

Vibrational spectroscopic studies and ab initio calculations of thorium chelate of 1, 2-naphthoquinone dioxime

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ABSTRACT: The FTIR spectrum of thorium chelate of 1,2-naphthoquinone dioxime was recorded and analyzed. The vibrational wavenumbers have been compared using Gaussian 09 software code, employing RHF / SDD basis set and compared with experimental values. The fundamental modes are assigned by using animation software. The predicted infrared intensities and Raman activities are reported. The calculated frequencies are in good agreement with the experimental values. The calculated geometrical parameters are also given. The study is extended to calculate the HOMO-LUMO energy gap, Ionization potential (I), Electron affinity (A), Global hardness (η), chemical potential (μ) and global electrophilicity (ω). The calculated HOMO-LUMO energies show the charge transfer occurs in the molecule. Optimized geometrical parameters of the title compound are in agreement with similar reported structures.

Keywords: 1-2 naphthoquinone dioxime, IR, HF, Energy gap, Thorium dioximate

I. INTRODUCTION

Quinones and naphthoquinones are widely distributed in nature and play a vital role in certain cellular functions. Owing to the large variety of coordination geometries, coordination numbers, and modes of interactions with their ligands, metal complexes or mostly chelates give access to a different field of pathways in cancer treatment than do organic compounds. The discovery of the anticancer properties of cisplatin was a breakthrough event as far as interest in metal complexes was concerned (1,2). A tremendous number of novel metal complexes have been synthesized and evaluated to find species with better anticancer properties, lower toxic side effects and less tumor resistance to cisplatin (3-5). The structure of 1-2 naphthoquinone dioxime is examined by use of the HF (6-31 G*level), density functional theory DFT (6-31 G* level) & hybrid functional B3LYP. Using the optimized structure of the titled compound IR, NMR, and ultraviolet data is calculated and compared with experimental data. It shows good relation between theoretically calculated IR wave numbers & observed values for Mid – Far IR data (6). Al, Zn, Cu (II), Ni (II) and alkali metal salts of dioximes were reported and the authors concluded that the colour of the quinone oximes is not related to quinone oxime structure (7). The polarographic behavior of the 1, 2-naphthoquinone has been investigated in the pH range 3 to 14. All of the compounds produce well defined polarographic reduction waves which can be used for analytical purposes. Polarographic evidence indicates that the monoximes and the dioximes exhibit tautomerism (8). This paper describes synthesis and vibrational spectra of thorium chelate of 1, 2-naphthoquinone dioxime calculated by HF basis set, the data is compared with experimental values. Geometrical parameters, Mulliken atomic charges and HOMO – LUMO energy gap of the chelate is reported.

II. MATERIALS AND METHODS

The ligand 1, 2-naphthoquinone dioxime is synthesized in laboratory as per the reported method (9). A stock solution of zirconium oxychloride [Th (NO₃)₄] is prepared by using AR grade chemicals. Deionised water is used during synthesis.

2.1 Preparation of metal chelates.

The chelates were prepared by mixing metal salt solution and ligand in 1: 1 proportion for silver chelate and 1: 2 for other metals. The mixture was constantly stirred for one hour on magnetic stirrer. The pH of the mixture was maintained, in between 5.0 – 6.0 by adding ammonia solution to it. Warm the mixture on water bath for about 15 minutes. On cooling it was filtered and found to be coloured.

2.2 Instrumental Analysis.

Elemental analysis was carried out with a Perkin Elmer 2400 series for C, H, and O & N. The IR spectra are recorded on a Thermo Fischer FTIR spectrophotometer iS5 model in a KBr matrix and in the range of 4000 – 400 cm⁻¹ as well as in the range of 1000 – 300 cm⁻¹.

2.2.1 Computational details

The entire calculations conducted in the present work were performed at Hartree – Fock (HF/ SDD) basis set in the Gaussian 09 software code. The geometries were first determined at the Hartree – Fock level of employing SDD basis set (10,11).

