

The chelate formation of thorium with 1, 2-naphthoquinone, 1-oxime

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Abstract: Thorium chelate of 1,2-naphthoquinone, 1-oxime was synthesized. The vibrational wave numbers of thorium with 1,2-naphthoquinone, 1-oxime have been calculated using Gaussian 09 software code, employing RHF / SDD basis set and IR data is compared with experimental values. 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, 1-oxime, IR, HF, Energy gap, Thorium monoximate

I. Introduction

It was shown that 2-nitroso 1-naphthol (1-oxime) ($pK_a = 7.24$) is a stronger acid than 1-nitroso 2-naphthol (2-oxime) ($pK_a = 7.63$) (1). The chemistry of coordination compounds has shown a rapid development in diverse disciplines as a result of the possible use of these new compounds in biological applications. Oximes have often been used as chelating ligands in the field of coordination chemistry and their metal complexes have been of great interest for many years. Oxime metal chelates are biologically active (2). 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 (3). The structure of 1-2 naphthoquinone 1-oxime 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 (4). 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 (5). Ab initio, Hartree-Fock and Density Functional Theoretical study of vibrational spectra of zirconium chelate of 1, 2-naphthoquinone-1, oxime have been reported by G. S. Jagtap et al. (6). This paper describes synthesis and vibrational spectra of thorium chelate of 1, 2-naphthoquinone 2-oxime 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 1-oxime or 1-nitroso 2-naphthol is used as it is supplied by (Fluka, chemicals). A stock solution of thorium nitrate $[Th(NO_3)_4]$ is prepared by using AR grade chemicals. Deionised water is used during synthesis.

2.1 Synthesis of metal chelate

The chelate was prepared by mixing metal salt solution and ligand in 1: 1 proportion. 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 was 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 (7,8).

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 confirms that the structure corresponds to minimum energy. HOMO-LUMO energy gap and other related molecular parameters are calculated.

III. Results and Discussion

The infra red absorption frequencies of Th(NQO)₂ are analysed 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 are used for identifying modes unambiguously. The harmonics vibrational frequencies calculated for Th (NQO)₂ at HF using the SDD basis set have been presented in 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: Infra red Wave numbers of Thorium1-oximate

Sr.No	Cald.cm ⁻¹	Intensity	Raman Activity	Exp cm ⁻¹	Int.	Assignment
1.	23.84	0.933	21.286736	--	--	Deformation
2.	98.79	7.425	88.209591	--	--	Deformation
3.	147.26	7.928	131.488454	--	--	Deformation
4.	174.59	11.114	155.891411	--	--	Deformation
5.	188.37	21.776	168.195573	--	--	Deformation
6.	196.23	10.981	175.213767	--	--	Deformation
7.	211.34	0.203	188.705486	--	--	Deformation
8.	215.49	22.116	192.411021	--	--	
9.	249.01	0.967	222.341029	--	--	
10.	254.08	3.384	226.868032	--	--	
11.	328.82	122.9	293.603378	--	--	M-O Stretching
12.	349.19	30.389	311.791751	--	--	M-O Bending
13.	372.74	121.32	332.819546	376.21	0.0453	C-N Stretching
14.	388.8	23.681	347.15952			O-H Bending
15.	399.67	3.384	356.865343	489.60	0.718	M-O Stretching
16.	423.17	7.604	377.848493	--	--	M-O Stretching
17.	437.76	7.977	390.875904	--	--	C-H Bending o.p.
18.	447.86	4.139	399.894194	--	--	C-H Bending o.p.
19.	508.96	87.017	454.450384	501.94	0.507	O-H Bending
20.	520.83	19.002	465.049107	--	--	M-O Bending
21.	530.76	25.625	473.915604	529.31	0.596	O-H Bending
22.	558.44	2.178	498.631076	554.60	0.696	C-H Bending o.p
23.	560.25	6.702	500.247225	577.80	0.793	C-H Bending o.p
24.	594.37	57.46	530.712973	590.50	0.730	O-H Bending
25.	597.06	0.105	533.114874	--	--	deformation
26.	610.51	23.902	545.124379	603.00	0.862	C-H Bending o.p
27.	620.11	25.178	553.696219	--	--	C-H Bending o.p
28.	648.96	34.546	579.456384	--	--	M-O Bending
29.	654.45	39.802	584.358405	--	--	M-O Bending
30.	689.59	78.236	615.734911	680.90	0.385	deformation
31.	694.94	26.047	620.511926	--	--	M-N
32.	742.68	9.808	663.138972	739.40	0.780	C-H Bending o.p
33.	745.02	8.827	665.228358	758.18	0.821	C-H Bending o.p
34.	788.90	152.176	704.40881	783.40	0.772	O-H Bending
35.	831.28	19.856	742.249912	--	--	C-C Stretching
36.	832.53	14.176	743.366037	--	--	C-C Stretching
37.	836.96	101.404	747.321584	--	--	deformation
38.	842.27	27.852	752.062883	841.36	0.722	
39.	864.06	52.234	771.519174	--	--	C-H Bending o.p

