

Physico-Chemical Properties and Quantum Chemical Calculation of Methyleugenol (1,2-dimethoxy-4-(prop-2-en-1-yl)benzene)

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Abstract - Physico-chemical properties play 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, Revision A.01, software package was used for the theoretical quantum chemical calculations of 1,2-dimethoxy-4-(prop-2-en-1-yl)benzene commonly called Methyleugenol. 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 Methyl eugenol (1,2-dimethoxy-4-(prop-2-en-1-yl)benzene). 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 Methyl eugenol (1,2-dimethoxy-4-(prop-2-en-1-yl)benzene) 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.

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

I. INTRODUCTION

Methyl eugenol is a volatile Phenylpropanoid present in the essential oils from flowers, stems, roots, or whole plant extracts of over 450 species of plant from 80 families including both angiosperm and gymnosperm families [1]. In the essential oil of several species, like *Cinnamomum cordatum* Kosterm (Lauraceae) and *Croton malambo* H.Karst (Euphorbiaceae), more than 90% methyl eugenol can be found [2]. Chemical name for Methyl eugenol is 1,2-dimethoxy-4-prop-2-enylbenzene in accordance with International Union Of Pure and Applied Chemistry and other synonyms are 4-allylveratrole; 4-allyl-1,2-dimethoxybenzene; eugenyl methyl ether; 1,2-dimethoxy-4-(2-propenyl)benzene; 3,4-dimethoxy-allylbenzene; 3-(3,4-dimethoxyphenyl)prop-1-ene; O-methyl eugenol and methyl eugenol ether. Structural formula of Methyl eugenol is depicted in Figure -1.

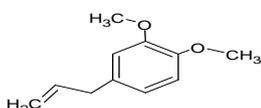


Figure-1: Structural formula of Methyl eugenol (1,2-dimethoxy-4-(prop-2-en-1-yl)benzene)

Methyl eugenol is colourless to pale yellow liquid with a clove-carnation odour and a bitter taste [3], soluble in ethanol, ethyl ether, chloroform and most organic solvents but insoluble in water, glycol and propylene glycol [3]. Methyl eugenol evaporates readily at room temperature but darkens and slowly thickens when exposed to air [3]. Methyl eugenol has been known to possess antifungal [4-5], antibacterial [6], nematocidal [7], anti-inflammation [8], anticancer [9], anaesthetic [10], anti-allergen activity [11], anti-anaphylaxis [12], anti-nociceptive [13] effects etc. It is widely used in foods as a flavouring agent and in cosmetics, soaps, and shampoos as a fragrance agent [14]. Methyl 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, Methyl 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 [15-16]. Growing interest of researchers in this molecule motivated us to calculate physico-chemical properties and carry out quantum chemical calculations (computational study) of Methyl 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 Methyl eugenol(1,2-dimethoxy-4-(prop-2-en-1-yl)benzene) are done using acdlab/chemsketch [17] and the predicted data is generated using the ACD/Labs Percepta Platform - PhysChem Module. Quantum chemical calculation of Methyl eugenol(1,2-dimethoxy-4-(prop-2-en-1-yl)benzene) have been performed using personal laptop using Gaussian 09, Revision A, 01 software package [18] 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 Methyl eugenol(1,2-dimethoxy-4-(prop-2-en-1-yl)benzene). 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 Methyl eugenol(1,2-dimethoxy-4-(prop-2-en-1-yl)benzene) were computed using Time Dependent DFT (TD-DFT) method using the same basis set.

III. RESULTS AND DISCUSSION

A. Physico-chemical Properties of Methyl eugenol(1,2-dimethoxy-4-(prop-2-en-1-yl)benzene)

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 Methyl eugenol(1,2-dimethoxy-4-(prop-2-en-1-yl)benzene) were calculated using acdlab/chemsketch [17] 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 of Methyl eugenol(1,2-dimethoxy-4-(prop-2-en-1-yl)benzene)

S.No.	Physico-chemical property	Calculated values of the property
1	Molecular Formula:	C ₁₁ H ₁₄ O ₂
2	Formula Weight:	178.22766
3	Composition:	C(74.13%) H(7.92%) O(17.95%)
4	Molar Refractivity:	53.51 ± 0.3 cm ³
5	Molar Volume:	181.8 ± 3.0 cm ³
6	Parachor:	425.9 ± 4.0 cm ³
7	Index of Refraction:	1.500 ± 0.02
8	Surface Tension:	30.1 ± 3.0 dyne/cm
9	Density:	0.980 ± 0.06 g/cm ³
10	Dielectric Constant:	Not available
11	Polarizability:	21.21 ± 0.5 10 ⁻²⁴ cm ³
12	Topological Polar Surface Area	18.5 Å ²
13	RDBE:	5

14	Monoisotopic Mass:	178.09938 Da
15	Nominal Mass:	178 Da
16	Average Mass:	178.2277 Da
17	M+:	178.098831 Da
18	M-:	178.099928 Da
19	[M+H] ⁺ :	179.106656 Da
20	[M+H] ⁻ :	179.107753 Da
21	[M-H] ⁺ :	177.091006 Da
22	[M-H] ⁻ :	177.092103 Da

B. Geometrical analysis

The molecular structure of Methyl eugenol(1,2-dimethoxy-4-(prop-2-en-1-yl)benzene) having Molecular formula C₁₁H₁₄O₂ Molecular mass: 178.09938 amu, is an asymmetric top type of molecule with 75 degrees of freedom. Gaussian 09, Revision A.01, and Gauss View 6.0.16 programme was used for the optimisation of molecular structure of Methyl eugenol(1,2-dimethoxy-4-(prop-2-en-1-yl)benzene) and the obtained optimised molecular structure along with the atom numbering scheme is shown in Figure 2.

