antisymmetric -CH_3 bending of methoxy

				group
50	1496.27	1437.62	80.7124	Antisymmetric -CH_3 bending
51	1538.41	1478.11	309.1886	C=C stretching vibration of benzene ring
52	1639.02	1574.77	20.6970	C=C stretching vibration of benzene ring
53	1646.59	1582.04	32.6908	C=C stretching vibration of benzene ring
54	1695.49	1629.03	23.1308	C=C stretching vibration of unconjugated o alkene
55	3017.60	2899.31	40.6947	C-H stretching of methylene of allyl group
56	3019.32	2900.96	71.0568	C-H stretching of methyl of methoxy group
57	3063.96	2943.85	26.0541	Symmetrical stretching vibration of C-H group other than terminal C-H group of alkenes.
58	3083.25	2962.39	49.7805	C-H stretching of methyl of methoxy
59	3117.84	2995.62	33.9985	Asymmetrical stretching vibration of terminal C-H group of alkenes.
60	3127.33	3004.74	10.7246	Symmetrical stretching vibration of terminal C-H group of alkenes.
61	3146.27	3022.94	27.4379	Antisymmetric -CH_3 stretching vibration of -CH_3 group of methoxy group
62	3167.74	3043.57	15.5257	Symmetrical =C-H stretch of aromatic ring
63	3185.63	3060.76	22.8109	Asymmetrical =C–H stretches of aromatic ring
64	3190.61	3065.54	3.5714	Symmetrical=C-H Stretches of aromatic ring
65	3204.55	3078.93	28.1753	C-H vibration of ethene
66	3755.84	3608.61	187.8432	O-H stretching vibration of non-hydrogen bonded hydroxyl group of phenol

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 1640cm^{-1} with moderate intensity.

Alkene C-H stretching vibrations

In general, any C-H stretching bands above 3000cm^{-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 .

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 1416cm^{-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.

Alkanes C-H Stretching Vibrations

Absorption arising from C-H stretching in alkanes occurs 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 2962cm^{-1} result 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 are very weak and usually lost in other aliphatic C-H absorption and are observed near 2890 cm^{-1}.

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 720cm^{-1}. Configuration in which two methyl groups are attached to the same carbon atoms exhibits distinctive absorption in the C-H bending region

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 1300-1000cm^{-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 depend 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}.

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 absorbs at 1390-1330 and 1260-1180 cm^{-1}. These bands apparently result from interaction between O-H bending and C-O stretching.

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.

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 atom results in greater change in dipole moments than those involving carbon atoms hence more intnse bands are observed for ethers.The C-O-C stretching bands of ethers, as is the case of C-O stretching band of alconols, involve coupling with other vibrations with in molecule.The spectra of aryl-alkyl ethers display an asymmetrical C-O-C stretching band at 1275-1200cm^{-1} with symmetrical stretching band near 1075-1020 cm^{-1}. Resonance, which results in stregthening of the C-O bond , is responsible for the shift in the asymmetrical absorption band of aryl alkyl ethers.

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 Eugenol molecule and are compiled in Table 4. The statistical thermo chemical analysis of Eugenol (2-methoxy-4-(prop-2-en-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) has 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 Eugenol (2-methoxy-4-(prop-2-en-1-yl) phenol) as computed by frequency calculations

Thermodynamic Functions	**Value**
Zero-point vibrational energy	518243.3 (Joules/Mol)
	123.86313 (Kcal/Mol)
Zero-point correction	0.197388 (Hartree/Particle)
Thermal correction to Energy	0.209361
Thermal correction to Enthalpy	0.210305
Thermal correction to Gibbs Free Energy	0.158355
Sum of electronic and zero-point Energies	-538.654814
Sum of electronic and thermal Energies	-538.642841
Sum of electronic and thermal Enthalpies	-538.641897
Sum of electronic and thermal Free Energies	-538.693847

Table 5 : Thermodynamic properties of Eugenol (2-methoxy-4-(prop-2-en-1-yl) phenol) as calculated by DFT/B3LYP/6-311 G (d, p) level basis set

Type	**E (Thermal) (KCal/Mol)**	**C_v (Cal/Mol-Kelvin)**	**S (Cal/Mol-Kelvin)**
Total	131.376	44.865	109.338
Electronic	0.000	0.000	0.000
Translational	0.889	2.981	41.194
Rotational	0.889	2.981	31.116
Vibrational	129.599	38.903	37.028
Vibration 1	0.593	1.985	6.245
Vibration 2	0.598	1.969	4.199
Vibration 3	0.599	1.966	4.046

