International Journal for Research in Engineering Application & Management (IJREAM)
ISSN : 2454-9150 Vol-07, Issue-10, JAN 2022

PHYSICO-CHEMICAL, STRUCTURAL AND OPTICAL PROPERTIES OF METHYL ISOEUGENOL (1,2-dimethoxy-4-(prop-1-en-1-yl) benzene): QUANTUM CHEMICAL CALCULATIONS BY DFT

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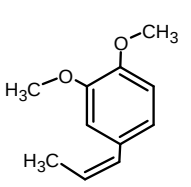
Abstract - Physico-chemical properties plays an important role in determining toxicity of a material hence were calculated using acdlab/chemsketch and the data predicted is generated using ACD/Labs Percepta Platform - PhysChem Module. Gaussian 09, RevisionA.01, software package was used for the theoretical quantum chemical calculations of 1,2-dimethoxy-4-(prop-1-en-1-yl) benzene commonly called Methyl 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 (Δα), first order hyperpolarizability (β), second order hyperpolarizability (γ) in terms of x, y, z components for Methyl isoeugenol (1,2-dimethoxy-4-(prop-1-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 isoeugenol (1,2-dimethoxy-4-(prop-1-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, acdlab /chemsketch, DFT, FMO, Mulliken population analysis, TD-DFT, NLO properties, ECD, Global reactive descriptors

I. INTRODUCTION

Methyl isoeugenol is a volatile Phenylpropanoid naturally occurring as a mixture of cis/trans (E/Z) isomers in essential oils of Asarum arifolium, Cymbopogon javanensis, Daucus carota subsp,sativus ,Ylang-Ylang and in nearly 60 other essential oils [1]. The chemical name of Methyl isoeugenol is 1,2-dimethoxy-4-(prop-1-en-1-yl) benzene in accordance with International Union of Pure and Applied Chemistry and other synonyms are 1,2-dimethoxy-4-propenylbenzene, isoeugenyl methyl ether, O-methyl isoeugenol, Methyl isoeugenol etc. Methyl isoeugenol can exist as either the cis (Z) or trans (E) isomer. Structural formula of both cis (Z) and trans (E) the isomers of Methyl isoeugenol are depicted in Figure -1(a) and 1 (b) respectively.



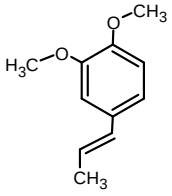


Fig.-1(a) 1,2-dimethoxy-4-[(1*Z*)-prop-1-en-1-yl] benzene
Fig.-1(b) 1,2-dimethoxy-4-[(1*E*)-prop-1-en-1-yl] benzene

Methyl isoeugenol (1,2-dimethoxy-4-(prop-1-en-1-yl) benzene) is colourless to pale yellow liquid, delicate with clove carnation aroma and a bitter taste, insoluble in glycerine and propylene glycol but soluble in ethanol and most fixed oils [2]. Methyl isoeugenol (1,2-dimethoxy-4-(prop-1-en-1-yl) benzene) is a naturally occurring food flavour hence besides its effect on the central nervous system and use as food flavour, Methyl isoeugenol (1,2-dimethoxy-4-(prop-1-en-1-yl) benzene) can exert hypotensive, vasorelaxant activities by influencing calcium channels, economize heart functions and possess an anticonvulsant, anxiolytic and antidepressant activity [3],[4],[5]. Methyl isoeugenol (1,2-dimethoxy-4-(prop-1-en-1-yl) benzene) is reported to possess antibacterial activity [6], Nematocidal activity [7], insecticidal and repellent activities [8],[9], anti-fungal activities [10]. It is widely used in foods as a flavouring agent and in cosmetics, soaps, and shampoos as a fragrance agent [11]. Scientists have reported that essential oil extracted from the flowers of plant Lavandula vera and Rosa damascene contain Methyl isoeugenol (1,2-dimethoxy-4-(prop-1-en-1-yl) benzene) and is used in skin creams, lotions, and ointment foe beautification, smoothness, and protection from sunburns [12],[13]. Due to its numerous

 DOI : 10.35291/2454-9150.2022.0032

properties, Methyl isoeugenol (1,2-dimethoxy-4-(prop-1-en-1-yl) benzene) has found a wide range of uses in many areas of life. Besides, due to the growing interest in traditional and unconventional medicines that contain natural ingredients, Methyl isoeugenol (1,2-dimethoxy-4-(prop-1-en-1-yl) benzene) 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 [14],[15]. Growing interest of researchers in this molecule motivated us to calculate physico-chemical properties and carry out quantum chemical calculations (computational study) of Methyl isoeugenol (1,2-dimethoxy-4-(prop-1-en-1-yl) benzene). 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 isoeugenol (1,2-dimethoxy-4-(prop-1-en-1-yl) benzene) are done using acdlab/chemsketch [16] and the predicted data is generated using the ACD/Labs Percepta Platform - PhysChem Module. Quantum chemical calculation of Methyl isoeugenol (1,2-dimethoxy-4-(prop-1-en-1-yl) benzene) have been performed using personal laptop using Gaussian 09, Revision A, 01 software package [17] 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 isoeugenol (1,2-dimethoxy-4-(prop-1-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 isoeugenol (1,2-dimethoxy-4-(prop-1-en-1-yl) benzene) were computed using Time Dependent DFT (TD-DFT) method using the same basis set.