The wave number value computed theoretically contains known systematic error due to the negligence of electron correlation. We have used the scaling factor value of 0.9393 for HF /SDD basic set. The absence of imaginary wave number on the calculated Vibrating Spectrum conform that the structure corresponds to minimum energy. HOMO-LUMO energy gap and other related molecular parameters are calculated.

III. RESULTS AND DISCUSSION

The vibrational analysis of Th(NQO)₂ is performed on the basis of the characteristics vibration of hydroxyl, Carbonyl, C=N, N-O and Th-N modes. The computed vibrational wave numbers of IR with intensity used for identifying modes unambiguously. The harmonics vibrational frequencies calculated for Th (NQO)₂ at HF using the SDD basis set have been summarized Table -1. It can be noted that calculated results are harmonics frequencies while the observed contains unharmonic contribution also. The value of the wave number is lower than the former due to anharmonicity. Comparison between the calculated and the observed vibration spectra help us to understand the observed spectral frequency.

Table 1: Wave numbers and Raman activity of Thoriumdioximate by HF

Sr. No.	HF cm ⁻¹	INT	RAMA N	EXPT cm ⁻¹	INT	ASSIGNMENTS
1	60.50031	5.85	2.39	--	--	Th-N Bending
2	76.68445	34.27	1.79	--	--	N-O Bending
3	103.896	6.98	0.5	--	--	N-O Bending
4	133.1082	100.82	21.16	--	--	Th-N Bending
5	150.5228	43.72	0.54	--	--	Th-N Bending
6	164.7814	44.65	10.18	--	--	Th-N Bending
7	191.8426	122.11	0.35	--	--	Th-N Bending
8	199.4228	21.5	4.73	--	--	C-H Bending O.P.
9	202.1186	6.78	1.11	--	--	C-H Bending O.P.
10	227.3482	241.12	19.38	--	--	O-H Bending
11	238.6386	4.06	2.11	--	--	C-H Bending O.P.
12	246.9795	108.1	2.78	--	--	O-H Bending
13	313.4726	27.14	1851	--	--	O-H Bending
14	336.0628	74.39	18.81	--	--	O-H Bending
15	352.9138	122.49	0.95	356.00	30.1	C-H Bending I.P.
16	360.8603	8.71	10.28	--	--	N-O Bending
17	385.8081	230.21	23.38	--	--	O-H Bending
18	397.4084	253.96	16.21	398.7	27.5	O-H Bending
19	406.7357	1.377	14.34	--	--	O-H Bending
20	425.4278	45.95	10.75	--	--	C-H Bending O.P.
21	430.3027	4.93	9.46	--	--	C-H Bending O.P.
22	458.9232	132.96	14.19	459.73	25.1	O-H Bending
23	480.0668	23.91	1.61	476.2	76.56	C=N Bending
24	484.1904	1.32	21.3	498.01	25.3	C=N Bending
25	527.0694	13.88	7.6	529.3	56.85	C-H Bending O.P.
26	528.3469	4.52	11.48	539.3	63.46	C-H Bending O.P.
27	552.6747	49.35	16.28	553.23	43.4	Th-N Bending
28	555.239	2.47	195.21	559.04	31.3	Th-N Bending
29	580.0929	33.93	8.17	583.9	67.06	C-H Bending O.P.
30	586.4989	47.46	5.55	591.46	28.4	C-H Bending O.P.
31	636.4509	78.73	7.04	642.7	7.61	Th-N Stretching
32	641.5701	12.44	55.31	664.5	42.9	Th-N Bending
33	695.2135	23.13	11.16	685.65	38.3	N-O Bending
34	697.0357	12.14	9.5	704.2	85.61	Th-N Bending
35	711.6513	9.76	19.19	--	--	C-H Bending O.P.
36	712.0645	21	12.74	755.63	39.7	N-O Bending
37	774.8474	64.38	17.15	781.0	81.53	C=N Bending

