THEORETICAL INVESTIGATIONS ON THE MOLECULAR STRUCTURE, VIBRATIONAL SPECTROSCOPIC ANALYSIS OF 2,4-DINITRO-1-NAPHTHOL

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Abstract

The FT-IR & FT-Raman spectra of 2,4-dinitro-1-naphthol have been recorded in the region 4000- 400 cm-1 and 3500-50 cm-1 respectively. The spectra were interpreted with the aid of normal coordination analysis following full structure optimization and force field calculations on the Density Functional Theory (DFT) use in the standard B3LYP method and 6-31+G basis set combination. A close agreement was achieved between the observed and calculated frequencies by refinement of the scale factors.

Keywords: FTIR, FT-Raman Spectra, DFT calculations, Vibrational analysis, 2,4-dinitro-1-naphthol

Introduction

Aromatic rings provide the framework for most of dyes. The dyes owe their colour because of the functional group present in it. The naphthalene plays vital role in this field besides it is also a valuable insecticide. The major commercial use of naphthalene is in the manufacture of polyvinyl chloride (PVC) Plastics. The major consumer use, in mouth repellents, toilet deodorant blocks and to make other chemicals [1].

Naphthalene and its derivatives are biologically, pharmaceutically and industrially useful compounds. The structure of naphthol was benzene-like, having two six member rings fused together. Particularly, naphthol was studied because of its technological applications in a vast amount of industrial process. It is used for the syntheses of plastics and dyes, Gamma ray detector in photo multiplier tubes and also in dye stuffs, synthetic resins, coatings, tanning agent and celluloid [2].

Photo resist compositions are used in micro lithography processes for making miniaturized electronic components such as in the fabrication of components such as in the fabrication of computer chips and integrated circuits. Generally in this process, a thin coating of film of photo resist composition is first applied to a substrate material such as silicon wafers. Now 2,4-dinitro-1-naphthol is one among the composition of a light sensitive positive photo resist material increases it efficiency [3]. Considering the above aspects give a complete description of the molecular geometry and molecular vibrations of its derivative known as 2,4-dinitro-1-naphthol

Experimental details

Pure chemical of 2,4-dinitro-1-naphthol was obtained from Lancaster Chemical Company, UK and used as such without any further purification.

The FTIR spectrum of the title compound was recorded in the region 4000 – 400 cm-1 using KBr. The BRUCKER IFS 66 V model FTIR spectrometer was used for the spectral measurements. The golbar and mercury arc sources.

The FT-Raman spectrum was recorded on a BRUCKER IFS 66V model interferometer equipped with an FRA-106 FT-Raman accessory. The spectrum was recorded in the region 3500- 50 cm-1 using the 1064 nm line on a Nd;YAG laser for excitation operating a 200 mW power. The frequencies of all the sharp bands are accurate to ±1 cm.

Computational details

Theoretically the vibrational wave numbers of the compound were calculated in order to provide data for making a complete vibrational assignments and to give additional information with regard to the structural characteristics and the normal vibrational modes of 2,4-Dinitro-1-naphthol, the restricted DFT-B3LYP correlation functional calculations have been performed with Gaussian (03) [4] program package adopting the standard 6-31+G basis set. The Cartesian representation of the theoretical force constants have been computed at optimized geometry by assuming Cs point group symmetry. Scaling of the force field was performed according to the SQM procedure [5,6] using selective scaling in the natural internal coordinate representation [7,8]. Transformations of the force field and subsequent normal coordinate analysis including

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the least square refinement of the scaling factors, are calculated. The Force constants, Reduced Mass, IR intensities obtained from the same basis set.

Result and Discussions
Molecular geometry

The molecular structure of the said molecule is shown in Fig 1.