III. RESULTS AND DISCUSSION

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

Physico-chemical properties are the intrinsic physical and chemical characteristics of a substance. These includes appearance, boiling point, density, volatility, water solubility, vapour pressure etc. These properties have a significant effect on the absorption, distribution, excretion and a strong influence on the environmental behaviour and toxic activity of a molecule hence are essential indicators used in hazard, exposure, risk assessments Physico-chemical properties can also be used to assess the requirement for higher tier data. This compels the researchers to evaluate the role of these properties in determining associated toxicity, hazard, exposure, risk issues. The physico-chemical properties of Methyl isoeugenol (1,2-dimethoxy-4-(prop-1-en-1-yl) benzene) were calculated using acdlab/chemsketch [16] 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 Methyl isoeugenol (1,2-dimethoxy-4-(prop-1-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	Boiling Point	271.1±20.0 °C at 760 mmHg
5	Vapour Pressure	0.0±0.5 mmHg at 25°C
6	Enthalpy of Vaporization	48.9±3.0 kJ/mol
7	Flash Point	104.5±21.3 °C
8	Molar Refractivity	53.51 ± 0.3 cm^3
9	Molar Volume	181.8 ± 3.0 cm^3
10	Parachor	425.9 ± 4.0 cm^3
11	Index of Refraction	1.500 ± 0.02
12	Surface Tension	30.1 ± 3.0 dyne/cm
13	Density	0.980 ± 0.06 g/cm^3
14	Dielectric Constant	Not available
15	Polarizability	21.21 ± 0.5 $10^{-24}cm^3$
16	Topological Polar Surface Area	18 $Å^2$
17	RDBE	5
18	Monoisotopic Mass	178.09938 Da
19	Nominal Mass	178 Da
20	Average Mass	178.2277 Da
21	#H bond acceptors	2
22	#H bond donors	0
23	#Freely Rotating Bonds	3
24	#Rule of 5 Violations	0
25	ACD/LogP	3.05
26	ACD/LogD (pH 5.5)	2.70
27	ACD/BCF (pH 5.5)	66.54
28	ACD/KOC (pH 5.5)	702.39
29	ACD/LogD (pH 7.4)	2.70
30	ACD/BCF (pH 7.4)	66.54
31	ACD/KOC (pH 7.4)	702.39
32	M+	178.098831 Da
33	M-	178.099928 Da
34	[M+H]+	179.106656 Da
35	[M+H]-	179.107753 Da
36	[M-H]+	177.091006 Da
37	[M-H]-	177.092103 Da

B. Geometrical analysis of Methyl isoeugenol (1,2-dimethoxy-4-(prop-1-en-1-yl) benzene)

The molecular structure of Methyl isoeugenol (1,2-dimethoxy-4-(prop-1-en-1-yl) benzene) having Molecular formula $C_{11}H_{14}O_2$ Molecular mass: 178.09938 amu, is an asymmetric top type of molecule with 75 degrees of freedom. Gaussian 09, Revision A.01,[17] and Gauss View 6.0.16 programme was used for the optimisation of molecular structure of Methyl isoeugenol (1,2-dimethoxy-4-(prop-1-en-1-yl) benzene) and the obtained optimised molecular structure along with the atom numbering scheme is shown in Figure 2. Geometrical parameters i.e., Bond Length, Bond Angle, Dihedral Angle of Methyl isoeugenol (1,2-dimethoxy-4-(prop-1-en-1-yl) benzene) after optimisation as

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calculated by DFT/ B3LYP/66-311G (d, p) level basis set are listed in Table 2.

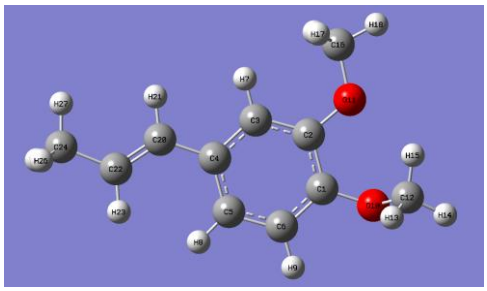

Figure 2: Optimised Geometrical Structure of Methyl isoeugenol (1,2-dimethoxy-4-(prop-1-en-1-yl) benzene)