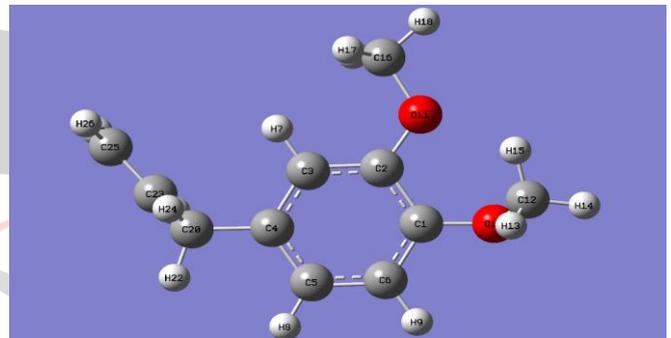


Figure 2: Optimised Geometrical Structure of Methyl eugenol(1,2-dimethoxy-4-(prop-2-en-1-yl)benzene)

Geometrical parameters i.e., Bond Length, Bond Angle, Dihedral Angle of Methyl eugenol(1,2-dimethoxy-4-(prop-2-en-1-yl)benzene) 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 Methyl eugenol(1,2-dimethoxy-4-(prop-2-en-1-yl)benzene) 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)	1.4127	A(2,1,6)	119.0667	D(6,1,2,3)	0.6258
2	R(1,6)	1.3869	A(2,1,10)	121.7831	D(6,1,2,11)	-178.9407
3	R(1,10)	1.3723	A(6,1,10)	119.0626	D(10,1,2,3)	177.1896
4	R(2,3)	1.3931	A(1,2,3)	119.4964	D(10,1,2,11)	-2.3769
5	R(2,11)	1.3653	A(1,2,11)	116.005	D(2,1,6,5)	0.0334
6	R(3,4)	1.4025	A(3,2,11)	124.497	D(2,1,6,9)	179.2005
7	R(3,7)	1.0824	A(2,3,4)	121.1758	D(10,1,6,5)	-176.625
8	R(4,5)	1.3912	A(2,3,7)	120.132	D(10,1,6,9)	2.5421
9	R(4,20)	1.5206	A(4,3,7)	118.6921	D(2,1,10,12)	68.8745
10	R(5,6)	1.396	A(3,4,5)	118.8321	D(6,1,10,12)	-114.5616
11	R(5,8)	1.0846	A(3,4,20)	119.897	D(1,2,3,4)	-0.7976
12	R(6,9)	1.0838	A(5,4,20)	121.265	D(1,2,3,7)	179.2922
13	R(10,12)	1.4311	A(4,5,6)	120.3245	D(11,2,3,4)	178.7297

14	R(11,16)	1.4206	A(4,5,8)	120.0009	D(11,2,3,7)	-1.1806
15	R(12,13)	1.0962	A(6,5,8)	119.6745	D(1,2,11,16)	177.6223
16	R(12,14)	1.0899	A(1,6,5)	121.0987	D(3,2,11,16)	-1.9199
17	R(12,15)	1.0918	A(1,6,9)	117.7015	D(2,3,4,5)	0.2967
18	R(16,17)	1.0956	A(5,6,9)	121.1944	D(2,3,4,20)	-178.8359
19	R(16,18)	1.0888	A(1,10,12)	116.1467	D(7,3,4,5)	-179.7918
20	R(16,19)	1.0954	A(2,11,16)	118.3798	D(7,3,4,20)	1.0756
21	R(20,21)	1.0962	A(10,12,13)	110.693	D(3,4,5,6)	0.3723
22	R(20,22)	1.096	A(10,12,14)	106.0214	D(3,4,5,8)	-179.7417
23	R(20,23)	1.5065	A(10,12,15)	111.418	D(20,4,5,6)	179.4926
24	R(23,24)	1.0885	A(13,12,14)	109.2599	D(20,4,5,8)	-0.6214
25	R(23,25)	1.3301	A(13,12,15)	109.7521	D(3,4,20,21)	65.7083
26	R(25,26)	1.0843	A(14,12,15)	109.6122	D(3,4,20,22)	-178.2803
27	R(25,27)	1.0862	A(11,16,17)	111.6199	D(3,4,20,23)	-56.9201
28			A(11,16,18)	105.7993	D(5,4,20,21)	-113.4028
29			A(11,16,19)	111.388	D(5,4,20,22)	2.6087
30			A(17,16,18)	109.3405	D(5,4,20,23)	123.9689
31			A(17,16,19)	109.3121	D(4,5,6,1)	-0.5394
32			A(18,16,19)	109.2951	D(4,5,6,9)	-179.6773
33			A(4,20,21)	109.938	D(8,5,6,1)	179.5743
34			A(4,20,22)	108.2589	D(8,5,6,9)	0.4364
35			A(4,20,23)	113.5525	D(1,10,12,13)	58.5527
36			A(21,20,22)	106.539	D(1,10,12,14)	176.9325
37			A(21,20,23)	109.1707	D(1,10,12,15)	-63.8742
38			A(22,20,23)	109.1381	D(2,11,16,17)	62.4801
39			A(20,23,24)	115.5596	D(2,11,16,18)	-178.6793
40			A(20,23,25)	125.0829	D(2,11,16,19)	-60.0183
41			A(24,23,25)	119.3568	D(4,20,23,24)	-57.7267
42			A(23,25,26)	121.6846	D(4,20,23,25)	121.9927
43			A(23,25,27)	121.5402	D(21,20,23,24)	179.2227
44			A(26,25,27)	116.7734	D(21,20,23,25)	-1.0579
45					D(22,20,23,24)	63.1404
46					D(22,20,23,25)	-117.1402
47					D(20,23,25,26)	179.6459
48					D(20,23,25,27)	0.1501
49					D(24,23,25,26)	-0.6446
50					D(24,23,25,27)	179.8596