The global minimum energy obtained by the DFT structure optimization for 2,4-dinitro-1-naphthol is calculated as -869.82373165 using B3LYP/6-31+G. The calculated optimized geometrical parameters obtained in this study are presented in Table 1.
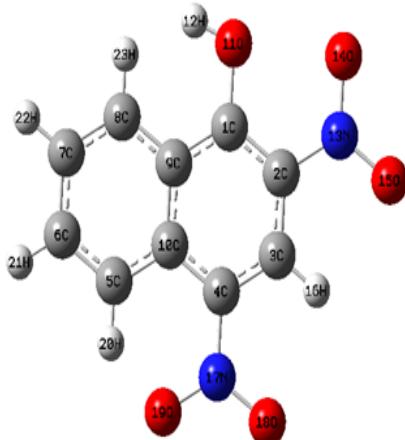
Fig. 1

Table 1– Optimized geometrical parameters of 2,4-dinitro -1- naphthol

Bond length	Value (A°)	Bond angle	Value (A°)
$C_1 - C_2$	1.40140	$C_1 - C_2 - C_3$	120.00002
$C_2 - C_3$	1.40140	$C_2 - C_3 - C_4$	119.99998
$C_3 - C_4$	1.40140	$C_3 - C_4 - C_{10}$	120.00003
$C_4 - C_{10}$	1.40140	$C_4 - C_{10} - C_9$	119.99999
$C_{10} - C_9$	1.40140	$C_{10} - C_9 - C_1$	119.99999
$C_9 - C_1$	1.40140	$C_9 - C_1 - C_2$	119.99999
$C_5 - C_6$	1.40140	$C_5 - C_6 - C_7$	119.99993
$C_6 - C_7$	1.40140	$C_6 - C_7 - C_8$	120.00004
$C_7 - C_8$	1.40140	$C_7 - C_8 - C_9$	120.00000
$C_8 - C_9$	1.40140	$C_8 - C_9 - C_{10}$	120.00002
$C_{10} - C_5$	1.40140	$C_9 - C_{10} - C_5$	119.99994
$C_1 - O_{11}$	1.43000	$C_{10} - C_5 - C_6$	120.00007
$O_{11} - H_{12}$	0.96000	$C_9 - C_1 - O_{11}$	120.00001
$C_2 - N_{13}$	1.47000	$C_2 - C_1 - O_{11}$	120.00000
$N_{13} - O_{14}$	1.36000	$C_1 - O_{11} - H_{12}$	109.47118
$N_{13} - O_{15}$	1.36000	$C_1 - C_2 - N_{13}$	120.00003

$C_3 - H_{16}$	1.07000	$C_3 - C_2 - N_{13}$	119.99995
$N_{17} - O_{18}$	1.36000	$C_2 - N_{13} - O_{14}$	119.99993
$N_{17} - O_{19}$	1.36000	$C_2 - N_{13} - O_{15}$	120.00003
$C_5 - H_{20}$	1.07000	$O_{14} - N_{13} - O_{15}$	120.00004
$C_6 - H_{21}$	1.07000	$C_2 - C_3 - H_{16}$	120.00001
$C_7 - H_{22}$	1.07000	$C_4 - C_3 - H_{16}$	120.00001
$C_8 - H_{23}$	1.07000	$C_3 - C_4 - N_{17}$	120.00001
$C_4 - N_{17}$	1.47000	$C_{10} - C_4 - N_{17}$	119.99996
		$C_4 - N_{17} - O_{18}$	120.00004
		$C_4 - N_{17} - O_{19}$	120.00000
		$O_{18} - N_{17} - O_{19}$	119.99996
		$C_4 - C_{10} - C_5$	120.00007
		$C_{10} - C_5 - H_{20}$	119.99995
		$C_6 - C_5 - H_{20}$	119.99998
		$C_5 - C_6 - H_{21}$	120.00006
		$H_{21} - C_6 - C_7$	120.00001
		$C_6 - C_7 - H_{22}$	119.99997
		$H_{22} - C_7 - C_8$	119.99999
		$C_7 - C_8 - H_{23}$	119.99999
		$H_{23} - C_8 - C_9$	120.00002
		$C_8 - C_9 - C_1$	119.99999