38	781.0937	7.07	98.88	797.5	57.96	C=N Bending
39	801.1571	45.24	3.69	797.66	37.7	C-H Bending O.P.
40	804.3883	33.92	3.66	803.7	66.86	C-H Bending O.P.
41	809.5827	76.27	40.87	813.14	46.5	O-H Bending
42	829.7307	26.54	20.74	--	--	C=C Stretching
43	832.774	27.61	15.71	846.0	85.88	O-H Bending
44	839.2739	51.34	78.91	--	--	N-O Bending
45	854.4718	152.5	43.93	958.7	19.08	O-H Bending
46	870.3272	205.22	22.97	870.22	28.4	C-H Bending O.P.
47	874.1971	201.78	21.49	--	--	C-H Bending O.P.
48	922.7683	22.4	15.77	--	--	C-H Bending O.P.
49	925.1166	6.6	59.69	--	--	C-H Bending O.P.
50	945.0391	2.17	15.2	--	--	C-H Bending O.P.
51	950.6655	1.79	13.12	958.64	91.2	C-H Bending O.P.
52	1024.391	5.38	19.63	989.06	23.8	C-H Bending I.P.
53	1028.712	1.51	17.39	--	--	C-H Bending I.P.
54	1030.638	330.57	3.05	1034.3	74.68	C=N Stretching
55	1034	96.06	17.82	--	--	C=N Stretching
56	1065.251	3.63	20.83	--	--	C-H Bending O.P.
57	1066.434	3.04	19.94	1070.0	84.08	C-H Bending O.P.
58	1097.394	167.3	99.39	1091.1	65.81	C=C Stretching
59	1098.107	27.49	203.59	1100.6	76.39	C-H Bending I.P.
60	1126.343	10.45	18.51	1140.1	59.99	C-H Bending O.P.
61	1144.349	364.75	90.48	1145.9	62.84	O-H Bending
62	1146.143	201.07	260.66	--	--	C-H Bending O.P.
63	1166.836	95.33	115.55	--	--	C-H Bending I.P.
64	1177.516	1199.62	148.62	--	--	N-O Stretching
65	1184.523	242.64	951.02	1191.2	18.20	C=C Stretching
66	1215.999	88.39	17.12	1192.24	94.0	C-H Bending I.P.
67	1216.816	35.72	182.64	1229.1	69.0	C-H Bending I.P.
68	1240.797	103.09	34.21	1249.89	73.0	N-O Stretching
69	1243.361	151.85	68.56	1249.9	28.18	N-O Stretching
70	1255.205	113.54	96.63	--	--	C-H Bending I.P.
71	1257.554	62.29	169.26	1267.8	69.94	C-H Bending I.P.
72	1273.766	8.18	2.44	--	--	N-O Bending
73	1275.1	2.14	84.89	1282.35	45.8	N-O Bending
74	1331.824	201.49	62.84	1319.05	40.7	C-H Bending I.P.
75	1334.172	103.11	265.14	1340.84	47.3	C-H Bending I.P.
76	1367.527	45.8	25.81	--	--	C-H Bending I.P.
77	1370.636	54.52	133.28	1383.95	156.0	C-H Bending I.P.
78	1392.963	160.66	28.98	--	--	C-H Bending I.P.
79	1399.228	63.76	123.5	1401.6	49.48	O-H Bending
80	1412.022	66.64	83.17	--	--	O-H Bending
81	1420.682	40.82	28.76	--	--	O-H Bending
82	1431.69	3.14	30.25	1438.84	100.2	O-H Bending
83	1476.786	178.31	152.16	--	--	O-H Bending
84	1499.574	29.61	256.71	--	--	C-H Bending I.P.
85	1503.077	1.32	90.06	--	--	C-H Bending I.P.
86	1524.625	166.69	99.45	--	--	O-H Bending
87	1535.784	254.09	22.63	1560.0	21.74	O-H Bending
88	1565.804	254.43	915.1	1564.66	88.8	C=C Stretching
89	1567.504	264.43	3519.43	--	--	C-H Bending I.P.
90	1597.505	116.4	153.87	1593.0	59.07	C-H Bending I.P.
91	1600.276	133.88	115.68	1607.95	59.7	C-H Bending I.P.
92	1645.522	254.55	399.34	1643.9	81.94	C-H Bending I.P.
93	1655.084	273.15	272.09	1650.5	84.66	O-H Bending
94	1664.815	373.99	264.74	1666.6	88.42	O-H Bending