C. 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 [19,20]. Methyl eugenol(1,2-dimethoxy-4-(prop-2-en-1-yl)benzene), the molecule under consideration, has an asymmetric top group symmetry and 27 atoms; hence 75 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 Methyl eugenol(1,2-dimethoxy-4-(prop-2-en-1-yl)benzene) molecule and theoretical IR spectra and Raman spectra so obtained are shown in Figure 3 and 4 respectively while frequencies, Reduced mass, Force constant, Intensities, and corresponding vibrational assignment for the theoretical IR spectra of Methyl eugenol(1,2-dimethoxy-4-(prop-2-en-1-yl)benzene) 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 [19]. A comprehensive account of the characteristic group absorptions and their relationship to molecular structure is discussed below.

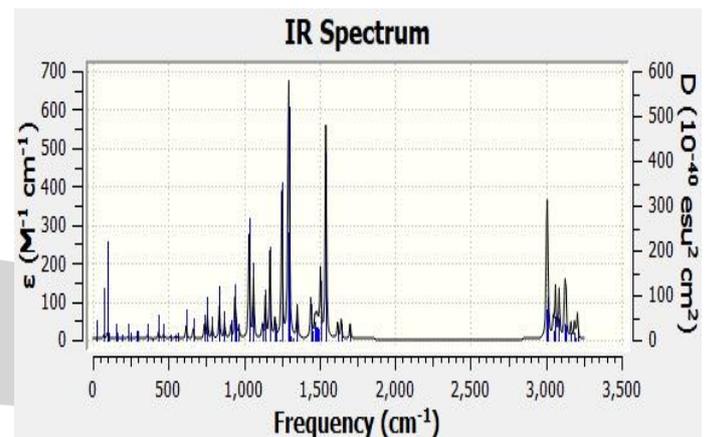


Figure 3: Theoretical IR Spectra of Methyl eugenol(1,2-dimethoxy-4-(prop-2-en-1-yl)benzene)

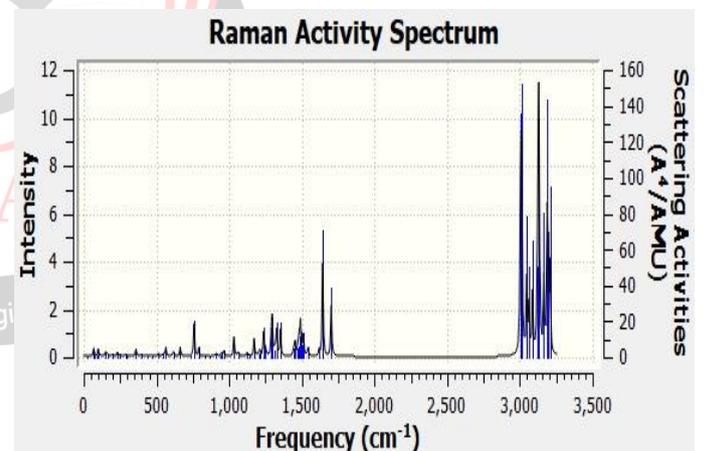


Figure 4: Theoretical Raman Spectra of Methyl eugenol(1,2-dimethoxy-4-(prop-2-en-1-yl)benzene)

Table 3: frequencies, Reduced mass, Force constant, Intensities, and corresponding vibrational assignment for the theoretical IR spectra of Methyl eugenol(1,2-dimethoxy-4-(prop-2-en-1-yl)benzene)

MOD E	Frequen cy	Reduc ed Mass	Force Consta nt	Infrare d	Raman Activit y	Depola r-P	Depola r-U
1	24.92	3.1939	0.0012	0.2624	0.4503	0.7472	0.8553
2	69.13	3.5938	0.0101	1.1451	4.5024	0.6624	0.7969
3	73.36	2.1871	0.0069	2.1298	0.6163	0.7063	0.8279
4	93.58	3.1949	0.0165	5.1154	0.5746	0.6259	0.7699
5	100.74	2.1617	0.0129	0.3665	4.0155	0.7383	0.8495
6	150.74	1.4619	0.0196	1.2969	2.7396	0.6875	0.8148
7	161.68	2.2584	0.0348	0.7034	1.7613	0.7491	0.8565
8	195.00	2.5608	0.0574	0.4982	1.4453	0.7494	0.8567
9	231.63	1.6878	0.0534	2.0160	2.6131	0.6358	0.7774
10	246.23	2.9835	0.1066	1.0747	1.1439	0.2765	0.4332
11	286.81	2.4468	0.1186	1.5709	1.1655	0.5747	0.7299
12	299.85	4.1796	0.2214	1.6195	0.8558	0.1020	0.1852