Vibration 4	0.607	1.938	3.198
Vibration 5	0.628	1.870	2.354
Vibration 6	0.633	1.856	2.247
Vibration 7	0.648	1.806	1.937
Vibration 8	0.681	1.707	1.522
Vibration 9	0.686	1.693	1.476
Vibration 10	0.729	1.569	1.153
Vibration 11	0.751	1.511	1.035
Vibration 12	0.763	1.477	0.974
Vibration 13	0.776	1.444	0.919
Vibration 14	0.821	1.331	0.756
Vibration 15	0.846	1.273	0.684
Vibration 16	0.903	1.144	0.548
Vibration 17	0.916	1.116	0.522
Vibration 18	0.971	1.007	0.430

Nonlinear optical properties of Eugenol

Molecular NLO properties of active compounds can be predicted with the help of quantum chemical calculations [22, 23]. The relationship between the nonlinear optical properties and the molecular structure can be better understood with the help of Hyperpolarizability [24-25]. 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 (Δα), 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 Eugenol molecule. Calculation of above mentioned NLO properties have been executed using equation-1 to equation-5[26-27] and the results are summarised in Table 6.

$$\mu = (\mu^2_x + \mu^2_y + \mu^2 z) \qquad (1)$$

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

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

$$\beta = (\beta^2_x+\beta^2_y+\beta^2_z)^{1/2} \qquad (4)$$

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

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

The conversion factor of α, β and γ in atomic unit are

For α 1 atomic unit (a.u.) = 0.1482 x 10^{-24} electrostatic unit (esu),

For β 1 a.u. = 8.6393x10^{-33}esu and

For γ 1a.u. = 5.0367x10^{-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 Eugenol. 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 Eugenol molecule (μ = 3.7864D)was calculated to be 1.5955 times that of the standard reference material of prototypical molecule urea (μ = 2.3732D) and first-order hyperpolarizability (β) of Eugenol molecule (β = 6.7409 x 10^{-31} esu) is about 1.81 times the first order hyperpolarizability of urea (β of urea = 3.728x10^{-31}esu).Thus it is recommended to use Eugenol molecule as a prospective building block for nonlinear optical material.

Table 6 : Nonlinear Optical components of Eugenol (2-methoxy-4-(prop-2-en-1-yl) phenol) 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	-0.4559	α_{XX}	-67.1836	β_{XXX}	-47.6636	γ_{XXXX}	-2324.1514
μ_Y	3.7414	α_{YY}	-65.9909	β_{YYY}	20.4356	γ_{YYYY}	-768.0847
μ_Z	0.3617	α_{ZZ}	-73.4884	β_{ZZZ}	-5.1247	γ_{ZZZZ}	-183.6064
Total μ	3.7864	α_{XY}	-10.0217	β_{XYY}	-14.3124	γ_{XXXY}	-110.5223
		α_{XZ}	1.3109	β_{XXY}	14.0975	γ_{XXXZ}	9.9362
		α_{YZ}	-1.1226	β_{XXZ}	-3.4332	γ_{YYYX}	-73.9495
		α	-68.88763333au	β_{XZZ}	-4.4824	γ_{YYYZ}	-1.5146
		Δα	-1.020914726x10^{-23}esu	β_{YZZ}	5.7562	γ_{ZZZX}	1.7675
				β_{YYZ}	1.6181	γ_{ZZZY}	0.7508
				β_{XYZ}	-2.3135	γ_{XXYY}	-549.7505
				β	78.0263 au	γ_{XXZZ}	-421.8113
					6.7409 x 10^{-31}esu	γ_{YYZZ}	-172.5652
						γ_{XXYZ}	-16.7900
						γ_{YYXZ}	3.9311
						γ_{ZZXY}	3.0906
						γ	-1112.8193 au
							-5.6049 x 10^{-37}esu

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 [28]. 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 Muliiken, APT, and Natural atomic charges are given in Table 7 and plotted in Figure 4. Atomic charge distribution is different due to the presence of polar -OH group on Carbon atom -1 and $-OCH_3$ 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.

