

Geometry optimization, vibrational analysis, HOMO-LUMO, MESP plot of 2-(3-NitroPhenyl) 1, 3-DITHIAN by using DFT method

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In this paper we study quantum chemical calculation of 2-(3-NitroPHENYL)1,3-DITHIAN molecule. Geometry optimization were done by using combination of DFT/B3LYP method and 6-311G(d, p) basis set without any symmetry constrain. Theoretical FT-IR, thermodynamic properties and electronic properties of title compound are reported by DFT/B3LYP method. Calculated frequencies were scaled by a scaling factor. Electronic properties of given molecule also predicated by using HOMO,LUMO orbital and MESP surfaces. Our finding is experimental and calculated geometry is well matched with each other. Electronic parameter shows that benzene ring acts as most nucleophile charge center.

Keywords:-2-(3-NitroPHENYL)1,3-DITHIAN, Normal mode Analysis, HOMO,LUMO, MESP electronic properties

INTRODUCTION

Vibrational spectroscopy gives important information about geometry, electronic properties UV spectra analysis as well NLO properties of given molecule.[1-9] A dithiane is a heterocyclic compound composed of a cyclohexane core structure wherein two methylene bridges (-CH₂- units) are replaced by sulfur centers. The three isomeric parent heterocycles are 1,2-dithiane, 1,3-dithiane and 1,4-dithiane. 1,3-Dithianes are protecting group of some carbonyl-containing compounds due to their inertness to many conditions. [10] In the title compound dithian molecule are joined with phenyl ring along with Nitro group (attached in 2,3 position). In this process the chemical as well physical and electronic properties are different from dithiane group.[11]Theoretical FT-IR ,thermodynamic properties and electronic properties of title compound are reported with Density Functional B3LYP method. To gain a better understanding of the performance and limitation of DFT/B3LYP method, as a general approach to the vibrational problems of organic molecules, we calculated optimized parameter of 2-(3-NitroPHENYL)1,3-DITHIAN and calculated parameter are compared with experimental ones

2. COMPUTATIONAL METHOD

The DFT calculations have been performed at B3LYP/6-31G (d, p) [11-15] level has been employed for the computation of molecular structure, vibrational frequencies, HOMO-LUMO, and energies of the optimized structures,

using G03 program [16], involving gradient optimized geometry [17]. The basis set 6-311G (d, p) augmented by d polarization functions on heavy atoms and p polarization functions on hydrogen atoms as well as diffuse functions for both hydrogen and heavy atoms were used. Initial geometry was generated from standard geometrical parameters and was minimized without any constraint in the potential energy surface.

RESULT AND DISCUSSION

OPTIMIZATION GEOMETRY

In the title compound, C₁₀H₁₁NO₂S₂, the 1,3-dithiane ring has a chair conformation with the 1,4-disposed C atoms being above and below the remaining four atoms. The nitrobenzene substituent occupies an equatorial position and forms a dihedral angle of 88.28 (5)^o with the least-squares plane through the 1,3-dithiane ring.

The nitro group is twisted out of the plane of the benzene ring to which it is connected, forming a dihedral angle of 10.12 (3)^o. Experimental value taken from literature [11] Nearly all the calculated bond length match well with the experimental values For example, the optimized bond lengths of C-C in ring R2 falls in the range from 1.38Å⁰-139Å⁰ which are in good agreement with the experimental bond lengths. Since all the carbon atoms in the benzene ring are sp² hybridized so they have equal bond lengths and bond angles but this is not happen in our study this clearly show that substitution of hydrogen in benzene ring results in a perturbation of the valence electron distribution of the molecule followed by changes in the various chemical and physical properties. The angular changes in

benzene ring geometry have proved to be a sensitive indicator of the interaction between the substituent and the benzene ring. [18] The optimized bond lengths of C-S in ring R1 falls in the range from 1.83\AA to 1.84\AA , which are also in good agreement with those of the experimental bond lengths. The bond length of C-N of ring R1 is lies at 1.49\AA which are also in good agreement with those of the experimental bond lengths. The other calculated bond lengths also show an excellent agreement with experimental value by allowing the relaxation of all parameters. As animated Gauss view of molecule no ring lies in plane and also shows that, a single Nitrogen atom of each NO_2 unit lies in the plane of adjacent ring while both oxygen atom are symmetrically positioned above and below the plane of adjacent ring.