For numbering of an atom refer Fig. 1

Table 2 – Definition of internal co-ordinates of 2,4-dinitro-1- naphthol

No.	Symbol	Type	Definition
Stretching			
1 – 5	a_i	C - H	$C_3 - H_{16}$, $C_5 - H_{20}$, $C_6 - H_{21}$, $C_7 - H_{22}$, $C_8 - H_{23}$
6 - 16	b_i	C - C	$C_1 - C_2$, $C_2 - C_3$, $C_3 - C_4$, $C_4 - C_{10}$, $C_{10} - C_9$, $C_9 - C_1$
			$C_{10} - C_5$, $C_5 - C_6$, $C_6 - C_7$, $C_7 - C_8$, $C_8 - C_9$
17,18	c_i	C - N	$C_2 - N_{13}$, $C_4 - N_{17}$
19	d_i	C - O	$C_1 - O_{11}$
20	e_i	O - H	$O_{11} - H_{12}$
21 - 24	f_i	N - O	$N_{13} - O_{14}$, $N_{13} - O_{15}$, $N_{17} - O_{18}$, $N_{17} - O_{19}$
In-plane bending			
25 - 30	β_i	Ring 1	$C_1 - C_2 - C_3$, $C_2 - C_3 - C_4$, $C_3 - C_4 - C_5$,
			$C_4 - C_5 - C_6$, $C_5 - C_6 - C_1$, $C_6 - C_1 - C_2$

31 - 36	β_i	Ring 2	$C_{10} - C_5 - C_6$, $C_5 - C_6 - C_7$, $C_6 - C_7 - C_8$,
			$C_7 - C_8 - C_9$, $C_8 - C_9 - C_{10}$, $C_9 - C_{10} - C_5$
37 - 46	α_i	b C - H	$C_2 - C_3 - H_{16}$, $C_4 - C_3 - H_{16}$, $C_6 - C_5 - H_{20}$,
			$C_{10} - C_5 - H_{20}$, $C_5 - C_6 - H_{21}$, $C_7 - C_6 - H_{21}$,
			$C_6 - C_7 - H_{22}$, $C_8 - C_7 - H_{22}$, $C_7 - C_8 - H_{23}$,
			$C_9 - C_8 - H_{23}$,
47, 48	γ_i	b C - O	$C_2 - C_1 - O_{11}$, $C_9 - C_1 - O_{11}$
49 - 52	π_i	b C - N	$C_1 - C_2 - N_{13}$, $C_3 - C_2 - N_{13}$, $C_3 - C_4 - N_{17}$,
			$C_{10} - C_4 - N_{17}$,
53 - 56	ϕ_i	b N - O	$C_2 - N_{13} - O_{14}$, $C_2 - N_{13} - O_{15}$, $C_4 - N_{17} - O_{18}$,
			$C_4 - N_{17} - O_{19}$,
57, 58	σ_i	O - N - O	$O_{14} - N_{13} - O_{15}$, $O_{18} - N_{17} - O_{19}$
59	ε_i	C - O - H	$C_1 - O_{11} - H_{12}$
Out-of-plane bending			
60 - 64	ω_i	C - H	$H_{16} - C_3 - C_2 - C_4$, $H_{20} - C_5 - C_6 - C_{10}$
			$H_{21} - C_6 - C_5 - C_7$, $H_{22} - C_7 - C_6 - C_8$
			$H_{23} - C_8 - C_7 - C_9$
65, 66	ρ_i	C - N	$N_{13} - C_2 - C_3 - C_1$, $N_{17} - C_4 - C_3 - C_{10}$
67	χ_i	C - O	$O_{11} - C_1 - C_2 - C_9$
68	ω_i	C – O - H	$H_{12} - O_{11} - C_1 - C_2 (C_9)$
Torsion			
69 - 74	τ_i	Ring 1	$C_1 - C_2 - C_3 - C_4$, $C_2 - C_3 - C_4 - C_5$,
			$C_3 - C_4 - C_{10} - C_9$, $C_4 - C_{10} - C_9 - C_1$,
			$C_{10} - C_9 - C_1 - C_2$, $C_9 - C_1 - C_2 - C_3$
75 - 80	τ_i	Ring 2	$C_{10} - C_5 - C_6 - C_7$, $C_5 - C_6 - C_7 - C_8$,
			$C_6 - C_7 - C_8 - C_9$, $C_7 - C_8 - C_9 - C_{10}$,
			$C_8 - C_9 - C_{10} - C_5$, $C_9 - C_{10} - C_5 - C_6$
81,82	τ_i	NO_2	$C_2 - N_{13} - O_{14} - O_{15}$, $C_4 - N_{17} - O_{18} - O_{19}$,
83,84	T_i	Butterfly	$C_5 - C_{10} - C_9 - C_1$, $C_4 - C_{10} - C_9 - C_8$