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40.	864.60	26.269	772.00134	--	--	C-H Bending o.p
41.	887.34	19.067	792.305886	888.20	0.722	C-H Bending o.p
42.	888.99	3.801	793.779171	--	--	C-H Bending o.p
43.	938.97	87.821	838.406313	930.60	0.169	C-H Bending o.p
44.	940.61	134.87	839.870669			C-H Bending o.p
45.	989.33	10.91	883.372757	--	--	
46.	989.56	5.025	883.578124	--	--	
47.	1007.42	10.118	899.525318	--	--	C-H Bending o.p
48.	1018.38	1.4897	909.311502	--	--	C-H Bending o.p
49.	1106.25	0.494	987.770625	1086.27	0.652	C-H Bending o.p
50.	1108.75	0.951	990.002875	1101.00	0.668	C-H Bending o.p
51.	1121.19	56.567	1001.110551	--	--	C-C stretching
52.	1126.75	34.831	1006.075075	--	--	C-C stretching
53.	1135.00	3.03	1013.4415	--	--	C-H Bending o.p
54.	1140.01	2.664	1017.914929	1137.56	0.641	C-H Bending o.p
55.	1155.38	1.579	1031.638802	1153.97	0.892	C-H Bending o.p
56.	1178.41	28.939	1052.202289	1173.73	0.746	N-O stretching
57.	1183.92	22.953	1057.122168	--	--	N-O stretching
58.	1203.34	6.03	1074.462286	1216.08	1.117	C-H Bending
59.	1234.76	36.16	1102.517204	1235.80	0.623	C-H Bending i.p
60.	1234.97	21.513	1102.704713	--	--	C-H Bending i.p
61.	1272.69	295.78	1136.384901	1260.83	0.595	C-C stretching
62.	1276.43	17.158	1139.724347	--	--	C-H Bending i.p
63.	1293.40	8.155	1154.87686	1293.80	0.468	C-H Bending i.p
64.	1301.11	44.614	1161.761119	--	--	C-H Bending i.p
65.	1315.08	3.136	1174.234932	1310.05	0.854	N-O Stretching
66.	1319.46	7.436	1178.145834	--	--	C-C stretching
67.	1352.35	27.845	1207.513315	1344.56	0.966	C-H Bending i.p
68.	1361.95	5.062	1216.085155	--	--	C-H Bending i.p
69.	1399.10	57.883	1249.25639	1384.34	1.279	C-H Bending i.p
70.	1400.93	36.446	1250.890397	1404.22	1.073	C-H Bending i.p
71.	1461.15	0.782	1304.660835	--	--	C-C stretching
72.	1463.29	3.442	1306.571641	1454.65	0.592	C-H Bending i.p
73.	1490.81	19.061	1331.144249	1477.82	0.694	O-H Bending
74.	1498.75	19.426	1338.233875	--	--	C-C stretching
75.	1520.52	7.031	1357.672308	1524.57	0.911	O-H Bending
76.	1562.67	83.886	1395.308043	1557.50	1.292	C-O Stretching
77.	1568.74	133.628	1400.727946	--	--	C-O Stretching
78.	1584.10	84.426	1414.44289	1580.40	0.329	O-H Bending
79.	1621.60	110.588	1447.92664	1609.65	1.073	C-H Bending i.p
80.	1624.00	24.559	1450.0696	--	--	C-C stretching
81.	1654.30	44.195	1477.12447	1647.70	0.545	C-C stretching
82.	1654.96	3.726	1477.713784	--	--	C-C stretching
83.	1707.27	28.746	1524.421383	--	--	C-N stretching
84.	1722.45	4.71	1537.975605	--	--	C-O stretching
85.	1747.15	201.235	1560.030235	1746.10	0.884	C-C stretching
86.	1750.47	104.291	1562.994663	--	--	C-C stretching
87.	1803.65	70.667	1610.479085	--	--	C-C stretching
88.	1807.98	71.047	1614.345342	--	--	C-O stretching
89.	1826.90	356.751	1631.23901	--	--	C-N stretching
90.	1837.13	89.831	1640.373377	--	--	C-N stretching
91.	1885.21	0.984	1683.304009	--	--	C-C stretching
92.	1886.08	0.824	1684.080832	--	--	C-C stretching
93.	1920.72	33.52	1715.010888	--	--	C-C stretching
94.	1923.07	89.096	1717.109203	1944.30	0.837	C-C stretching
95.	3391.55	9.168	3028.314995	3247.80	0.240	C-H stretching
96.	3394.27	5.116	3030.743683	--	--	C-H stretching
97.	3400.34	3.233	3036.163586	--	--	C-H stretching
98.	3402.25	3.736	3037.869025	--	--	C-H stretching
99.	3407.15	42.564	3042.244235	--	--	C-H stretching
100.	3410.00	31.001	3044.789	--	--	C-H stretching
101.	3425.22	34.35	3058.378938	--	--	C-H stretching
102.	3427.13	40.34	3060.084377	--	--	C-H stretching
103.	3428.04	32.9	3060.896916	--	--	C-H stretching
104.	3430.02	51.187	3062.664858	--	--	C-H stretching
105.	3436.92	105.19	3068.825868	--	--	C-H stretching
106.	3484.14	40.911	3110.988606	--	--	C-H stretching