Table-7: Mulliken, APT and Natural atomic charges on each of the constituent atom of Eugenol (2-methoxy-4-(prop-2-en-1-yl) phenol) molecule as calculated by DFT/B3LYP/6-311 G (d, p) level basis set

Atoms	Mulliken Charge	APT	Natural Charge
1 C	0.140144	0.596244	0.28865
2 C	0.154751	0.622668	0.26899
3 C	-0.100449	-0.130899	-0.29107
4 C	-0.128772	0.008106	-0.02547
5 C	-0.075602	-0.104159	-0.22183
6 C	-0.110946	-0.057445	-0.25451
7 H	0.120818	0.075289	0.21986
8 H	0.096928	0.041359	0.20849
9 H	0.108971	0.050048	0.21737
10 O	-0.389111	-0.964476	-0.68994
11 H	0.271691	0.414110	0.48641
12 O	-0.406821	-1.144331	-0.55955
13 C	-0.128646	0.644225	-0.19491
14 H	0.127306	-0.039590	0.17402
15 H	0.140245	-0.001360	0.19194
16 H	0.127272	-0.040384	0.17388
17 C	-0.196545	0.148439	-0.42707
18 H	0.133828	-0.046587	0.21254
19 H	0.126712	-0.049222	0.20868
20 C	-0.116591	0.081632	-0.15869
21 H	0.107984	0.010157	0.18878
22 C	-0.229089	-0.172489	-0.39031
23 H	0.115960	0.029736	0.19056
24 H	0.109964	0.028929	0.18318

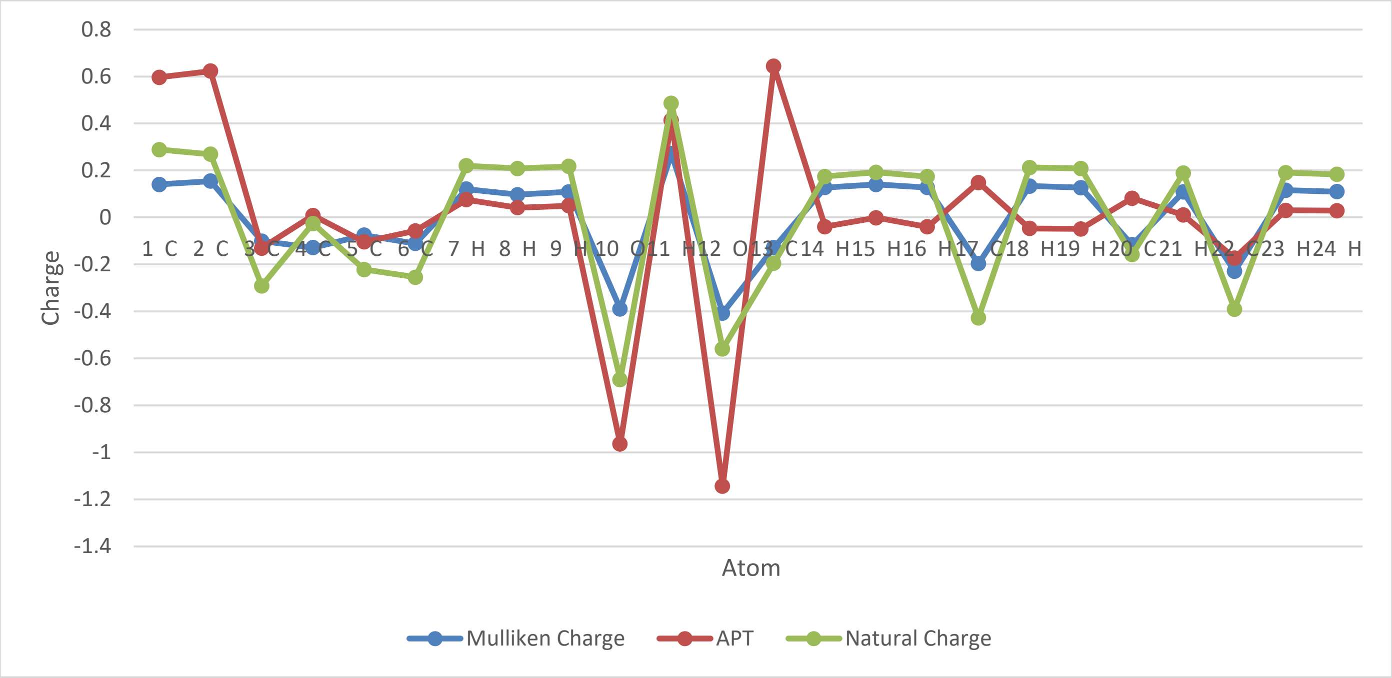


Figure 4: Mulliken, APT, and Natural charges on each of the constituent atom of Eugenol (2-methoxy-4-(prop-2-en-1-yl) phenol)

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 [25]. 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 Eugenol compound as obtained from TD-DFT calculations is shown in Figure 5.