For numbering of an atom refer Fig. 1

Table 3 - Definition of local symmetry co-ordinates of 2,4-dinitro-1-naphthol

No.	Symbol	Definition
1 – 5	CH	a_1, a_2, a_3, a_4, a_5
6 - 16	CC	$b_6, b_7, b_8, b_9, b_{10}, b_{11}, b_{12}, b_{13}, b_{14}, b_{15}, b_{16}$
17,18	CN	c_{17}, c_{18}
19	CO	d_{19}
20-22	NO$_2$ ss	$(f_{21} + f_{22}) / \sqrt{2}$, $(f_{23} + f_{24})/ \sqrt{2}$
23 - 24	NO$_2$ ass	$(f_{21} - f_{22}) / \sqrt{2}$, $(f_{23} - f_{24})/ \sqrt{2}$
25	R$_1$ trigd	$(\beta_{25} - \beta_{26} + \beta_2 - \beta_{28} + \beta_{29} - \beta_{30})/ \sqrt{6}$
26	R$_1$ symd	$(-\beta_{25} - \beta_{26} + 2\beta_2 - \beta_{28} - \beta_{29} + 2\beta_{30})/ \sqrt{12}$
27	R$_1$ asymd	$(\beta_{25} - \beta_{26} + \beta_{28} - \beta_{29})/ 2$
28	R$_2$ trigd	$(\beta_{31} - \beta_{32} + \beta_{33} - \beta_{34} + \beta_{35} - \beta_{36})/ \sqrt{6}$
29	R$_2$ symd	$(-\beta_{31} - \beta_{32} + 2\beta_{33} - \beta_{34} + \beta_{35} - 2\beta_{36})/ \sqrt{2}$
30	R$_2$ asymd	$(\beta_{31} - \beta_{32} + \beta_{34} - \beta_{35})/ \sqrt{2}$
31 - 35	bCH	$(\alpha_{37} - \alpha_{38})/ \sqrt{2}$, $(\alpha_{39} - \alpha_{40})/ \sqrt{2}$, $(\alpha_{41} - \alpha_{42})/ \sqrt{2}$ $(\alpha_{43} - \alpha_{44})/ \sqrt{2}$, $(\alpha_{45} - \alpha_{46})/ \sqrt{2}$
36	bCO	$(\rho_{47} - \rho_{48})/ \sqrt{2}$
37,38	b CN	$(\theta_{49} - \theta_{50})/ \sqrt{2}$, $(\theta_{51} - \theta_{52})/ \sqrt{2}$
39, 40	NO$_2$ twist	$(\psi_{53} + \psi_{54})/ \sqrt{2}$, $(\psi_{55} + \psi_{56})/ \sqrt{2}$
41,42	NO$_2$ rock	$(\psi_{53} - \psi_{54})/ \sqrt{2}$, $(\psi_{55} - \psi_{56})/ \sqrt{2}$
43,44	NO$_2$ sciss	$(2\psi_{56} - \psi_{53} - \psi_{54})/ \sqrt{6}$
45	b OH	π_{57}
46 - 50	ωCH	$\varepsilon_{60}, \varepsilon_{61}, \varepsilon_{62}, \varepsilon_{63}, \varepsilon_{64}$
51,52	ωCN	$\varepsilon_{65}, \varepsilon_{66}$
53	ωCO	ε_{67}
54	ωOH	ε_{68}
55	t R$_1$ trigd	$(\tau_{69} - \tau_{70} + \tau_{71} - \tau_{72} + \tau_{73} - \tau_{74}) / \sqrt{6}$
56	t R$_1$ symd	$(\tau_{69} - \tau_{71} + \tau_{72} - \tau_{74}) / \sqrt{2}$
57	t R$_1$ asymd	$(-\tau_{69} + 2\tau_{70} - \tau_{71} - \tau_{72} + 2\tau_{73} - \tau_{74}) / \sqrt{6}$
58	t R$_2$ trigd	$(\tau_{75} - \tau_{76} + \tau_{77} - \tau_{78} + \tau_{79} - \tau_{80}) / \sqrt{6}$
59	t R$_2$ symd	$(\tau_{75} - \tau_{77} + \tau_{78} - \tau_{80}) / \sqrt{2}$
60	t R$_2$ asymd	$(-\tau_{75} + 2\tau_{76} - \tau_{77} - \tau_{78} + 2\tau_{79} - \tau_{80}) / \sqrt{6}$
61,62	NO$_2$ wag	τ_{81}, τ_{82}
63	Butterfly	$(\tau_{83} - \tau_{84}) / \sqrt{2}$