13	358.85	3.8652	0.2933	3.2740	4.6237	0.1496	0.2602
14	394.21	2.2226	0.2035	0.3056	1.2824	0.3953	0.5666
15	435.11	3.6004	0.4016	6.1411	1.0907	0.7500	0.8571
16	468.06	3.2845	0.4240	4.2304	1.1540	0.4287	0.6001
17	514.24	3.4369	0.5355	1.5612	2.2420	0.6486	0.7869
18	546.40	3.4855	0.6131	1.6282	1.6760	0.6857	0.8136
19	564.75	5.0637	0.9516	2.3304	5.7680	0.3501	0.5186
20	616.76	2.2585	0.5062	10.5530	3.3214	0.6974	0.8217
21	663.29	3.1543	0.8176	8.2205	5.9036	0.4720	0.6413
22	738.00	3.4023	1.0918	10.5569	0.6097	0.7056	0.8274
23	758.22	4.2104	1.4261	18.5463	20.5835	0.1182	0.2114
24	790.31	3.4218	1.2592	10.3052	5.4781	0.1134	0.2037
25	837.44	1.5300	0.6322	25.4300	1.0291	0.4371	0.6083
26	870.73	1.5168	0.6776	13.6540	0.4917	0.4311	0.6025
27	911.98	1.6311	0.7993	10.1614	2.3715	0.1590	0.2743
28	940.34	1.5897	0.8282	29.0918	0.5261	0.0972	0.1772
29	946.55	1.4356	0.7578	3.9163	0.5700	0.7401	0.8507
30	948.53	1.6830	0.8921	8.5573	2.1168	0.4470	0.6178
31	965.96	2.9535	1.6237	8.5591	3.5429	0.1153	0.2068
32	1032.86	4.6959	2.9516	70.3183	8.6034	0.7292	0.8434
33	1034.30	1.2457	0.7852	9.5668	5.4423	0.5901	0.7422
34	1063.02	4.7027	3.1309	45.4164	3.1776	0.3044	0.4667
35	1121.10	1.6709	1.2374	10.5233	2.5347	0.3799	0.5506
36	1142.13	1.4625	1.1241	31.5705	1.4151	0.0769	0.1428
37	1168.50	1.2618	1.0151	5.8777	2.6913	0.7161	0.8345
38	1170.95	1.2956	1.0467	2.2288	2.9561	0.6690	0.8017
39	1172.30	2.2530	1.8243	60.6676	7.5220	0.0856	0.1578
40	1204.61	1.4215	1.2153	12.6042	2.3357	0.7078	0.8289
41	1211.43	1.4816	1.2811	5.6346	4.2173	0.4200	0.5915
42	1236.15	1.3689	1.2324	0.2044	16.7563	0.4799	0.6486
43	1249.92	2.5730	2.3684	110.0337	5.9735	0.5254	0.6889
44	1290.98	1.7168	1.6858	77.2875	16.5290	0.2113	0.3489
45	1296.67	2.6232	2.5986	168.4152	22.5070	0.1159	0.2077
46	1312.05	1.7765	1.8019	3.1683	4.3072	0.2198	0.3604
47	1325.57	1.3610	1.4091	0.9049	18.9229	0.4091	0.5807
48	1352.52	3.2770	3.5320	25.1321	19.2295	0.1579	0.2727
49	1441.90	2.1774	2.6673	29.4136	4.4407	0.7365	0.8483
50	1450.64	1.2148	1.5061	6.6874	10.0350	0.5300	0.6928
51	1469.22	1.2004	1.5267	14.7567	5.0101	0.7354	0.8475
52	1478.10	1.1082	1.4265	10.6678	5.6634	0.7070	0.8284
53	1482.29	1.0743	1.3907	10.4807	11.7584	0.7496	0.8569
54	1489.76	1.3302	1.7394	3.0729	10.5969	0.6855	0.8134
55	1491.04	1.0456	1.3696	8.5453	14.6418	0.7497	0.8570
56	1505.85	1.0652	1.4231	49.0961	6.7926	0.6423	0.7822
57	1510.93	1.0474	1.4088	7.3560	13.4819	0.7109	0.8311
58	1541.50	2.8839	4.0376	160.7115	6.0964	0.2708	0.4262
59	1619.51	7.0788	10.9391	12.5774	5.0419	0.3965	0.5678
60	1643.52	5.9786	9.5148	15.0049	70.6394	0.5994	0.7495
61	1702.49	4.5749	7.8127	12.1416	39.0779	0.1670	0.2861
62	3003.49	1.0346	5.4990	52.2399	94.1155	0.0356	0.0688
63	3007.79	1.0401	5.5439	71.2955	135.6738	0.0491	0.0935
64	3012.97	1.0587	5.6625	25.8068	152.0856	0.0394	0.0758