Table 2: Optimised Geometrical Parameters (bond length, bond angle, dihedral angle) of Methyl isoeugenol (1,2-dimethoxy-4-(prop-1-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(°)
R1	R(1,2)	1.4097	A(2,1,6)	118.9062	D(6,1,2,3)	0.8275
R2	R(1,6)	1.3911	A(2,1,10)	122.1295	D(6,1,2,11)	-178.616
R3	R(1,10)	1.3712	A(6,1,10)	118.8589	D(10,1,2,3)	177.0503
R4	R(2,3)	1.3934	A(1,2,3)	119.3478	D(10,1,2,11)	-2.3933
R5	R(2,11)	1.3661	A(1,2,11)	116.1879	D(2,1,6,5)	-0.1745
R6	R(3,4)	1.4064	A(3,2,11)	124.4617	D(2,1,6,9)	178.789
R7	R(3,7)	1.0824	A(2,3,4)	121.7758	D(10,1,6,5)	-176.5223
R8	R(4,5)	1.3998	A(2,3,7)	119.8133	D(10,1,6,9)	2.4412
R9	R(4,20)	1.4707	A(4,3,7)	118.4096	D(2,1,10,12)	67.6447
R10	R(5,6)	1.39	A(3,4,5)	118.0668	D(6,1,10,12)	-116.1308
R11	R(5,8)	1.0829	A(3,4,20)	118.2814	D(1,2,3,4)	-0.591
R12	R(6,9)	1.0838	A(5,4,20)	123.6511	D(1,2,3,7)	179.831
R13	R(10,12)	1.4316	A(4,5,6)	120.3863	D(11,2,3,4)	178.8034
R14	R(11,16)	1.4202	A(4,5,8)	120.4662	D(11,2,3,7)	-0.7746
R15	R(12,13)	1.0961	A(6,5,8)	119.1475	D(1,2,11,16)	177.4096
R16	R(12,14)	1.0898	A(1,6,5)	121.507	D(3,2,11,16)	-2.0022
R17	R(12,15)	1.0916	A(1,6,9)	117.4624	D(2,3,4,5)	-0.3071
R18	R(16,17)	1.0959	A(5,6,9)	121.0223	D(2,3,4,20)	179.9785
R19	R(16,18)	1.0889	A(1,10,12)	116.377	D(7,3,4,5)	179.2766
R20	R(16,19)	1.0954	A(2,11,16)	118.4815	D(7,3,4,20)	-0.4377
R21	R(20,21)	1.0893	A(10,12,13)	110.6644	D(3,4,5,6)	0.968
R22	R(20,22)	1.3375	A(10,12,14)	105.9637	D(3,4,5,8)	-179.0505
R23	R(22,23)	1.0878	A(10,12,15)	111.437	D(20,4,5,6)	-179.3342
R24	R(22,24)	1.4989	A(13,12,14)	109.2656	D(20,4,5,8)	0.6473
R25	R(24,25)	1.0963	A(13,12,15)	109.7634	D(3,4,20,21)	4.0232
R26	R(24,26)	1.0963	A(14,12,15)	109.6614	D(3,4,20,22)	-175.5847
R27	R(24,27)	1.0927	A(11,16,17)	111.6333	D(5,4,20,21)	-175.674
			A(11,16,18)	105.7986	D(5,4,20,22)	4.7181
			A(11,16,19)	111.4254	D(4,5,6,1)	-0.7416
			A(17,16,18)	109.2637	D(4,5,6,9)	-179.6683
			A(17,16,19)	109.3672	D(8,5,6,1)	179.2767
			A(18,16,19)	109.2601	D(8,5,6,9)	0.3499
			A(4,20,21)	114.6893	D(1,10,12,13)	58.2809
			A(4,20,22)	127.7262	D(1,10,12,14)	176.6187
			A(21,20,22)	117.5834	D(1,10,12,15)	-64.1534
			A(20,22,23)	119.6281	D(2,11,16,17)	62.8008
			A(20,22,24)	124.6249	D(2,11,16,18)	-178.4442
			A(23,22,24)	115.7468	D(2,11,16,19)	-59.8055
			A(22,24,25)	111.2083	D(4,20,22,23)	0.1748
			A(22,24,26)	111.2056	D(4,20,22,24)	-179.989
			A(22,24,27)	111.6245	D(21,20,22,23)	-179.4232
			A(25,24,26)	106.4616	D(21,20,22,24)	0.4129
			A(25,24,27)	108.0389	D(20,22,24,25)	120.7072
			A(26,24,27)	108.086	D(20,22,24,26)	-120.8299
					D(20,22,24,27)	-0.0323
					D(23,22,24,25)	-59.451
					D(23,22,24,26)	59.012
					D(23,22,24,27)	179.8096

C. Vibrational Assignments

For a non-linear molecule with N atoms, total number of degrees of freedom is 3N. This includes three translational and three rotational degrees of freedom and the remaining(3N-6) degrees of freedom constitutes vibrational motions [18],[19]. Methyl isoeugenol (1,2-dimethoxy-4-(prop-1-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 isoeugenol (1,2-dimethoxy-4-(prop-1-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

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corresponding vibrational assignment for the theoretical IR spectra of Methyl isoeugenol (1,2-dimethoxy-4-(prop-1-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 [18]. A comprehensive account of the characteristic group absorptions and their relationship to molecular structure is discussed below.

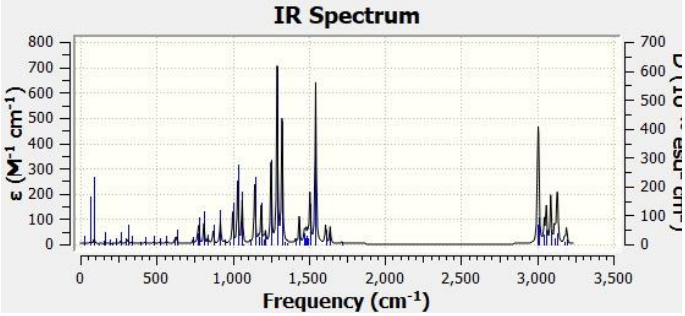


Figure 3: Theoretical IR Spectra of Methyl isoeugenol (1,2-dimethoxy-4-(prop-1-en-1-yl) benzene)

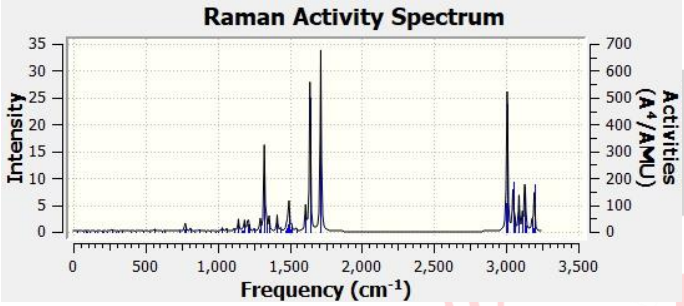


Figure 4: Theoretical Raman Spectra of Methyl isoeugenol (1,2-dimethoxy-4-(prop-1-en-1-yl) benzene)

Table 3: Frequencies, Reduced mass, Force constant, IR and Raman Intensities, Depolar-P and Depolar-U for the theoretical IR and Raman spectra of Methyl isoeugenol (1,2-dimethoxy-4-(prop-1-en-1-yl) benzene)