Table 8 : UV-visible spectral results (Excitation energy, Absorption wavelength, Oscillator strength, Transition energy) of eugenol 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	2.2441eV	552.50nm	0.0234	44-> 45 44 <- 45	0.72654 -0.17963
2	3.7154eV	333.70nm	0.0159	43 -> 45	0.70301
3	3.9052eV	317.48nm	0.0348	44 -> 46	0.70227

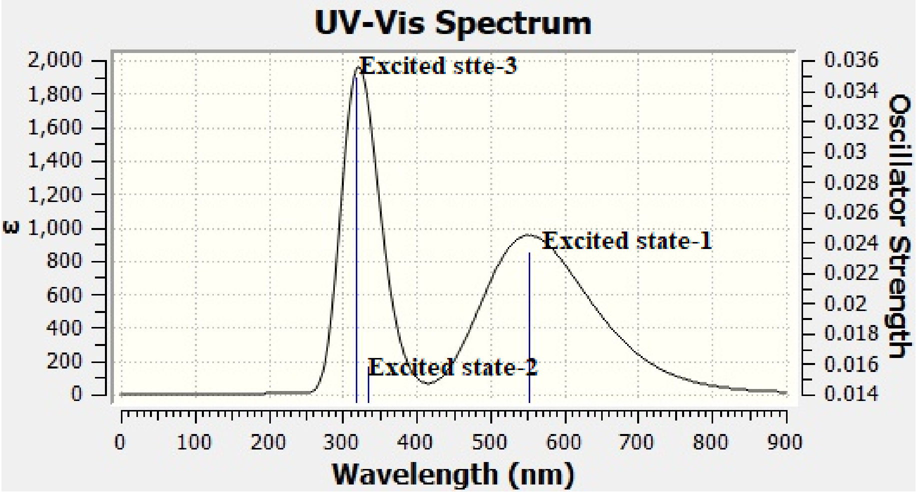


Figure 5: Theoretical UV-Visible spectra of Eugenol (2-methoxy-4-(prop-2-en-1-yl) phenol)

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 [29-30]. 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 $\Delta\varepsilon = \varepsilon_l - \varepsilon_r$ (L mol^{-1} cm^{-1}) [31]. TD-DFT method allows the simulation of the ECD spectrum of a medium size molecule on a desktop or PC in a reasonable time [32-33]. ECD spectra of Eugenol were studied using B3LYP/TD-DFT/6-311G (d, p) level and the results are presented in Table-9 and spectra in Fig. 6. In Eugenol molecule common chromophore and auxochrome groups are an aromatic ring, a phenolic and a methoxy group. The absorption bands are due to aromatic $\pi - \pi^*$ and $n - \pi^*$ transitions. A positive CE at 552.50nm, Rvel > 100 corresponds to R-configuration while almost zero CE at 333.70nm and 317.48nm corresponds to planar structure.