65	3047.47	1.1023	6.0316	14.4348	78.3016	0.7449	0.8538
66	3062.09	1.1062	6.1112	38.5783	50.4293	0.7410	0.8513
67	3086.32	1.0943	6.1412	36.9586	64.9459	0.4115	0.5831
68	3120.99	1.0616	6.0925	17.2404	50.0146	0.2492	0.3990
69	3125.97	1.1044	6.3583	28.3041	132.1707	0.5339	0.6961
70	3129.79	1.0886	6.2827	6.4346	133.1552	0.2166	0.3561
71	3132.38	1.0992	6.3544	24.0667	118.1354	0.4620	0.6320
72	3164.90	1.0885	6.4236	12.2416	80.5509	0.5133	0.6784
73	3188.37	1.0934	6.5487	12.2345	143.9387	0.2335	0.3786
74	3195.20	1.0891	6.5512	2.7121	69.6941	0.2104	0.3477
75	3207.35	1.1150	6.7578	19.3768	94.8245	0.6153	0.7619

a) 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.

b) 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.

c) 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.

d) 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} .

e) 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

f) Mononuclear Aromatic Hydrocarbon

In the spectra of aromatic compounds most prominent and informative bands occur in the frequency region between $900\text{--}675\text{ cm}^{-1}$. These strong absorption bands are the result of out-of-plane ("oop") bending C-H bonds of the ring. In the $1300\text{--}1000\text{ cm}^{-1}$ region In-plane bending bands are observed. Skeletal vibrations, involving stretching of carbon-carbon bonds within the benzene ring, absorb in the $1600\text{--}1585$ and $1500\text{--}1400\text{ cm}^{-1}$ 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 $2000\text{--}1650\text{ cm}^{-1}$ 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 $900\text{--}675\text{ cm}^{-1}$.

g) 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 intense bands are observed for ethers. The C-O-C stretching bands of ethers, as is the case of C-O stretching band of alcohols, involve coupling with other vibrations within molecule. The spectra of aryl-alkyl ethers display an asymmetrical C-O-C stretching band at $1275\text{--}1200\text{ cm}^{-1}$ with symmetrical stretching band near $1075\text{--}1020\text{ cm}^{-1}$. Resonance, which results in strengthening of the C-O bond, is responsible for the shift in the asymmetrical absorption band of aryl alkyl ethers.

D. 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 Methyl eugenol(1,2-dimethoxy-4-(prop-2-en-1-yl)benzene) molecule and are compiled in Table 4. The

statistical thermo chemical analysis of Methyl eugenol(1,2-dimethoxy-4-(prop-2-en-1-yl)benzene) is carried out by assuming the molecule under consideration to be at room temperature of 300 K 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 Methyl eugenol(1,2-dimethoxy-4-(prop-2-en-1-yl)benzene) as computed by frequency calculations

Thermodynamic Functions	Value
Zero-point correction	0.225312 (Hartree/Particle)
Thermal correction to Energy	0.238846
Thermal correction to Enthalpy	0.239790
Thermal correction to Gibbs Free Energy	0.184162
Sum of electronic and zero-point Energies	-577.921617
Sum of electronic and thermal Energies	-577.908083
Sum of electronic and thermal Enthalpies	-577.907139
Sum of electronic and thermal Free Energies	-577.962766

Table 5: Thermodynamic properties of Methyl eugenol(1,2-dimethoxy-4-(prop-2-en-1-yl)benzene) as calculated BY DFT/B3LYP/6-311 G (d, p) level basis set

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	149.878	49.547	117.078
Electronic	0.000	0.000	0.000
Translational	0.889	2.981	41.438
Rotational	0.889	2.981	31.555
Vibrational	148.101	43.586	44.085
Vibration 1	0.593	1.985	6.198
Vibration 2	0.598	1.969	4.178
Vibration 3	0.599	1.967	4.061
Vibration 4	0.603	1.954	3.584
Vibration 5	0.604	1.949	3.440
Vibration 6	0.618	1.902	2.663
Vibration 7	0.622	1.889	2.530
Vibration 8	0.636	1.847	2.180
Vibration 9	0.653	1.793	1.866
Vibration 10	0.661	1.769	1.757
Vibration 11	0.684	1.698	1.493
Vibration 12	0.692	1.674	1.418
Vibration 13	0.734	1.557	1.127
Vibration 14	0.761	1.483	0.984
Vibration 15	0.796	1.394	0.842
Vibration 16	0.825	1.321	0.743
Vibration 17	0.869	1.218	0.623
Vibration 18	0.902	1.148	0.552
Vibration 19	0.921	1.108	0.514
Vibration 20	0.976	0.996	0.422

E. Nonlinear optical properties of Methyl eugenol(1,2-dimethoxy-4-(prop-2-en-1-yl)benzene)

Molecular NLO properties of active compounds can be predicted with the help of quantum chemical calculations [21-22]. The relationship between the nonlinear optical properties and the molecular structure can be better understood with the help of Hyperpolarizability [23-24].