95	1679.919	436.79	301.7	1681.5	93.7	O-H Bending
96	1722.657	939.18	131.57	1718.1	88.99	C-N Stretching
97	1728.509	192.56	1518.24	1731.1	97.2	C-N Stretching
98	1765.574	14.7	126.61	1766.9	96.94	C=C Stretching
99	1766.372	19.7	128.94	1773.3	92.57	C=C Stretching
100	1781.458	35.97	2545.3	1789.3	99.48	C=C Stretching
101	1781.843	360.27	500.78	1792.7	95.62	C=C Stretching
102	3183.851	21.8	98.01	3058.7	62.94	C-H Stretching asym.
103	3184.218	20.07	90.01	3136.7	68.54	C-H Stretching asym.
104	3189.299	10.24	81.62	--	--	C-H Stretching asym.
105	3190.398	9.71	80.24	--	--	C-H Stretching asym.
106	3196.945	92.4	237.37	--	--	C-H Stretching asym.
107	3197.368	88.44	242.16	--	--	C-H Stretching asym.
108	3211.448	6.16	78.38	--	--	C-H Stretching asym.
109	3211.608	8.31	93.37	--	--	C-H Stretching asym.
110	3214.754	66.35	163.54	--	--	C-H Stretching asym.
111	3215.402	68.83	159.26	--	--	C-H Stretching asym.
112	3219.197	263.04	417.52	--	--	C-H Stretching asym.
112	3219.319	99.76	1122.44	3241.64	38.6	C-H Stretching sym.
114	3676.364	62.93	324.23	3562.23	5 6.2	O-H Stretching
115	3685.794	48.28	391.79	3576.99	45.2	O-H Stretching
116	3691.759	70.34	272.05	3645.03	23.5	O-H Stretching
117	3709.906	237.69	415.49	3668.69	23.1	O-H Stretching

O-H vibrations

The hydroxyl OH group provides four normal vibrations, ν_{OH} , δ_{OH} and γ_{OH} , of which not only the stretching vibration but also the out-of-plane deformation is good group vibrations (12). HF level calculations give the ν_{OH} mode at 3714.066, 3710.179, 3697.957 and 3689.395 cm^{-1} . We observed these values at 3562.23, 3576.99, 3645.03 and 3668.69 cm^{-1} . The moderate to strong absorption at $1350 \pm 40 \text{ cm}^{-1}$ in the spectrum of phenol is assigned to δ_{OH} mode (13). In the FTIR spectrum of title compound, the vibration at 1438.84 is observed for δ_{OH} mode. This band is predicted by HF at 1489.65, 1503.27, 1512.49, 1524.21 and 1572.22 cm^{-1} . The γ_{OH} mode is observed in the FTIR spectrum at 459.73 and 398.7 cm^{-1} . The vibration for γ_{OH} are predicted by HF at 488.58, 433.02, 423.09, 410.74, 357.78, 333.73 and 262.94 cm^{-1} .

C-H vibration

The Naphthalene structure shows the presence of structural vibration in the region 3250-2950 cm^{-1} which is characteristics for the zero identification of C-H stretching vibration. The region 3250-3100 cm^{-1} is for symmetric stretching. and 3100-2950 cm^{-1} for asymmetric stretching modes of vibration.(14). For most cases, the naphtholic C-H vibration absorption bands are usually weak and it is too weak for detection. In the present work, for the $\text{Th}(\text{NQO})_2$ the FTIR band is observed at 3241.64, 3058.7 and 3136.7 cm^{-1} have been assigned to C-H stretching vibration. The HF level predicted absorption at 3427.36, 3427.23, 3423.19, 3422.5, 3419.15, 3418.98, 3403.99, 3403.54, 3396.57, 3395.4, 3389.99 and 3389.6 cm^{-1} .