107.	3902.01	46.244	3484.104729	3904.00	0.553	O-H stretching
108.	3914.88	188.044	3495.596352	3912.70	0.599	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 (9). HF level calculations give the ν OH mode at 3902.01 and 3914.88 cm^{-1} and we observed these values at 3904.00 and 3912.70 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 (10). In the FTIR spectrum of title compound, the vibration at 1344.56 is observed for δ OH mode. This band is predicted by HF at 1400.93 cm^{-1} . The γ OH mode is observed in the FTIR spectrum at 376.21 cm^{-1} . The vibrations for γ OH are predicted by HF at 388.80 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 are asymmetric stretching modes of vibration.(11). 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 3247.8 cm^{-1} have been assigned to C-H stretching vibration. The HF level predicted absorptions at 3391.55, 3394.27, 3400.34, 3402.25, 3407.15, 3410.00, 3425.22, 3427.13, 3428.04, 3430.02, 3436.92 and 3484.14, 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 predicted at 437-648, 742-1155 cm^{-1} and in experimental values found at 554-603, 739-1153 cm^{-1} . These frequencies are well in agreement with the experimental and predicted data. 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 regions is predicted at 1234-1463 cm^{-1} which is comparable with the experimental recorded data at 1272-1454 cm^{-1} .

C=N Vibrations.

The stretching frequency of C=N bond is observed at 1700.2 and 1693.8 cm^{-1} in the FTIR spectra of $\text{Th}(\text{NQO})_2$ while these are predicted by HF/ SDD at 1923.07 and 1707.27 cm^{-1} . The bending frequency of C=N is found in the FTIR spectrum at 797.2 cm^{-1} while HF / SDD predicted at 831.28 and 372.74 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 $\gamma(\text{N}-\text{O})$ wave number is not observed in the FTIR spectrum. HF/SDD level predicted IR frequencies at 196.23, 188.37 and 98.79 cm^{-1} . The absorption of this $\gamma(\text{N}-\text{O})$ 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 (12,13).

N-O Stretching Vibration

The observation of (N-O) stretching vibration is found at 1192.2 cm^{-1} while HF/SDD level predicted IR frequencies at 1178.41 and 1183.92 cm^{-1} .

Th-N Stretching.