MODE	Frequency	Reduced Mass	Force Constant	Infrared Intensity	Raman Intensity	Depolar-P	Depolar-U
1	27.65	2.4434	0.0011	0.2064	2.4194	0.6955	0.8204
2	67.40	2.0701	0.0055	2.7677	1.1908	0.5030	0.6693
3	88.87	2.1139	0.0098	1.0277	3.5750	0.7016	0.8246
4	91.65	2.9498	0.0146	5.3382	0.0881	0.3831	0.5540
5	116.50	2.7840	0.0223	0.0341	1.7707	0.7210	0.8379
6	149.21	2.3168	0.0304	0.5257	1.4704	0.5719	0.7276
7	161.92	1.6069	0.0248	1.7951	0.9877	0.6920	0.8180
8	194.74	1.2336	0.0276	0.8045	1.3049	0.7500	0.8571
9	207.03	2.8737	0.0726	0.1150	1.1324	0.7408	0.8511
10	229.46	1.7717	0.0550	1.3256	1.2740	0.2945	0.4550
11	264.94	2.4074	0.0996	2.8995	5.9498	0.2123	0.3503
12	296.68	2.5444	0.1319	1.6197	2.2244	0.2346	0.3801
13	312.42	4.2769	0.2460	5.3678	0.2313	0.7497	0.8570
14	340.84	4.6454	0.3180	2.3915	3.4182	0.1897	0.3189
15	396.77	3.6397	0.3376	0.8203	1.8555	0.7497	0.8570
16	427.79	3.7171	0.4008	2.6149	0.4793	0.5408	0.7020
17	484.35	3.9554	0.5467	3.3540	0.7405	0.7235	0.8396
18	523.81	4.0550	0.6555	2.5202	0.8789	0.6891	0.8160
19	565.62	5.9530	1.1221	4.0238	7.4644	0.3476	0.5159
20	617.17	3.7719	0.8465	3.8249	0.9423	0.5995	0.7496
21	632.46	3.9237	0.9247	8.2488	3.6301	0.1690	0.2891
22	738.49	3.7004	1.1890	4.5140	4.8460	0.1866	0.3145
23	771.51	4.4690	1.5673	7.4606	7.6495	0.6667	0.8000
24	776.34	3.7737	1.3401	18.1783	20.3165	0.1235	0.2199
25	811.41	1.4768	0.5729	22.9287	10.2018	0.7360	0.8480
26	837.66	1.6925	0.6997	7.0873	1.1845	0.7497	0.8569
27	871.29	1.6904	0.7561	14.7024	4.7145	0.7500	0.8571
28	919.09	2.3974	1.1932	26.9904	1.0973	0.0406	0.0781
29	949.16	1.3205	0.7009	3.6689	0.6542	0.7298	0.8438
30	982.67	2.2832	1.2990	2.5818	2.1511	0.5501	0.7098
31	999.70	1.0935	0.6439	35.6971	1.2206	0.3024	0.4644
32	1032.34	7.8426	4.9244	70.9276	12.0895	0.6981	0.8222
33	1062.31	4.4901	2.9854	48.9485	4.9550	0.2291	0.3728
34	1063.94	1.5354	1.0240	0.1478	2.3683	0.7498	0.8570
35	1116.63	2.2893	1.6818	3.3374	8.6099	0.5726	0.7282
36	1144.30	1.6324	1.2594	67.4463	37.5191	0.1985	0.3313
37	1168.84	1.2570	1.0118	6.9530	3.1744	0.6373	0.7784
38	1171.70	1.2730	1.0297	0.7191	3.3063	0.7409	0.8512
39	1187.01	1.7446	1.4483	42.8692	33.4620	0.2926	0.4528
40	1207.45	1.3689	1.1759	5.4522	26.2642	0.5222	0.6861
41	1215.38	1.5795	1.3746	11.8963	29.2174	0.3645	0.5342
42	1251.80	2.5198	2.3264	91.2188	7.3684	0.4000	0.5714
43	1291.70	2.9615	2.9113	199.7162	9.9382	0.2961	0.4570
44	1296.33	1.5701	1.5546	2.8610	29.3996	0.2482	0.3977
45	1323.84	3.3523	3.4615	140.4851	266.2487	0.2471	0.3962
46	1336.60	1.7046	1.7942	3.4005	36.5863	0.3564	0.5255
47	1356.29	1.7042	1.8470	1.7428	42.6910	0.2941	0.4545
48	1412.73	1.2646	1.4871	5.0276	52.3147	0.4304	0.6018
49	1437.29	2.4531	2.9857	30.2481	11.2591	0.4100	0.5816
50	1471.25	1.1990	1.5292	13.4932	4.7105	0.6750	0.8060