The title compound has both C-H out of plane and in plane bending vibration. The out of plane bending mode of C-H vibration of $\text{Th}(\text{NQO})_2$ is found well in agreement with the experimental predicted in the region 1095-617 cm^{-1} and 562-254 cm^{-1} . HF level and SDD basis shows this region which gives number of vibration and are comparable with experimental results as shown in Fig 1. In plane bending vibration, the region is 1450-1087 cm^{-1} . Which are comparable with the predicted data. The in plane C-H deformation vibration of $\text{Th}(\text{NQO})_2$

is experimentally observed in the region 1250-1080 cm^{-1} which is supported by the vibration values predicted by HF.

C=N Vibrations.

The stretching frequency of C=N bond is observed at 1034.3, 1731.1 and 1718.1 cm^{-1} in the FTIR spectra of $\text{Th}(\text{NQO})_2$ while these are predicted by HF/ SDD at 1034.0, 1030.638, 1728.509 and 1722.657 cm^{-1} . The bending frequency of C=N is found in the FTIR spectrum at 797.5, 781.53, 498.01 and 476.2 cm^{-1} while HF / SDD predicted at 781.0937, 774.8474, 484.1904 and 480.0668 cm^{-1} . The $\nu(\text{C}=\text{N})$ in chelates shows lower frequency owing to elongation of these bonds on co-ordination.

N-O Bending Vibration.

The observation of $\nu(\text{N}-\text{O})$ wave number is observed at 1282.35 and 755.63 cm^{-1} in the FTIR spectrum. HF/SDD level predicted IR frequencies at 1275.1, 1273.766, 839.2739, 712.0645, 360.8603 and 103.896 cm^{-1} . The absorption of this $\nu(\text{N}-\text{O})$ at higher wave number indicates that this bond is significantly shorter in the chelates. The higher wave length of the N-O indicates that nitroso atoms of the oxime group coordinate to the centre (15,16).

Th-N Stretching.

The frequencies of Th-N stretching is observed in the FTIR spectrum at 642.7 cm^{-1} but the predicted IR values is at 636.4509 cm^{-1} by HF level. These values are in good agreement with experimental data.

Th-N bending vibration

The IR absorption frequencies of Th- N bending are predicted at 697.0357, 641.5701, 555.239, 552.6747, 191.8426, 164.7814, 150.5228, 133.1082, and 60.5031 cm^{-1} with HF level. Experimental values are recorded at 704.2, 664.5, 559.04 and 553.23 cm^{-1} only.

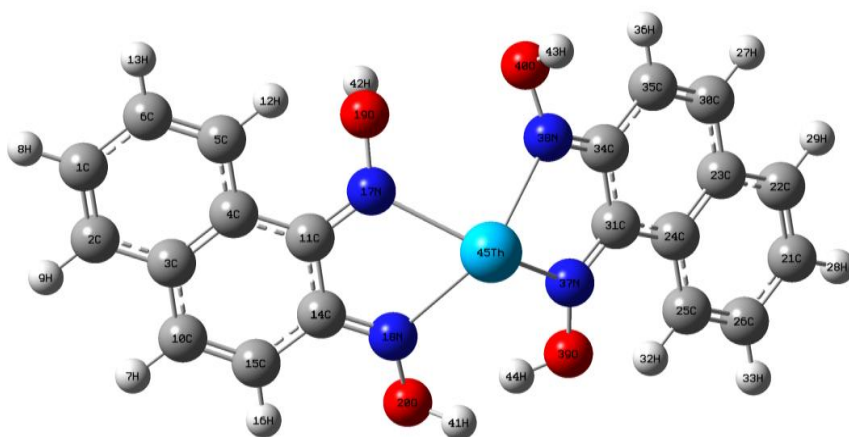


Fig.1 Molecular structure of thorium dioximate

Molecular geometry.

The optimized structure parameters of $\text{Th}(\text{NQO})_2$ calculated by ab initio, HF/SDD basis set are listed in Table 2 in accordance with the atom numbering scheme given in Fig -1. The values of bond length in \AA , bond angles and dihedral angles in degree are given in Table 2.