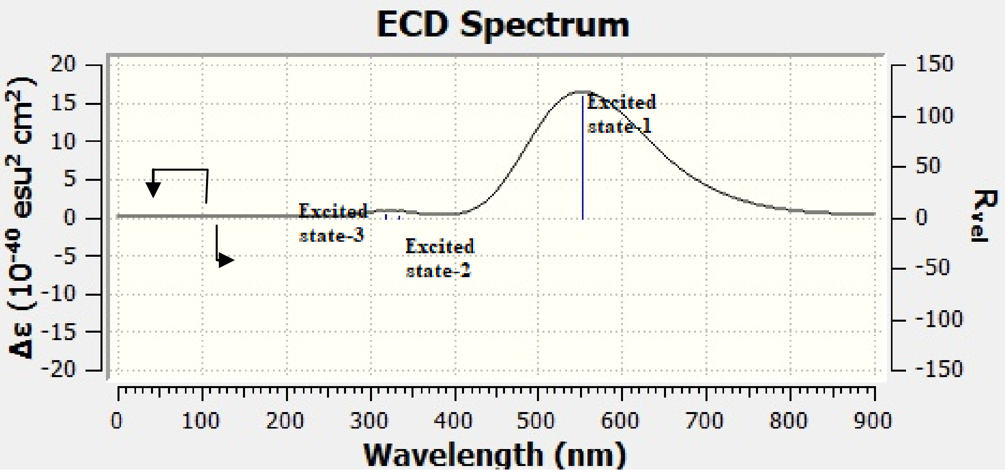


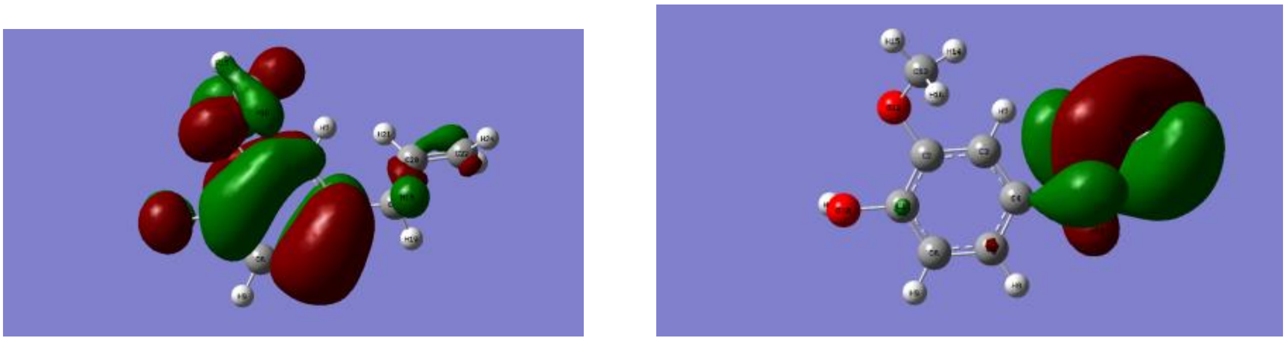
Figure 6: Theoretical ECD spectra of Eugenol (2-methoxy-4-(prop-2-en-1-yl) phenol)

Table 9: ECD spectral results of Eugenol (2-methoxy-4-(prop-2-en-1-yl) phenol)

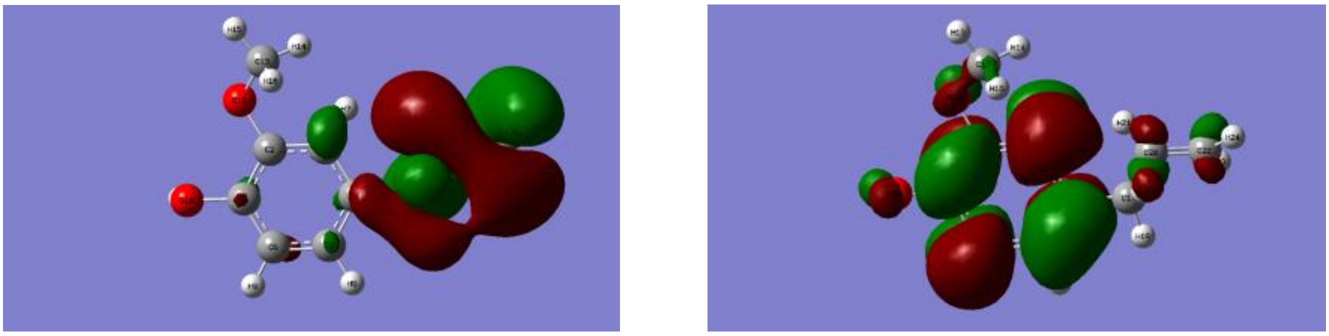
Excited State	**Wavelength (nm)**	**R_{vel}**	**Δε (10^{-40} esu^2 cm^2)**
1	552.50nm	≈ 130	≈ 17
2	333.70nm	≈ 0	≈ 0
3	317.48nm	≈ 0	≈ 0

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 Eugenol 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 7. In Table 10 energies of molecular orbitals undergoing major transitions and their energy gap (ΔE) have been presented.



HOMO MO-43 E= -0.2371eV **HOMO MO-44 E = -0.18684eV**



LUMO MO-45 E =-0.07794eV **LUMO MO-46 E = -0.01873eV**

Figure 7: FMO analysis Results

Table 10 : Energy gap (ΔE) of major electronic transitions in Eugenol (2-methoxy-4-(prop-2-en-1-yl) phenol) molecule

HOMO Energy (E_{LUMO})	**LUMO Energy (E_{HOMO})**	**Energy gap (ΔE) (E_{LUMO}-E_{HOMO})**
43 (-.0.2371 eV)	45 (-0.07794eV)	0.15916
44 (-0.18684eV)	45 (-0.07794eV)	0.1089
44 (-0.18684eV)	46 (-0.01873eV)	0.16811