The frequencies of Th-N stretching are not observed in the FTIR spectrum but the predicted IR values are at 196.23 cm^{-1} by HF level.

Th-N bending vibration

The IR absorption frequencies of Th- N bending is predicted at 174.89 cm^{-1} with HF level.

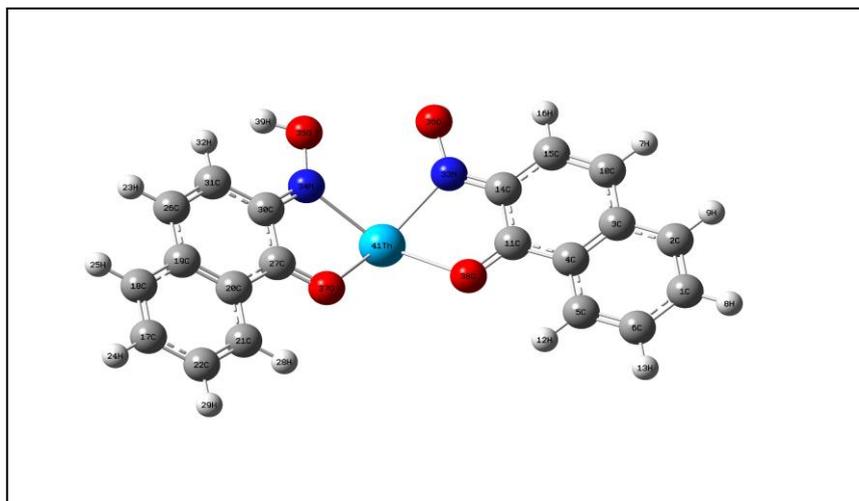


Fig.1 Molecular structure of thorium 1-oximate

Molecular geometry.

The optimized structure parameters of Th (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 Å⁰, bond angles and dihedral angles in degree are given in Table 2.

Table No:-2 Bond Length and Bong Angle and Dihedral Angle of Th1-oximate

Bond	Bond Length Å ⁰	Bong Angle (°)	Dihedral Angle (°)	A ⁰	
H41-O39	0.96	H41-O39-N34	109.472	H41-O39-N34-C27	90.207
H40-O38	0.96	H40-O38-N35	109.471	H40-O38-N35-C11	149.792
O39-N34	1.36	O39-N34-C27	123.707	O39-N34-C27-C20	-8.688
O38-N35	1.36	O38-N35-C11	123.707	O38-N35-C11-C4	8.688
O37-C14	1.287	O37-C14-C11	120.490	O37-C14-C11-C4	-178.644
O36-C30	1.287	O36-C30-C27	120.490	O36-C30-C27-C3	178.644
N35-C11	1.305	N35-C11-C4	121.392	N35-C11-C4-C3	-179.938
N34-C27	1.305	N34-C27-C20	121.392	N34-C27-C20-C19	179.937
Th33-N34	2.297	O39-N34-Th33	123.726	Th33-O37-C14-C11	-10.177
Th33-N37	2.272	C14-C37-Th33	113.215	Th33-N34-C27-C20	171.685
H32-C31	1.07	H32-C31-C26	120.008	H32-C31-C26-C19	-179.974
C31-C26	1.359	C31-C26-C19	120.926	C31-C26-C19-C18	179.725
C30-C27	1.436	C30-C27-C20	119.602	C30-C27-C20-C19	0.623
H29-C22	1.70	H29-C22-C21	120.006	H29-C22-C21-C20	-179.966
H28-C21	1.07	H28-C21-C20	120.007	H28-C21-C20-C19	-179.957
C27-C20	1.397	C27-C20-C19	119.776	C27-C20-C19-C18	179.870
C26-C19	1.408	C26-C19-C18	119.552	C26-C19-C18-C17	-179.94
H25-C18	1.07	H25-C18-C17	119.94	H25-C18-C17-C22	-179.998
H24-C17	1.07	H24-C17-C18	119.972	H24-C17-C22-C21	179.972
C2-C1	1.355	C1-C2-C3	120.120	C4-C3-C2-C1	-0.0613
C3-C2	1.401	C2-C3-C4	119.700	C5-C4-C3-C2	0.0834
C4-C3	1.358	C5-C4-C3	120.151	C6-C5-C4-C3	-0.0493
C5-C4	1.401	6C-C5-C4	119.985	H8-C3-C2-C1	-179.998
C6-C5	1.354	C10-C3-C2	119.522	C10-C3-C2-C1	179.988
H7-C10	1.070	H8-C1-C2	119.972	C11-C4-C3-C2	-179.871
H8-C1	1.07	C11-C4-C3	119.776	H12-C5-C4-C3	179.995