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 Methyl eugenol(1,2-dimethoxy-4-(prop-2-en-1-yl)benzene) molecule. Calculation of above mentioned NLO properties have been executed using equation-1 to equation-5[25-26] 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 1 a.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 Methyl eugenol(1,2-dimethoxy-4-(prop-2-en-1-yl)benzene). 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 Methyl eugenol(1,2-dimethoxy-4-(prop-2-en-1-yl)benzene) molecule ($\mu = 2.0638$ D) was calculated to be 0.8697 times that of the standard reference material of prototypical molecule urea ($\mu = 2.3732$ D) and first-order hyperpolarizability (β) of Methyl eugenol(1,2-dimethoxy-4-(prop-2-en-1-yl)benzene) molecule ($\beta = 5.487519 \times 10^{-31}$ esu) is about 1.4720 times the first order hyperpolarizability of urea (β of urea = 3.728×10^{-31} esu). Thus it is recommended to use Methyl eugenol(1,2-dimethoxy-4-(prop-2-en-1-yl)benzene) molecule as a prospective building block for nonlinear optical material.

Table 6: Nonlinear Optical components of Methyl eugenol(1,2-dimethoxy-4-(prop-2-en-1-yl)benzene) 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
2.0638D			

μ_x	0.9370	α_x x	-78.6061	β_x xx	39.5537	γ_{xx} xx	-2777.7614
μ_y	1.5648	α_y y	-69.6262	β_y yy	18.8232	γ_{yy} yy	-919.6656
μ_z	0.9657	α_z z	-78.8948	β_z z	2.9751	γ_{zz} z	-225.1523
Total μ	2.0638D	α_x y	1.0967	β_x yy	8.0816	γ_{xx} xy	-26.8750
		α_x z	5.0167	β_x xy	10.6030	γ_{xx} xz	62.9901
		α_y z	-1.3848	β_x xz	14.0407	γ_{yy} yx	32.5217
		α	-75.7090au	β_{xz} z	4.3618	γ_{yy} yz	-8.5249
			-11.2200738x 10^{-24} esu	β_{yz} z	6.3928	γ_{zz} x	-4.6974
		Δ α	12.96832877 78au	β_y yz	-3.2602	γ_{zz} y	-6.3491
				β_x yz	-2.3545	γ_{xx} yy	-617.9757
				β	63.5181a u	γ_{xx} zz	-477.9801
					5.487519 $\times 10^{-31}$ esu	γ_{yy} zz	-214.6450
						γ_{xx} yz	-0.9878
						γ_{yy} xz	-1.3590
						γ_{zz} y	-4.0656
						γ	1308.7562 au
							6591.8123 $\times 10^{-40}$ esu

F. 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 [27]. 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 and APT atomic charges. Calculated values of Mulliken and APT atomic charges are given in Table 7 and plotted in Figure 5. Atomic charge distribution is different due to the presence of $-OCH_3$ group on carbon atom-1 and 2. Oxygen atom -10 and 11 have maximum negative due to the presence of methyl group which has +I effect. Carbon atoms 1, 2, 12 and 16 have positive charge as they are directly attached to electronegative oxygen atom of two methoxy groups.

Table 7: Mulliken and APT atomic charges on each of the constituent atom of Methyl eugenol(1,2-dimethoxy-4-(prop-2-en-1-yl)benzene) molecule as calculated BY DFT/B3LYP/6-311 g (d, p) level basis set.

Atoms	Mulliken Charge	APT Charge
1 C	0.128758	0.422967
2 C	0.176669	0.501442
3 C	-0.057676	-0.182609
4 C	-0.128786	0.061477

5 C	-0.078132	-0.119727
6 C	-0.075551	-0.023972
7 H	0.103055	0.059557
8 H	0.078845	0.024649
9 H	0.095212	0.041398
10 O	-0.367628	-0.849136
11 O	-0.355583	-0.845228
12 C	-0.110094	0.526042
13 H	0.089426	-0.048386
14 H	0.111774	-0.028774
15 H	0.115057	-0.008025
16 C	-0.131983	0.507995
17 H	0.112887	-0.038196
18 H	0.129003	-0.001867
19 H	0.112970	-0.035925
20 C	-0.170280	0.125319
21 H	0.122599	-0.050406
22 H	0.119967	-0.028110
23 C	-0.122345	0.043737
24 H	0.095367	0.013026
25 C	-0.196753	-0.119636
26 H	0.105721	0.025743
27 H	0.097500	0.026645

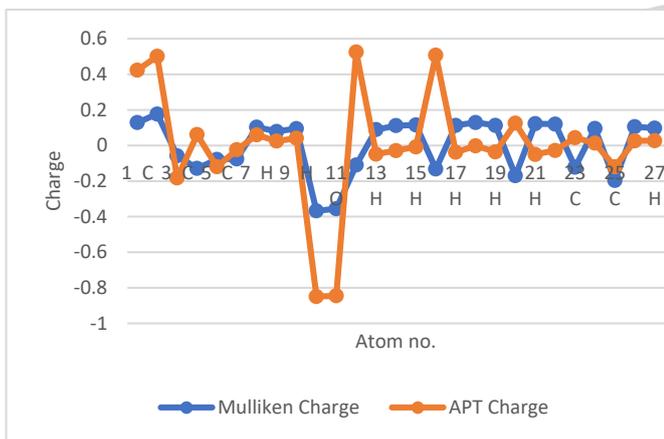


Figure-5: Mulliken and APT atomic charges on each of the constituent atom of Methyl eugenol(1,2-dimethoxy-4-(prop-2-en-1-yl)benzene) molecule