 DOI : 10.35291/2454-9150.2022.0032

51	1478.92	1.0445	1.3460	7.3557	14.6696	0.7500	0.8571
52	1482.84	1.1015	1.4270	10.3501	8.1915	0.7366	0.8484
53	1486.72	1.1737	1.5285	0.7594	26.4161	0.6900	0.8166
54	1491.97	1.0456	1.3713	7.7410	16.5262	0.7499	0.8571
55	1494.71	1.1361	1.4955	3.3801	78.9323	0.3785	0.5491
56	1506.86	1.0624	1.4213	52.5963	7.9850	0.7078	0.8289
57	1511.27	1.0475	1.4096	8.4904	16.9920	0.6863	0.8140
58	1544.97	2.8915	4.0665	184.2607	10.7245	0.7294	0.8436
59	1609.85	6.7188	10.2592	21.2932	81.3435	0.3042	0.4665
60	1640.01	5.9462	9.4227	19.4704	499.1383	0.4262	0.5977
61	1714.94	5.4570	9.4558	3.0572	618.4885	0.3157	0.4798
62	3002.03	1.0349	5.4950	52.6230	108.8791	0.0437	0.0837
63	3006.60	1.0372	5.5241	62.6233	477.9322	0.1281	0.2271
64	3009.32	1.0400	5.5491	70.7983	186.1655	0.0392	0.0754
65	3046.43	1.0991	6.0100	25.3058	184.6160	0.7498	0.8570
66	3060.31	1.1060	6.1030	40.5075	55.3503	0.7387	0.8497
67	3088.52	1.0942	6.1494	38.9785	73.0344	0.3974	0.5687
68	3089.46	1.0988	6.1791	15.7160	96.2514	0.7440	0.8532
69	3112.65	1.0884	6.2132	17.8772	76.9370	0.2348	0.3804
70	3127.21	1.1047	6.3653	27.6663	147.4487	0.5367	0.6985
71	3131.99	1.0989	6.3514	25.5366	134.2547	0.4590	0.6292
72	3134.58	1.0877	6.2969	30.3133	23.9441	0.2540	0.4051
73	3178.40	1.0869	6.4696	7.1121	48.9130	0.6844	0.8126
74	3191.88	1.0890	6.5369	14.7093	14.4048	0.4819	0.6504
75	3194.55	1.0939	6.5771	4.5944	177.8661	0.2161	0.3554

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 1640cm^{-1} with moderate intensity.

b) 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 .

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 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.

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 2962cm^{-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 720cm^{-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 900-675 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 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}.

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 intnse bands are observed for ethers.The C-O-C

 DOI : 10.35291/2454-9150.2022.0032

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.

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 isoeugenol (1,2-dimethoxy-4-(prop-1-en-1-yl) benzene) molecule and are compiled in Table 4. The statistical thermo chemical analysis of Methyl isoeugenol (1,2-dimethoxy-4-(prop-1-en-1-yl) benzene) 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 Methyl isoeugenol (1,2-dimethoxy-4-(prop-1-en-1-yl) benzene) as computed by frequency calculations

Thermodynamic Functions	Value
Zero-point correction	0.224945 (Hartree/Particle)
Thermal correction to Energy	0.238749
Thermal correction to Enthalpy	0.239694
Thermal correction to Gibbs Free Energy	0.183706
Sum of electronic and zero-point Energies	-577.931149
Sum of electronic and thermal Energies	-577.917344
Sum of electronic and thermal Enthalpies	-577.916400
Sum of electronic and thermal Free Energies	-577.972387

Table 5: Thermodynamic properties of Methyl isoeugenol (1,2-dimethoxy-4-(prop-1-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	149.818	50.135	117.835
Electronic	0.000	0.000	0.000
Translational	0.889	2.981	41.438
Rotational	0.889	2.981	31.706
Vibrational	148.040	44.173	44.690
Vibration 1	0.593	1.984	5.992
Vibration 2	0.598	1.970	4.228
Vibration 3	0.602	1.957	3.685
Vibration 4	0.602	1.955	3.625
Vibration 5	0.608	1.936	3.158
Vibration 6	0.618	1.904	2.682
Vibration 7	0.622	1.889	2.527
Vibration 8	0.635	1.847	2.182
Vibration 9	0.641	1.830	2.070
Vibration 10	0.652	1.796	1.883
Vibration 11	0.671	1.737	1.629
Vibration 12	0.690	1.680	1.436
Vibration 13	0.701	1.650	1.349
Vibration 14	0.720	1.594	1.208
Vibration 15	0.763	1.477	0.975
Vibration 16	0.789	1.410	0.866
Vibration 17	0.840	1.285	0.698
Vibration 18	0.879	1.197	0.601
Vibration 19	0.921	1.106	0.513
Vibration 20	0.977	0.996	0.421

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

Quantum chemical calculations helps to predict the molecular NLO properties of active compounds [20],[21]. The relationship between the nonlinear optical properties and the molecular structure can be better understood with the help of Hyperpolarizability [22],[23]. 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 Methyl isoeugenol (1,2-dimethoxy-4-(prop-1-en-1-yl) benzene) molecule. Calculation of above mentioned NLO properties have been executed using equation-1 to equation-5[24],[25] and the results are summarised in Table 6

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

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

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

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

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

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

The conversion factor of α, β and γ in atomic unit are
For α 1 atomic unit (a.u.) = 0.1482 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 Methyl isoeugenol (1,2-dimethoxy-4-(prop-1-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

 DOI : 10.35291/2454-9150.2022.0032

dipole moment (μ) of Methyl isoeugenol (1,2-dimethoxy-4-(prop-1-en-1-yl) benzene) (μ = 2.2185D)was calculated to be 0.9348 times that of the standard reference material of prototypical molecule urea (μ = 2.3732D) and first-order hyperpolarizability (β) of Methyl isoeugenol (1,2-dimethoxy-4-(prop-1-en-1-yl) benzene)) molecule (β = 4.19699x 10^{-31}esu) is about 1.13 times the first order hyperpolarizability of urea (β of urea = 3.728x10^{-31}esu). Since dipole moment and hyperpolarizability of Methyl isoeugenol (1,2-dimethoxy-4-(prop-1-en-1-yl) benzene)) is comparable to that of prototype urea hence it is recommended to use Methyl isoeugenol (1,2-dimethoxy-4-(prop-1-en-1-yl) benzene)) molecule as a prospective building block for nonlinear optical material.