Table No:-2 Bond Length and Bong Angle and Dihedral Angle of Thdioximate

Bond Length	A ⁰	Bong Angle	(⁰)	Dihedral Angle	A ⁰
Th45-N18	2.304	Th45-N18-C14	113.477	Th45-N18-C14-C11	9.793
H44-O39	0.956	H44-O39-N37	109.471	H44-O39-N37-C31	-149.841
H43-O40	0.960	H43-O40-N38	109.471	H43-O40-N38-C34	-90.159
H42-O19	0.959	H42-O19-N17	109.471	H42-O19-N17-C11	-89.847
H41-O20	0.959	H41-O20-N18	109.471	H41-O20-N18-C14	-150.161
O41-N38	1.359	O40-N38-C34	123.253	O40-N38-C34-C31	-169.916
O39-N37	1.360	O39-N37-C31	123.251	O39-N37-C31-C24	-9.180
N38-C34	1.314	N38-C34-C31	119.413	N38-C34-C31-C24	179.119
N37-C31	1.314	N37-C31-C24	121.265	N37-C31-C24-C23	179.286
N17-C11	1.314	N38-C34-C35	121.413	N17-C11-C4-C3	179.285
N18-C14	1.314	N37-C31-C34	119.408	N18-C14-C11-C4	179.115
O19-N17	1.360	N17-C11-C4	121.265	O19-N17-C11-C4	-9.179
O20-N18	1.360	N18-C14-C11	119.414	O20-N18-C14-C11	-169.918
Th45-N38	2.304	O19-N17-C11	123.253	Th45-N38-C34-C35	-171.106
C6-C5	1.354	C14-C11-C4	123.253	C10-C3-C2-C1	-179.888
C3-C10	1.409	C6-C5-C4	119.321	C6-C5-C4-C3	0.091
C11-C14	1.436	C10-C3-C2	119.993	C14-C11-C4-C3	0.183
C34-C31	1.436	C34-C31-C24	119.476	C24-C23-C22-C21	0.085
C35-C30	1.359	C24-C25-C26	119.320	C34-C31-C24-C23	0.185
C22-C21	1.355	C22-C21-C26	120.064	C35-C30-C23-C22	179.922
H16-C15	1.070	H7-C10-C3	119.552	H7-C10-C3-C4	179.982
H27-C30	1.070	H27-C30-C23	119.551	H27-C30-C23-C24	179.981

Mulliken Atomic Charges

Mulliken charges arise from the Mulliken population analysis (17,18) and provide a means of estimating partial atomic charges from calculations carried out by the methods of computational chemistry, particularly those based on the linear combination of atomic orbitals molecular orbital method, and are routinely used as variables in linear regression QSAR procedures(19).

In the application of quantum mechanical calculation to molecular system, the calculation of effective atomic charges plays an important role. The electron distribution of ZrO (NQO)₂ is compared in the two different mechanical methods and the sensitivity of the calculated charges to charge in choice of methods is studied. By determining electron population of each atom in the defined basis function, the Mulliken charges are calculated by HF/SDD. The results are presented in Table-3 which the values of atomic charges of each atom of the concerned molecule. Fig. 2 shows Atomic charge against atoms of the said molecule.

Table-3 :- Mulliken Atomic Charges of Th(NQO)₂

Sr. No.	Atom	Atomic charge	Sr. No.	Atom	Atomic charge
1	1 C	-0.294187	24	24 C	0.105229
2	2 C	-0.424752	25	25 C	-0.314506
3	3 C	0.360551	26	26 C	-0.362768
4	4 C	0.130517	27	27 H	0.229500
5	5 C	-0.346707	28	28 H	0.226204
6	6 C	-0.347381	29	29 H	0.233657
7	7 H	0.230570	30	30 C	-0.509079
8	8 H	0.226993	31	31 C	0.254845
9	9 H	0.234242	32	32 H	0.328427
10	10 C	-0.502205	33	33 H	0.224702
11	11C	0.261046	34	34 C	0.378388
12	12H	0.317340	35	35 C	-0.472258
13	13H	0.224987	36	36 H	0.246183
14	14C	0.356095	37	37 N	-0.679602
15	15 C	-0.465568	38	38 N	-0.715136
16	16 H	0.252585	39	39 O	-0.631435
17	17 N	-0.703970	40	40 O	-0.568583