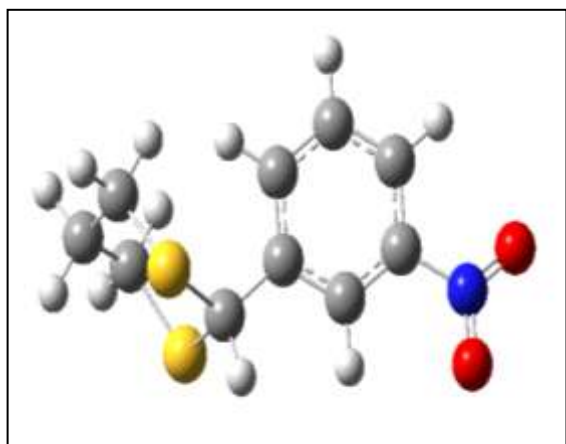


Fig-1 Optimized fig of Title molecule

TABLE-1
BOND LENGTH (\AA) AND BOND ANGLE OF 2-(3-NITROPHENYL)1,3-DITHIANE

S.No.	parameter	Experimental	Calculated
1.	(C ₁ -C ₂)	1.511	1.5177
2.	(C ₁ -C ₄)	1.509	1.5171
3.	(C ₁ -H ₁₅)	0.9700	1.1094
4.	(C ₁ -H ₁₆)	0.9700	1.1092
5.	(C ₂ -S ₅)	1.8048	1.8194
6.	(C ₂ -H ₁₃)	0.9700	1.1068
7.	(C ₂ -H ₁₄)	0.9700	1.1075
8.	(C ₃ -S ₅)	1.8102	1.8342
9.	(C ₃ -S ₆)	1.8069	1.8305
10.	(C ₃ -C ₇)	1.500	1.4966
11.	(C ₃ -H ₂₃)	0.9800	1.1209
12.	(C ₄ -S ₆)	1.8128	1.8216

13.	(C ₄ -H ₁₇)	0.9700	1.1119
14.	(C ₄ -H ₁₈)	0.9700	1.1065
15.	(C ₇ -C ₈)	1.391	1.3976
16.	(C ₇ -C ₉)	1.389	1.3973
17.	(C ₈ -C ₁₀)	1.377	1.3893
18.	(C ₈ -H ₁₉)	0.9300	1.1027
19.	(C ₉ -C ₁₁)	1.375	1.3987
20.	(C ₉ -H ₂₂)	0.9300	1.1014
21.	(C ₁₀ -C ₂₁)	1.377	1.3892
22.	(C ₁₀ -H ₂₀)	0.9300	1.0958
23.	(C ₁₁ -C ₁₂)	1.379	1.3992
24.	(C ₁₁ -N ₂₄)	1.471	1.4993
25.	(C ₁₂ -H ₂₁)	0.9300	1.0992
26.	(N ₂₄ -O ₂₅)	1.214	1.2148
27.	(N ₂₄ -O ₂₆)	1.215	1.215

BOND ANGLES

26.	(C ₂ -C ₁ -C ₄)	113.89	112.4032
21.	(C ₂ -C ₁ -H ₁₅)	108.7	110.3536
22.	(C ₂ -C ₁ -H ₁₆)	108.7	108.8873
23.	(C ₄ -C ₁ -H ₁₅)	108.7	110.2876
24.	(C ₄ -C ₁ -H ₁₆)	108.7	108.9373
25.	(H ₁₅ -C ₁ -H ₁₆)	107.7	105.7288
26.	(C ₁ -C ₂ -S ₅)	114.37	114.8341
27.	(C ₁ -C ₂ -H ₁₃)	108.8	110.2738
28.	(C ₁ -C ₂ -H ₁₄)	108.8	110.1891
29.	(S ₅ -C ₂ -H ₁₃)	108.7	110.3594
30.	(S ₅ -C ₂ -H ₁₄)	108.7	104.5182
31.	(H ₁₃ -C ₂ -H ₁₄)	107.6	106.1842
32.	(S ₅ -C ₃ -S ₆)	113.99	114.682
33.	(S ₅ -C ₃ -C ₇)	108.59	112.1431
34.	(S ₅ -C ₃ -H ₂₃)	108.7	103.0308
35.	(S ₆ -C ₃ -C ₇)	108.10	114.2175
36.	(S ₆ -C ₃ -H ₂₃)	108.7	102.8812
37.	(C ₇ -C ₃ -H ₂₃)	108.7	108.6088
38.	(C ₁ -C ₄ -S ₆)	114.22	114.6265
39.	(C ₁ -C ₄ -H ₁₇)	108.8	110.1453
40.	(C ₁ -C ₄ -H ₁₈)	108.8	110.4254
41.	(S ₆ -C ₄ -H ₁₇)	108.7	109.6729
42.	(S ₆ -C ₄ -H ₁₈)	108.7	104.996
43.	(H ₁₇ -C ₄ -H ₁₈)	107.6	106.5722
44.	(C ₂ -S ₅ -C ₃)	99.55	104.1164
45.	(C ₃ -S ₆ -C ₄)	100.11	103.3664
46.	(C ₃ -C ₇ -C ₈)	120.41	114.1554
47.	(C ₃ -C ₇ -C ₉)	120.46	118.5208
48.	(C ₈ -C ₇ -C ₉)	119.13	119.3233
49.	(C ₇ -C ₈ -C ₁₀)	120.67	120.3793
50.	(C ₇ -C ₈ -H ₁₉)	119.7	119.911
51.	(C ₁₀ -C ₈ -H ₁₉)	119.7	119.7041
52.	(C ₇ -C ₉ -C ₁₁)	118.65	120.1836
53.	(C ₇ -C ₉ -H ₂₂)	120.7	119.5206
54.	(C ₁₁ -C ₉ -H ₂₂)	120.7	120.2957