Table 6: Nonlinear Optical Components of for Methyl isoeugenol (1,2-dimethoxy-4-(prop-1-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	
μ_x	-0.5637	α_{xx}	-71.6443	β_{xxx}	14.9322	γ_{xxxx}	-3194.1577
μ_y	1.7494	α_{yy}	-68.4183	β_{yyy}	19.9192	γ_{yyyy}	-854.7858
μ_z	1.2424	α_{zz}	-82.0995	β_{zzz}	0.1443	γ_{zzzz}	-150.1358
Total μ	2.2185 D	α_{xy}	3.5800	β_{xyy}	13.5883	γ_{xxxy}	10.7753
		α_{xz}	3.9725	β_{xxy}	-0.1448	γ_{xxxz}	35.7792
		α_{yz}	-1.1074	β_{xxz}	15.2263	γ_{yyyx}	47.0027
		α	-74.0540 a.u	β_{xzz}	11.8390	γ_{yyyz}	1.0384
		α	-10.9748 1x 10^{-24}esu	β_{yzz}	2.5155	γ_{zzzx}	-2.3594
		Δα	15.5858 a.u	β_{yyz}	-0.0635	γ_{zzzy}	-2.3040
				β_{xyz}	-5.1299	γ_{xxyy}	-684.7735
				β	48.5802a.u.	γ_{xxzz}	-607.5508
				β	4.19699x 10^{-31}esu	γ_{yyzz}	-186.3838
						γ_{xxyz}	-15.1415
						γ_{yyxz}	3.8303
						γ_{zzxy}	2.0900
						γ	-1431.2991 a.u.
						γ	-7.20902x 10^{-37}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 [26]. 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 for Methyl isoeugenol (1,2-dimethoxy-4-(prop-1-en-1-yl) benzene). Calculated values of Muliiken, 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 -OCH_3 group on carbon atom-1 and 2. Oxygen atom -10 and 11 have more negative charge 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 methoxy groups.

Table 7: Mulliken, APT and Natural Atomic Charges on each of the constituent atom of Methyl isoeugenol (1,2-dimethoxy-4-(prop-1-en-1-yl) benzene) molecule as calculated by DFT/B3LYP/6-311 G (d, p) level basis set.

Atoms	Mulliken Charge	APT	Natural Charge
1 C	0.131984	0.451790	0.27720
2 C	0.172512	0.507407	0.28795
3 C	-0.100871	-0.148266	-0.27221
4 C	-0.064674	0.075879	-0.05563
5 C	-0.056506	-0.127479	-0.20408
6 C	-0.079925	-0.032081	-0.21808
7 H	0.097387	0.049256	0.20464
8 H	0.081678	0.034256	0.19899
9 H	0.095440	0.041624	0.21250
10 O	-0.367396	-0.915233	-0.55391
11 O	-0.356967	-0.864384	-0.53127
12 C	-0.110527	0.550725	-0.18768
13 H	0.090207	-0.048146	0.15490
14 H	0.111979	-0.032711	0.17482
15 H	0.115976	-0.008561	0.17319
16 C	-0.131375	0.520886	-0.19533
17 H	0.110812	-0.040178	0.16304
18 H	0.129497	-0.003882	0.18463
19 H	0.113805	-0.036221	0.16593
20 C	-0.076478	0.039159	-0.20926
21 H	0.076677	-0.001030	0.18383
22 C	-0.138243	0.016481	-0.14540
23 H	0.091806	0.011432	0.17937
24 C	-0.272052	0.067894	-0.59008
25 H	0.115867	-0.045846	0.20329
26 H	0.115334	-0.044268	0.20290
27 H	0.104052	-0.018502	0.19575

 DOI : 10.35291/2454-9150.2022.0032

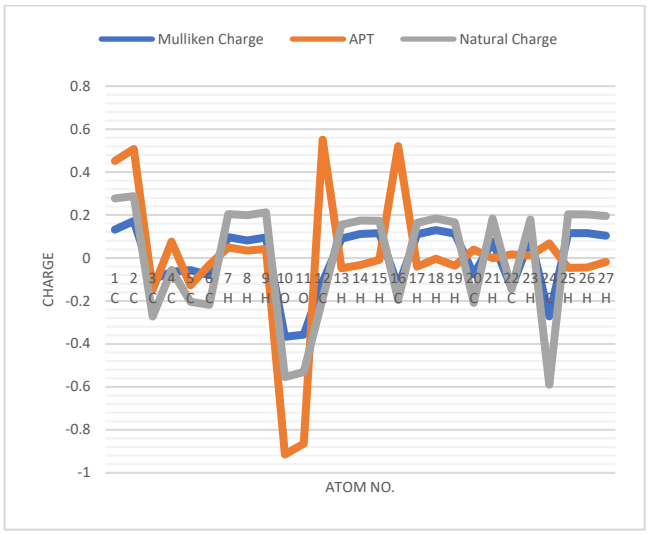


Figure 5: Mulliken, APT, and Natural Charges on each of the constituent atom of Methyl isoeugenol (1,2-dimethoxy-4-(prop-1-en-1-yl) benzene)

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 [23]. Molecular orbitals in Methyl isoeugenol (1,2-dimethoxy-4-(prop-1-en-1-yl) benzene) undergoing excitation transition, transition energy and excitation energy, absorption wavelength etc have been gathered in Table 8 and the UV – Visible spectra of Methyl isoeugenol (1,2-dimethoxy-4-(prop-1-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 isoeugenol (1,2-dimethoxy-4-(prop-1-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	2.6926 eV	460.46 nm	0.0987	48 -> 49 48 <- 49	0.71335 -0.13437
2	3.8148 eV	325.01 nm	0.0276	47 -> 49 48 -> 50	0.63894 -0.26804
3	4.1129 eV	301.45 nm	0.0306	46 -> 49 47 -> 49 48 -> 50	-0.10166 0.25691 0.63761