The CNO angle in typical oximes is relatively constant around 112-113° (14, 15). In the present chelate the C27-N34-O39 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 Å⁰ 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 C4-C11-N25 [121.392°] is significantly larger than the inside angle C14-C11-N35 [119.001°] . 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. Fig.2 shows atomic charges of atoms.

Mulliken Atomic Charges

Mulliken charges arise from the Mulliken population analysis (16,17) 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(18).

In the application of quantum mechanical calculation to molecular system, the calculation of effective atomic charges plays an important role. The electron distribution of Th (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	1C	-0.251275	22	22C	-0.326573
2	2 C	-0.410219	23	23 H	0.216324
3	3 C	0.413605	24	24 H	0.213478
4	4 C	0.144949	25	25 H	0.218348
5	5 C	-0.279177	26	26 C	-0.449054
6	6 C	-0.332238	27	27 C	0.229270
7	7 H	0.213163	28	28 H	0.201822
8	8 H	0.207409	29	29 H	0.208906
9	9 H	0.213888	30	30 C	0.364040
10	10 C	-0.455942	31	31 C	-0.402844
11	11 C	0.233087	32	32 H	0.235988
12	12 H	0.312284	33	33 Th	2.210392
13	13 H	0.206175	34	34 N	-0.651137
14	14 C	0.357746	35	35 N	-0.608482
15	15 C	-0.401937	36	36 O	-0.731165
16	16 H	0.230802	37	37 O	-0.730705
17	17 C	-0.260260	38	38 O	-0.614829
18	18 C	-0.399351	39	39 O	-0.578630
19	19 C	0.404330	40	40 H	0.490436
20	20 C	0.195699	41	41 H	0.429844
21	21 C	-0.268169			

Fig.2 Atomic charge on each 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 *EHOMO* is often associated with the electron donating ability of inhibitor molecule, higher values of *EHOMO* is an indication of the greater ease of donating electrons to the unoccupied d orbital of the receptor. The value of *ELUMO* is related to the ability of the molecule to accept electrons, lower values of *ELUMO* shows the receptor would accept electrons. Consequently, the value of *Egap* 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	-0.22404
LUMO eV	-0.03485
Energy gap	0.18559
Ionisation Potential (I)	0.22404
Electron Affinity(A)	0.03485
Global Hardness (η)	0.09279
Chemical Potential (μ)	0.09279
Global Electrophilicity (ω)	0.04639

Thermodynamic properties

On the basis of vibrational analysis at B3LYP / SDD and HF / SDD level, several thermodynamic parameters are calculated and are presented in Tabl-5. The zero point vibration energy (ZPVE) and the entropy, Svib.(T) are calculated to the extent of accuracy and the variations in ZPVE seem to be insignificant. The total energy and the change in total entropy of Th(NQO)₂ at room temperature at different methods is only marginal.

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	DFT/B3LYP/SDD
Total Energy e.u.	-1579.406
Zero Point Energy	206.305
Rotational constants	0.34303
	0.04830
	0.07317
Entropy Total	125.549
Translational	44.948
Rotational	36.272
vibrational	36.373
Dipole movement (D)	9.2314

IV. Conclusions

The calculated vibration frequencies are compared with experimental data 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 Th (NQO)₂ is best at the HF/ SDD level. The HOMO- LUMO energy was calculated and other related molecular properties were also discussed. The Mullikan atomic charges were calculated and the results were discussed. Thermodynamic parameters were calculated.

Acknowledgement

We thank Prin. K.D. Jadhav, Principal, Bharati Vidyapeeth Deemed University, Yashwantrao Mohite College, Pune for permission to Publish this work. RGS and GSJ are grateful to U.G.C. for providing financial assistance by Major Research Project [F. No. 40-84/2011(SR)].

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