Vibrational spectra

The 2,4-Dinitro-1-naphthol compound consists of 23 atoms and its 63 normal modes are distributed amongst the symmetry species as

$\overline{3N}$ - 6 = 43 A' (in-plane) + 20 A" (out-of-plane). All the vibrations are active both in the Raman scattering and infrared absorption. The molecular

belongs to Cs point group symmetry. The detailed vibrational assignment of fundamental modes of 2,4-dinitro-1-naphthol along with the calculated IR and Raman frequencies and normal mode descriptions are reported in table 4. The FTIR and FT Raman spectra of the 2,4-dinitro-1-naphthol are shown in Figs. 2 and 3.

Fig. 2. – FT-IR Spectrum of 2,4-dinitro-1- napthal
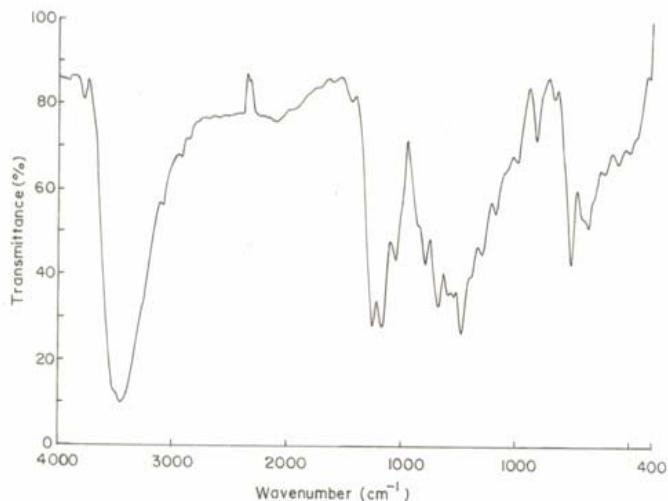
Fig. 3. - FT-Raman Spectrum of 2,4-dinitro-1- napthal
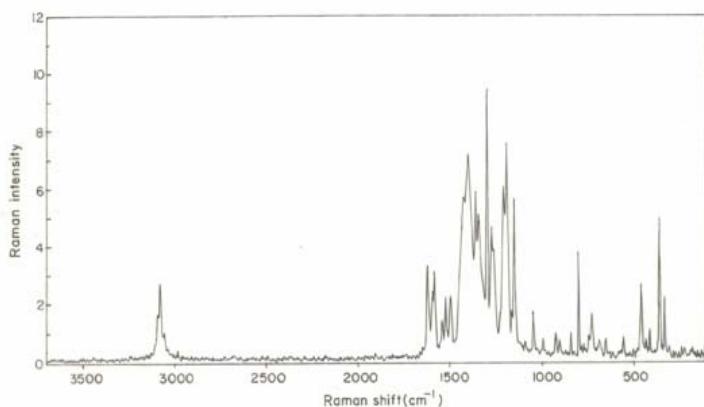
Table 4. Assignment of fundamental vibrational of 2,4-dinitro-1-napthal by normal mode analysis based on SQM force field calculations using selectively scaled B3LYP/6-31+G