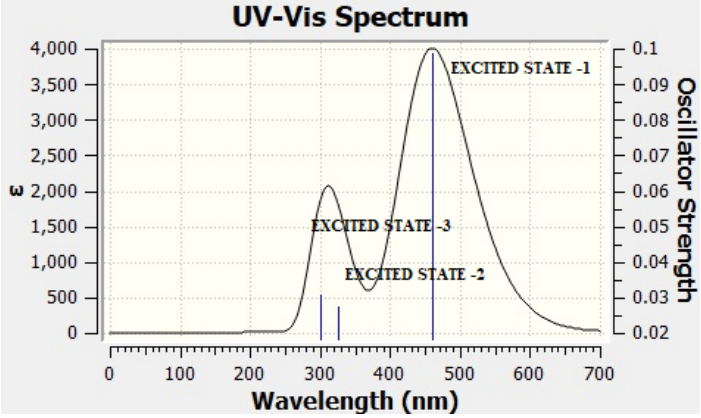


figure 6: Theoretical UV-Visible Spectra of Methyl isoeugenol (1,2-dimethoxy-4-(prop-1-en-1-yl) benzene)

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 [27],[28]. 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}) [29]. TD-DFT method allows the simulation of the ECD spectrum of a medium size molecule on a desktop or PC in a reasonable time [30],[31]. ECD spectra of Methyl isoeugenol (1,2-dimethoxy-4-(prop-1-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 isoeugenol (1,2-dimethoxy-4-(prop-1-en-1-yl) benzene) molecule common chromophore and auxochrome groups are an aromatic ring, two methoxy groups and an alkene group. The absorption bands are due to aromatic π – π* and n – π* transitions. A positive CE at 460.46 nm, Rvel > 100 corresponds to R-configuration while almost zero CE at 325.01 nm and 301.45 nm corresponds to planar structure.

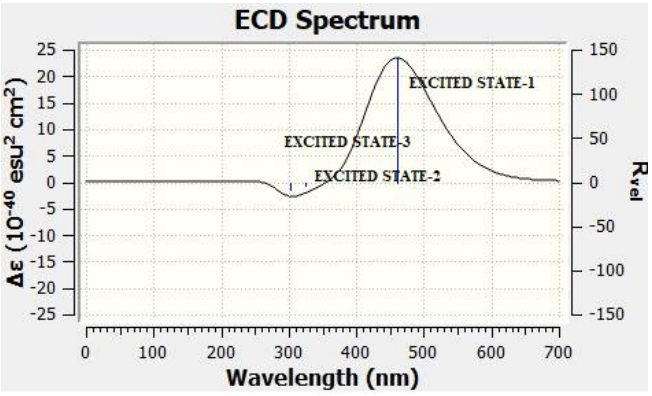


Figure 7: Theoretical ECD Spectra of Methyl isoeugenol (1,2-dimethoxy-4-(prop-1-en-1-yl) benzene)

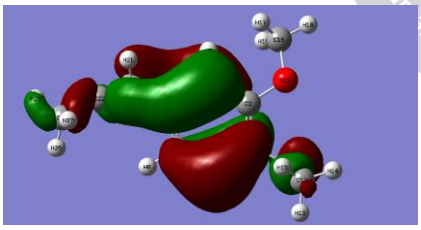
 DOI : 10.35291/2454-9150.2022.0032

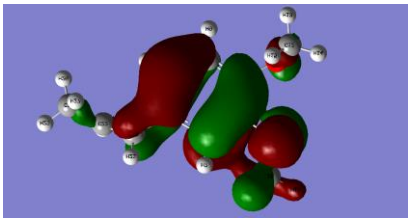
Table 9: ECD Spectral results of Methyl isoeugenol (1,2-dimethoxy-4-(prop-1-en-1-yl) benzene)

Excited State	Wavelength (nm)	R_{vel}	$\Delta\varepsilon$ (10^{-40} esu^2 cm^2)
1	460.46 nm	141.2308019	≈24
2	325.01 nm	-3.611512518	≈-1
3	301.45 nm	-9.189234744	≈-2

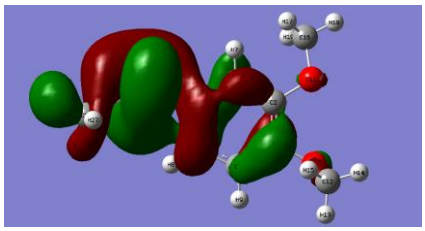
I. Frontier Molecular orbital analysis (FMO analysis)

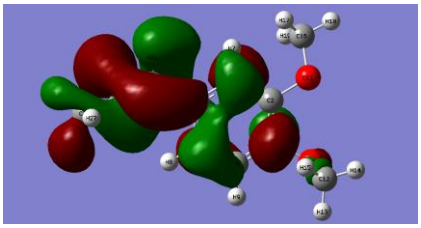
Interaction of two atomic orbitals with each other produces two new orbitals called molecular orbitals – bonding molecular orbital and antibonding molecular orbitals. The bonding molecular orbital has lower energy and is occupied by a pair of electrons (a Lewis base) and is called Highest Occupied Molecular 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 and are the main orbitals which takes part in chemical stability. They together are called Frontier Molecular Orbital (FMO) and are used for predicting the most reactive position in π-electron systems and explains several types of reaction in conjugated system [32]. The conjugated molecules are characterised by small HOMO-LUMO separation. The FMO analysis for Methyl isoeugenol (1,2-dimethoxy-4-(prop-1-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 7. In Table 10 energies of molecular orbitals undergoing major transitions and their energy gap (ΔE) have been presented.