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 [34-38]. Robert Parr and others [34] 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 [39] as the average value of the ionization potential and electron affinity. Robert G Parr and others [36] scrutinized the concept of electronegativity from the point of view of Density Functional Theory of Hohenberg and Kohn [40]. 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 [37-38]. 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 Eugenol 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 Eugenol (2-methoxy-4-(prop-2-en-1-yl) phenol)

Parameter	**Relation**	**Calculated Value**
Ionization Energy(I)	$-E_{HOMO}$	0.18684
Electron Affinity (A)	$-E_{LUMO}$	0.07794
Chemical Potential(ϕ)	$\frac{-(I+A)}{2}$	-0.13239
Absolute hardness(η)	$\frac{(I-A)}{2}$	0.05445
Softness(S)	$\frac{1}{\eta}$	18.36547291

Electronegativity (χ)	$\frac{(I + A)}{2}$	0.13239
Electrophilicity index (ω)	$\frac{\phi 2}{2\eta}$	0.16094685
Electron donating capability(ω-)	$\frac{(3I + A)2}{16(I - A)}$	0.233948101
Electron accepting capability (ω+)	$\frac{(I + 3A)2}{16(I - A)}$	0.101558101

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 Eugenol was computed using B3LYP/6-311G (d, p) basis set at DFT and is shown in Figure 8 and Figure 9 respectively. ESP for HOMO and LUMO are shown in Figure 10 and 11.

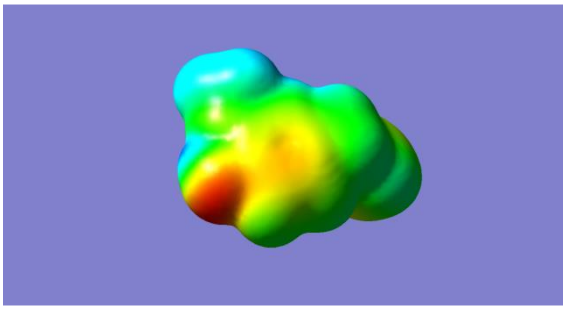


Figure 8: Electron density of Eugenol (2-methoxy-4-(prop-2-en-1-yl) phenol) from total scf density (isovalue =0.0004; mapped with esp)

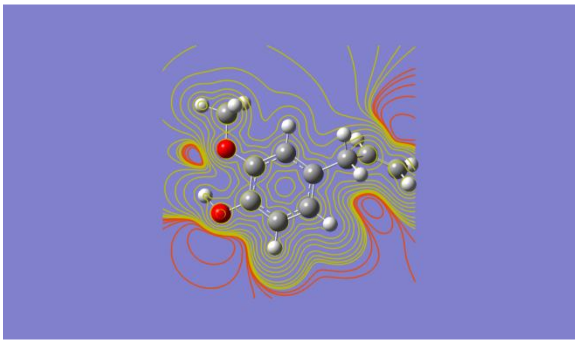


Figure-9: Electrostatic potential from total scf density (red- negative charge -yellow-green - blue positive charge)

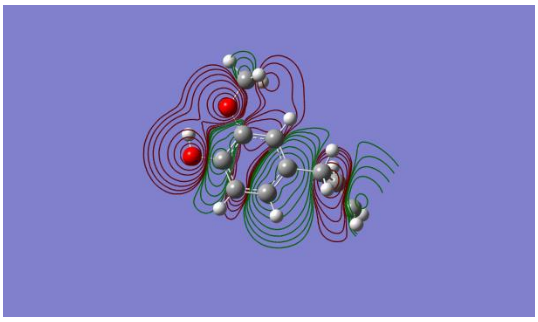


Figure-10 electrostatic potential from total scf density (mo-44) HOMO potential from total scf density (mo-45) LUMO

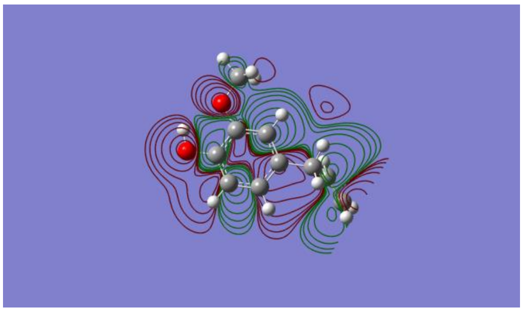


Figure-11 Electrostatic

IV. CONCLUSION

An attempt was made to calculate various physico-chemical properties of Eugenol 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 Eugenol 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 Eugenol were calculated and were observed to be greater than 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 Eugenol is quite stable and does not undergo decomposition readily.

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