55.	(C ₈ -C ₁₀ -C ₁₂)	120.77	120.5181
56.	(C ₈ -C ₁₀ -H ₂₀)	119.6	119.7878
57.	(C ₁₂ -C ₁₀ -H ₂₀)	119.6	119.6939
58.	(C ₉ -C ₁₁ -C ₁₂)	112.93	120.0337
59.	(C ₉ -C ₁₁ -N ₂₄)	118.60	119.9699
60.	(C ₁₂ -C ₁₁ -N ₂₄)	118.46	119.9964
61.	(C ₁₀ -C ₁₂ -C ₁₁)	117.84	119.5599
62.	(C ₁₀ -C ₁₂ -H ₂₁)	121.1	119.5984
63.	(C ₁₁ -C ₁₂ -H ₂₁)	119.6	120.8416
64.	(C ₁₁ -N ₂₄ -O ₂₅)	117.90	119.4268
65.	(C ₁₁ -N ₂₄ -O ₂₆)	118.32	119.3343
66.	(O ₂₅ -N ₂₄ -O ₂₆)	123.77	121.2389

VIBRATIONAL MODES ANALYSIS

The molecule has C₁ point group symmetry having 24 atoms and 66 normal modes of fundamental vibration. Out of these N-1 are stretching modes and remaining are bending modes. These normal modes of frequencies are divided in two parts, above 1000 cm⁻¹ are called functional region and below 1000 cm⁻¹ are called fingerprint region. The calculated normal mode vibrational frequencies provide thermodynamic properties by way of statistical mechanics by combining the results of the GAUSSVIEW'S Program [19].

It is well known that vibrational frequencies obtained by quantum chemistry calculation are typically larger than that of their experimental counterpart and thus experimental scaling factors of .9648 are usually employed to have better agreement with the experimental vibrational frequencies [20]. The scaling factor depends on both basis set and method used in the calculation and are determined from the mean deviation between calculated and experimental value of frequencies [21,22].

C-H VIBRATION

The hetero aromatic structure shows the presence of C-H stretching vibrations in the region 3000-3100 cm⁻¹, which

is the characteristic region for the ready identification of the C-H stretching vibration [23]. The frequencies obtained by B3LYP method in this region are 3002,2987,2969,2663 cm⁻¹ are polarized along perpendicular to the phenyl ring which are also supported by the literature [23]. Scissoring mode occurs higher region due to compact configuration. In plane bending mode lies higher frequency region however out of plane bending mode lies lower region. At lower region some mixing of mode of vibration occurs due to this it is difficult to identify mode of vibration and intensity goes higher region.

C-C Stretching

At low frequency range almost all the modes of vibrations belong to out of plane bending, rocking and ring torsion. The ring C-C stretching vibration obtained by DFT/B3LYP are lies in between 739 cm⁻¹-1154 cm⁻¹. The theoretically calculated C-C-C bending modes and C-C torsional modes have been found to be consistent with the recorded spectral values.