G. 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 [28]. 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 Methyl eugenol(1,2-dimethoxy-4-(prop-2-en-1-yl)benzene) 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 Methyl eugenol(1,2-dimethoxy-4-(prop-2-en-1-yl)benzene) 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	4.9634 eV	249.80 nm	0.0387	47 -> 49	-0.23857
				47 -> 50	0.21187
				47 -> 51	-0.15636
				48 -> 49	0.47038
2	5.2646 eV	235.51 nm	0.0861	48 -> 49	-0.14450
				48 -> 49	-0.42997
				48 -> 50	0.50932
				48 -> 51	0.15371
3	5.7595 eV	215.27 nm	0.0521	45 -> 49	-0.11633
				47 -> 49	0.37950
				47 -> 50	0.10469
				48 -> 49	0.12865
				48 -> 51	0.55173

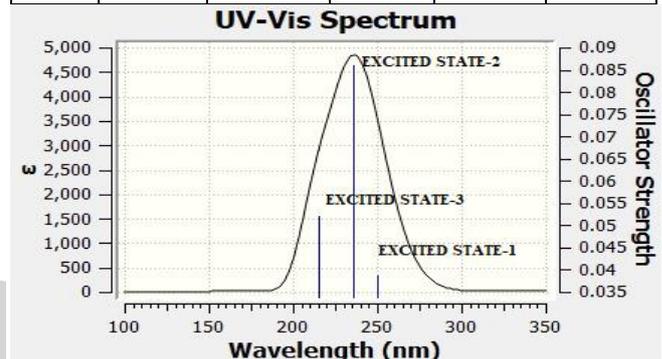


Figure 6: Theoretical UV-Visible Spectra of Methyl eugenol(1,2-dimethoxy-4-(prop-2-en-1-yl)benzene) molecule

H. 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 $\Delta\epsilon = \epsilon_l - \epsilon_r$ ($L \text{ mol}^{-1} \text{ cm}^{-1}$) [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 Methyl eugenol(1,2-dimethoxy-4-(prop-2-en-1-yl)benzene) 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 Methyl eugenol(1,2-dimethoxy-4-(prop-2-en-1-yl)benzene) molecule common chromophore and auxochrome groups are an aromatic ring, an alkene group and a methoxy group. The absorption bands are due to aromatic $\pi - \pi^*$ and $n - \pi^*$ transitions. A CE with $R_{\text{vel}} < 100$ at 249.80, 235.51 and 215.27 nm suggests a planar structure.

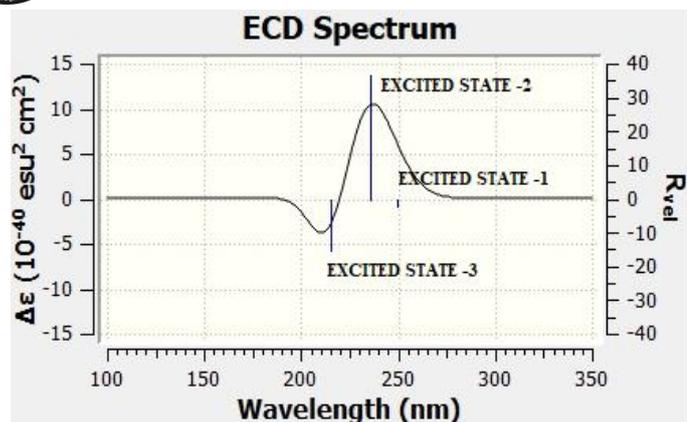


Figure 7: Theoretical ECD Spectra of Methyl eugenol(1,2-dimethoxy-4-(prop-2-en-1-yl)benzene) molecule

Table 9: ECD Spectral results of Methyl eugenol(1,2-dimethoxy-4-(prop-2-en-1-yl)benzene)

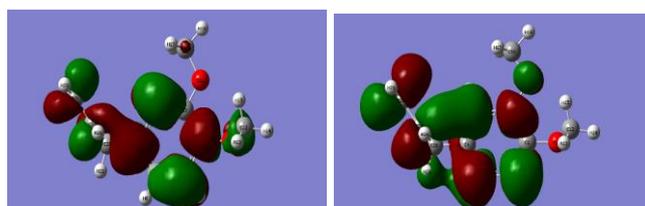
Excited State	Wavelength (nm)	R _{vel}	Δε (10 ⁻⁴⁰ esu ² cm ²)
1	249.80 nm	-2.228	≈ -2
2	235.51 nm	36.823	≈ 13
3	215.27 nm	-15.324	≈ -5

I. 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 Methyl eugenol(1,2-dimethoxy-4-(prop-2-en-1-yl)benzene) 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

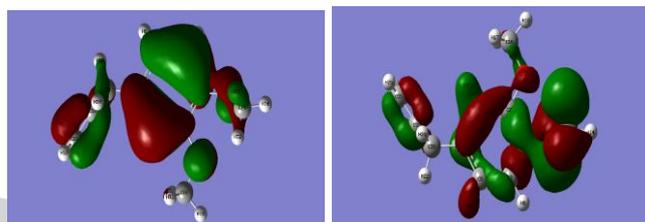
LUMO Energy (E _{LUMO})	HOMO Energy (E _{HOMO})	Energy gap (ΔE) (E _{LUMO} -E _{HOMO})
49 (-0.00685eV)	45(-0.27607ev)	0.26922eV
49 (-0.00685eV)	47(-0.24080eV)	0.23395 eV
49 (-0.00685eV)	48(-0.21698eV)	0.21013 eV
50 (-0.00332 ev)	47(-0.24080eV)	0.23748 eV
50 (-0.00332 ev)	48(-0.21698eV)	0.21366 eV
51 (0.01881 eV)	47(-0.24080eV)	0.22199 eV
51 (0.01881 eV)	48(-0.21698eV)	0.19817 eV