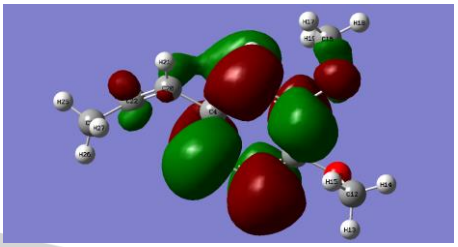


HOMO MO-46 E = -0.26211eV
HOMO MO-47 E = -0.23572eV





HOMO MO-48 E = -0.18804eV
LUMO MO-49 E = -0.07019eV



LUMO MO-50 E = -0.00985eV

Figure -8 – Frontier Molecular orbitals with Molecular Orbital No. and its energy indicated below each Molecular Orbital of Methyl isoeugenol (1,2-dimethoxy-4-(prop-1-en-1-yl) benzene)

Table 10: Energy gap (ΔE) of major electronic transitions in Methyl isoeugenol (1,2-dimethoxy-4-(prop-1-en-1-yl) benzene)

LUMO Energy (E_{LUMO})	HOMO Energy (E_{HOMO})	Energy gap (ΔE) (E_{LUMO}-E_{HOMO})
49 (-0.07019eV)	46(-0.26211eV)	0.19192eV
49(-0.07019eV)	47(-0.23572eV)	0.16553 eV
49(-0.07019eV)	48(-0.18804eV)	0.11785 eV
50(-0.00985eV)	48(-0.18804eV)	0.17819 eV

J. Global and Local Reactivity Descriptors of Methyl isoeugenol (1,2-dimethoxy-4-(prop-1-en-1-yl) benzene)

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 [33],[34],[35],[36],[37]. Robert Parr and others [33] 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 [38] as the average value of the ionization potential and electron affinity. Robert G Parr and others [35] scrutinized the concept of electronegativity from the point of view of Density Functional Theory of Hohenberg and Kohn [39]. In the

 DOI : 10.35291/2454-9150.2022.0032

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 [36-37]. 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 isoeugenol (1,2-dimethoxy-4-(prop-1-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 isoeugenol (1,2-dimethoxy-4-(prop-1-en-1-yl) benzene)

Parameter	Relation	Calculated Value
Ionization Energy(I)	$-E_{HOMO}$	0.18804
Electron Affinity (A)	$-E_{LUMO}$	0.07019
Chemical Potential(ϕ)	$\frac{-(I+A)}{2}$	-0.129115
Absolute hardness(η)	$\frac{(I-A)}{2}$	0.058925
Softness(S)	$\frac{1}{\eta}$	7.745033
Electronegativity (χ)	$\frac{(I+A)}{2}$	0.129115
Electrophilicity index (ω)	$\frac{\phi 2}{2\eta}$	0.141457
Electron donating capability(ω-)	$\frac{(3\,I+A)2}{16(I-A)}$	0.213380
Electron accepting capability (ω+)	$\frac{(I+3A)2}{16(I-A)}$	0.084265

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 isoeugenol (1,2-dimethoxy-4-(prop-1-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.

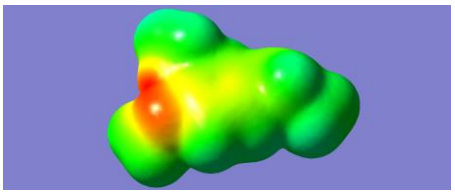


Figure 9: Electron Density of Methyl isoeugenol (1,2-dimethoxy-4-(prop-1-en-1-yl) benzene) from total SCF density (isovalue =0.0004; mapped with ESP)

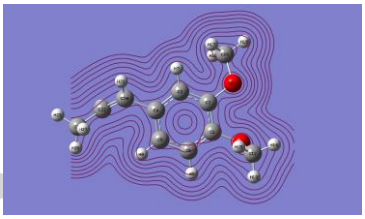


Figure-10: Electrostatic Potential from total SCF density (red-negative charge -yellow-green -blue positive charge)

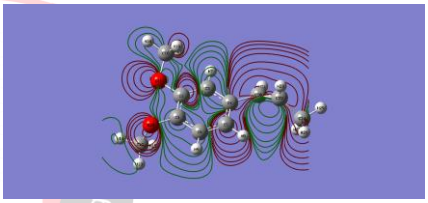


Figure-11 Electrostatic Potential from total scf density (MO-48) HOMO

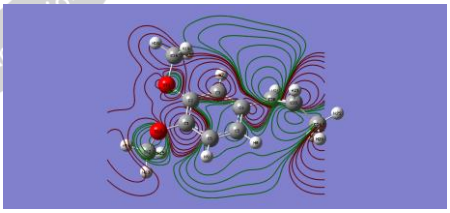


Figure-12 Electrostatic Potential from total scf density (MO-49) LUMO

IV. CONCLUSIONS

An attempt was made to calculate various physico-chemical properties of Methyl isoeugenol (1,2-dimethoxy-4-(prop-1-en-1-yl) benzene) using acdlab/chemsketch as these properties influence the toxic, hazards, exposure, and risk 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 isoeugenol (1,2-dimethoxy-4-(prop-1-en-1-yl) benzene) were discussed by

 DOI : 10.35291/2454-9150.2022.0032

analysing HOMO and LUMO calculated using B3LYP/6-311 G (d, p) basis set. The values of dipole moment (μ), hyperpolarizability (β) of Methyl isoeugenol (1,2-dimethoxy-4-(prop-1-en-1-yl) benzene)l were calculated and were observed to be comparable to the values of standard reference material of prototype molecule urea hence this molecule can be recommended for its use as a perspective building block for NLO material and a low value of hardness indicates that Methyl isoeugenol (1,2-dimethoxy-4-(prop-1-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 readily.

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