We can say that the IR intensities are very high as compared to those in the higher frequency region (Table 2). We also observe that the best agreement between the calculated and the experimental intensities are observed in the low frequency region only i.e. <704 cm⁻¹ (B3LYP) because of the electron correlation anharmonicity and incomplete approximation of vibrational intensity could not be computed very accurately using quantum chemistry software till now. So, it is obvious that frequency needs to be emphasized rather than intensity in the present work. Calculated intensity of vibration are not match well with experimental one because calculation done on single system in gas phase so we ignore inter molecular interaction in calculated system.

TABLE-2 CALCULATED WAVE NUMBERS AND RESPECTIVE IR INTENSITY

ν : stretching ν_s : symmetric stretching , ν_{as} : anti symmetric stretching, β : -in plane bending; γ : out of plane bending, w -wagging, τ : torsion, S : scissoring , R : rocking

OTHER MOLECULAR PROPERTIES:-

Several calculated thermodynamic properties based on

the vibrational analysis at B3LYP and 6-311G (d,p) level, like internal thermal energy (E), constant volume heat capacity (Cv), and entropy (S), have been calculated and listed in Table 3. At the room (270C) temperature, conduction band is almost empty so in electronic contribution in total energy negligible. The thermodynamic

42	1110	7.1431	β (C-C-C)
43	1128	3.9423	β (C-H)
44	1139	33.7246	β (C ₁₂ -H ₂₁)
45	1155	9.6886	β (C ₁₀ -H ₂₀)
46	1163	40.1902	Twist (C-C-C-H)
47	1189	0.3959	R (H ₁₃ -C ₂ -H ₁₄)
48	1215	3.0848	Twist (C-C-C-H)
49	1234	7.3207	R (H ₁₇ -C ₄ -H ₁₈)
50	1302	11.5872	Breathing R1
51	1305	13.1744	Breathing Ring
52	1349	4.1052	S (H ₁₆ -C ₁ -H ₁₅)
53	1358	3.6622	S (H ₁₃ -C ₂ -H ₁₄)
54	1362	37.4444	ν (Ring R1)
55	1388	4.4115	S (H ₁₇ -C ₄ -H ₁₈)
56	1518	140214 3	ν (Whole Ring)
57	1560	25.8133	ν (Whole Ring)
58	1572	538.140 8	ν_s (O ₂₅ -N ₂₄ -O ₂₆)
59	1739	19.3816	ν (Whole Ring)
60	1754	16.0976	ν (Whole Ring)
61	1858	637.121 3	ν_{as} (O ₂₅ -N ₂₄ -O ₂₆)
62	2809	51.9611	ω (C ₃ -H ₂₃)
63	2889	4.1743	ν_{as} (H ₁₆ -C ₁ -H ₁₅)
64	2898	14.9903	ν_{as} (H ₁₈ -C ₄ -H ₁₇)
65	2916	14.6339	ν_{as} (H ₁₄ -C ₂ -H ₁₃)
66	2951	42.3482	ν (C ₉ -H ₂₂)
67	2663	15.3934	ν (C ₈ -H ₁₉)
68	2967	1.083	ν_s (H ₁₅ -C ₁ -H ₁₆)
69	2969	40.2259	ν (C ₁₂ -H ₂₁)
70	2981	37.8967	ν (H ₁₇ -C ₄ -H ₁₈)
71	2987	16.8268	ν_s (H ₁₄ -C ₂ -H ₁₃)
72	3002	40.1631	ν (C ₁₀ -H ₂₀)

parameters clearly indicate that out of all motion vibration motion plays a crucial role in assessing thermodynamical behavior of title compound