18	18 N	-0.698357	41	41 H	0.424554
19	19 O	-0.595206	42	42 H	0.447924
20	20 H	-0.573341	43	43 H	0.431293
21	21 C	-0.291337	44	44 H	0.428777
22	22 C	-0.427755	45	45 Th	3.001389
23	23 C	-0.424752			

The CNO angle in typical oximes is relatively constant around 112-113°(20, 21). In the present chelate the C34-N38-O40 angle is opened up by about 10 ° from the expected value and found constant for all four angles. The naphthalene carbon ring is relatively planar, the largest deviation from the mean plane being 0.023 Å ° for the C1 carbon atom. The N and O atoms lie approximately in the naphthalene mean plane. A further interesting finding is that the outside angle C35-C34-N38 [121.27 °] is significantly larger than the inside angle C31-C35-N38 [119.41 °] . It may be noted that almost the same differences are predicted. It is obvious that the only marked distortions of the geometry and orientation of the present 1,2-oxime groups are associated with the oxime groups on the carbon atom.

HOMO-LUMO energy gap and related molecular properties.

The HOMO-LUMO energy gap of the molecule Th(NQO)₂ in the HF and SDD basis set has been calculated. The HOMO-LUMO energy gap is constant in both methods. It is known that the value of *E*_{HOMO} is often associated with the electron donating ability of inhibitor molecule, higher values of *E*_{HOMO} is an indication of the greater ease of donating electrons to the unoccupied d orbital of the receptor. The value of *E*_{LUMO} is related to the ability of the molecule to accept electrons, lower values of *E*_{LUMO} shows the receptor would accept electrons. Consequently, the value of *E*_{gap} provides a measure for the stability of the formed complex on the metal surface. The frame work of SCF MO theory, the ionization energy and electron affinity can be expressed through HOMO and LUMO energies AS I= -*E*_{HOMO}, A= -*E*_{LUMO}. The hardness compounds to the gap between the HOMO and LUMO orbital energies. If the gap energy is higher than the Hardness is also larger. The global hardness $\eta = \frac{1}{2} (E_{HOMO} - E_{LUMO})$. The hardness is associated with the stability of chemical potential (μ) can be expressed in combination of electron affinity and ionization potential. The global electrophilicity index (ω) is also calculated and listed in table- 4.

Table No: - 4 Comparison of HOMO-LUMO, Energy gap and related Molecular Properties of Th(NQO)₂

Molecular Properties	HF/SDD
HOMO eV	-0.20154
LUMO eV	0.02287
Energy gap	0.22441
Ionisation Potential (I)	0.20154
Electron Affinity(A)	-0.02287
Global Hardness (η)	0.112205
Chemical Potential (μ)	-0.089335
Global Electrophilicity (ω)	0.035563

Table 5 Theoretically computed Energies (a.u.), Zero point Energy (Kcal / mol) Rotational Constants (GHz), Entropy (cal mlo⁻¹K⁻¹) and Dipole moment D (Kcal. mlo⁻¹K⁻¹)

Parameter	HF/SDD
Total Energy e.u.	-1689.677
Zero Point Energy	227.01894
Rotational constants	0.33125
	0.07603
	0.06817
Entropy Total	130.173
Translational	45.099
Rotational	36.48
Vibrational	48.594
Dipole moment (D)	13.9118

IV. CONCLUSIONS

The proper frequency assignment for the chelate Th(NQO)₂ is performed from the FTIR spectra. The experimental vibration frequencies are compared with HF level calculation and found most of them are in good agreement. The assignments were confirmed with the help of animation process which is available in Gaussian 09 computer code. The results suggest that it shows the formation of chelates. The molecular geometry of ZrO(NQO)₂ is best at the HF/ SDD level. The HOMO- LUMO energy was calculated and other related molecular properties were also discussed. The Mulliken atomic charges were calculated and the results were discussed. Thermodynamic parameters were calculated.

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