LUMO MO-49 E= -0.00685eV LUMO MO -50 E = -0.00332 eV



LUMO MO -51 E = 0.01881 eV HOMO MO – 48 E = -0.21698eV



HOMO MO- 47 E = -0.24080eV HOMO MO-45 E= -0.27607eV

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

J. 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 Methyl eugenol(1,2-dimethoxy-4-(prop-2-en-1-yl)benzene)) 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 Methyl eugenol(1,2-dimethoxy-4-(prop-2-en-1-yl)benzene)

Parameter	Relation	Calculated Value
Ionization Energy(I)	$-E_{\text{HOMO}}$	0.21698
Electron Affinity (A)	$-E_{\text{LUMO}}$	0.00685
Chemical Potential(ϕ)	$\frac{-(I + A)}{2}$	-0.111915
Absolute hardness(η)	$\frac{(I - A)}{2}$	0.105065
Softness(S)	$\frac{1}{\eta}$	9.5179174797
Electronegativity (χ)	$\frac{(I + A)}{2}$	0.111915
Electrophilicity index (ω)	$\frac{\phi^2}{2\eta}$	0.0596058021
Electron donating capability(ω^-)	$\frac{(3I + A)^2}{16(I - A)}$	0.0056825414
Electron accepting capability (ω^+)	$\frac{(I + 3A)^2}{16(I - A)}$	0.0007409775

K. 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 Methyl eugenol(1,2-dimethoxy-4-(prop-2-en-1-yl)benzene) was computed using B3LYP/6-311G (d, p) basis set at DFT and are shown in Figure 9 and Figure 10 respectively. ESP for HOMO and LUMO are shown in Figure 11 and 12 respectively.

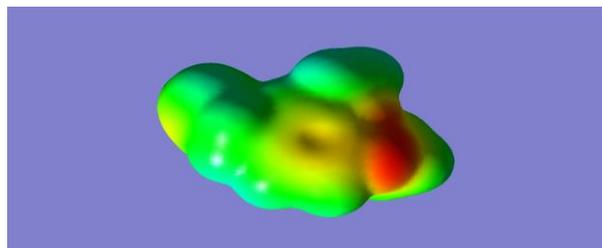


figure 9: electron density of Methyl eugenol(1,2-dimethoxy-4-(prop-2-en-1-yl)benzene)) from total scf density (isovalue =0.0004; mapped with esp)

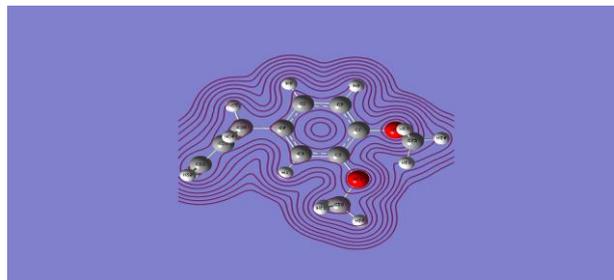


figure-10: electrostatic potential from total scf density (red-negative charge -yellow-green -blue positive charge)

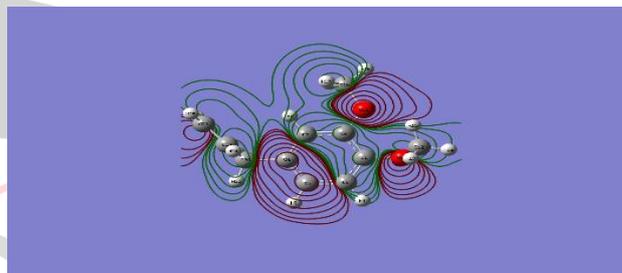


figure-11 electrostatic potential from total scf density (mo-48) homo

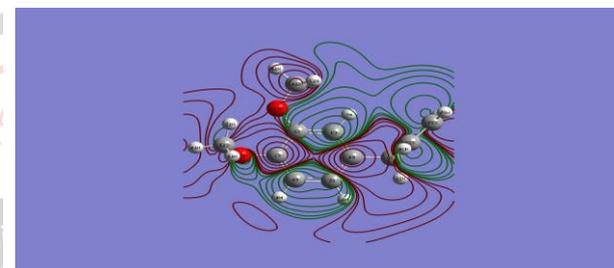


figure-12 electrostatic potential from total scf density (mo-49) lumo

IV. CONCLUSIONS

An attempt was made to calculate various physico-chemical properties of Methyl eugenol(1,2-dimethoxy-4-(prop-2-en-1-yl)benzene) 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 Methyl eugenol(1,2-dimethoxy-4-(prop-2-en-1-yl)benzene) 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 Methyl eugenol(1,2-dimethoxy-4-

(prop-2-en-1-yl)benzene) 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 Methyl eugenol(1,2-dimethoxy-4-(prop-2-en-1-yl)benzene) is quite stable and does not undergo decomposition readily.

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