**TABLE-3
THERMODYNAMIC PROPERTIES OF
TITLE MOLECULE**

S.N	Fre.	IR intensity	Vibrational Assignment
1	21	0.1768	τ (O25-N24-O26)
2	54	0.3579	Butterfly Motion
3	81	0.971	γ (C1-C2)
4	101	1.0488	τ (H ₁₅ -C ₁ -H ₁₆)
5	139	4.1303	τ (H ₁₅ -C ₁ -H ₁₆)
6	152	5.8737	τ (H ₁₅ -C ₁ -H ₁₆)
7	175	3.3119	γ (H ₁₅ -C ₁ -H ₁₆)
8	221	1.4889	τ (C1-C2-C4)
9	242	0.3791	τ (C7-C8-C10-C12)
10	285	291.12	γ (whole Ring)
11	302	4.3357	τ (H ₁₅ -C ₁ -H ₁₆)
12	331	2.7997	Twist in (H18-C ₄ -H ₁₇)
13	372	1.1927	γ (whole Ring)
14	388	0.3953	Twist in (C ₁₀ -H ₂₀)
15	418	1.0225	τ in whole molecule
16	493	1.0165	τ (C4-C1-C2)
17	509	11.691	τ (C7-C9-C1-C12)
18	530	2.0823	τ in Ring R1
19	605	6.3144	γ (Ring R1)
20	630	9.9958	ω (C ₈ -H ₁₉ -C ₉)
21	651	24.410	ω (H ₁₅ -C ₁ -H ₁₆)
22	663	65.659	γ (Ring R1)
23	681	25.850	τ (H ₁₆ -C ₁ -H ₁₄)
24	704	11.372	τ (H ₁₈ -C ₄ -H ₁₇)
25	739	194.43	R (H ₁₈ -C ₄ -H ₁₇)
26	779	5.1172	R (H ₁₈ -C ₄ -H ₁₇)
27	789	83.559	τ (C7-C8-C10-C12)
28	816	1.1883	Twist (C7-C8-C10-C12)
29	829	1.3321	τ (H ₁₇ -C ₄ -H ₁₈)
30	868	13.267	Twist in (H ₁₇ -C ₄ -H ₁₈)
31	938	0.3765	γ (C12-H21)
32	946	2.8055	Twis (H ₁₅ -C ₁ -H ₁₆)
33	950	3.4402	γ (C ₈ -H ₁₉)
34	974	0.433	γ (H ₁₃ -C ₂ -H ₁₄)
35	989	69.155	γ (C ₃ -H ₂₃)
36	999	1.4133	γ (C ₈ -H ₁₉)
37	1011	2.0047	R (H ₁₃ -C ₂ -H ₁₄)
38	1038	8.7715	τ (C ₁₁ - C ₉ -C ₇ -C ₈)
39	1058	0.0877	γ (C ₃ -H ₂₃)
40	1082	0.8571	R (H ₁₆ -C ₁ -H ₁₅)
41	1109	1.2599	R (H ₁₇ -C ₄ -H ₁₈)

PARAMETER	E (Thermal) Kcal/Mol	CV Cal/Mol- Kelvin	S Cal/Mol- Kelvin
Total	131.581	51.623	119.928
Translational	0.889	2.981	42.320
Rotational	0.889	2.981	32.879
Vibrational	129.80	45.66	44.70

ELECTRONIC PROPERTIES

The interaction with other species in a chemical system is also determined by frontier orbital's, HOMO and LUMO. It can also be determined by experimental data. The frontier orbital gape helps to distinguish the chemical reactivity and kinetic stability of the molecule. A molecule which has a larger orbital gape is more polarized having reactive part as far as reaction is concerted [24]. The frontier orbital gape in case of the given molecule is .235 eV. The contour plots of the HOMO, LUMO and MESP structures of the molecule are shown in Figure 2, 3, 4. LUMO is located over whole molecule however HOMO is located over whole molecule except benzene ring. The transition from HOMO→LUMO in given molecule indicates charge transfer Benzene ring. The importance of MESP lies in the fact that it simultaneously displays molecular size, shape as well as positive, negative, and neutral electrostatic potential region in terms of grading and is very useful in the investigation of molecular structure with its physiochemical property relationship [25,26]. In the present context, color code ranges between - 0.0563 a.u. for deepest red and +0.0783 a.u. for deepest blue. The electronegative region lies in the vicinity of O of nitro group with the value of - 0.0563 a.u. This possibly suggests that an nucleophile attack will favor the positively charged region of ring.

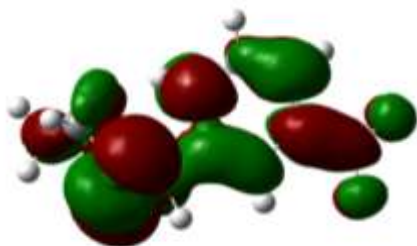


FIG-2 HOMO OF TITLE MOLECULE



FIG-3 LUMO OF OF TITLE MOLECULE

CONCLUSION

In this paper we study vibrational mode analysis geometry optimization, electronic properties as well as thermal properties of title molecule by using combination of DFT/B3LYP and 6-311G(d, p) method. Optimized structure well matches with experimental one. Vibrational motion plays important role in thermal vibration. HOMO-LUMO and MESP plot shows that oxygen of nitro group is strong center for nucleophile substitution reaction. All frequency is positive so above molecule is real and at higher region stretching modes are dominated and at lower region bending modes are effective. Some modes show mixing of several vibration so intensity at these places are effective.

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