Symmetry species	Observed frequencies (cm^{-1})		Calculated frequencies (cm^{-1}) (Unscaled)	Scaling frequency (cm^{-1})	Reduced mass (AMU)	Force constant (mDyne/A)	IR intensity (KM/Mole)	Assignment
	FTIR	FT-Raman						
A'	3448(s)	-	3723	3451	1.0670	8.7128	212.2790	ν OH
A'	3110(w)	-	3381	3111	1.0914	7.3512	26.7864	ν CH
A'	-	3085(s)	3376	3088	1.0960	7.3612	12.4446	ν CH
A'	-	3059(w)	3366	3055	1.0927	7.2958	14.1617	ν CH
A'	2995(w)	-	3355	2997	1.0890	7.2218	21.0146	ν CH

A'	2975(w)	-	3349	2973	1.0890	7.1948	47.7083	ν CH
A'	1721(w)	-	1692	1719	7.1431	12.0450	151.9195	ν CC
A'	1629(m)	-	1655	1633	8.5693	13.8364	133.6828	ν CC
A'	-	1624(vs)	1609	1624	4.9267	7.5175	15.2291	ν CC
A'	-	1595(w)	1596	1592	4.5714	6.8649	38.0951	ν CC
A'	-	1588(vs)	1516	1590	7.9378	10.7505	149.9477	ν CC
A'	1583(m)	-	1495	1581	2.4798	3.2673	30.5704	ν CC
A'	-	1545(s)	1479	1549	2.2102	2.8494	28.6024	ν CC
A'	1528(m)	-	1433	1530	4.0015	4.8417	1.0238	ν CC
A'	-	1523(s)	1409	1523	4.7305	5.5348	36.2628	ν CC
A'	-	1498(s)	1348	1501	1.6183	1.7333	1.0033	ν CC
A'	1479(vw)	-	1267	1471	1.7207	1.6275	83.3881	ν CC
A'	-	1413(w)	1231	1417	2.6278	2.3460	4.8467	NO_2 ass
A'	-	1399(s)	1218	1393	1.2910	1.1275	11.0366	NO_2 ass
A'	1394(m)	-	1179	1397	1.6091	1.3179	12.0818	ν CN
A'	-	1361(vs)	1169	1361	1.7335	1.3954	52.9841	ν CN
A'	-	1344(s)	1106	1340	3.2654	2.3545	112.7925	ν CO
A'	1338(ms)	-	1070	1335	3.5449	2.3924	80.3020	NO_2 ss
A'	-	1298(vs)	1022	1300	1.4717	0.9063	3.2544	NO_2 ss
A'	1275(w)	1276(s)	1022	1277	6.8818	4.2362	709.9662	b OH
A'	1237(ms)	-	993	1230	7.5830	4.4097	320.8951	b CH
A'	-	1210(s)	988	1214	1.4758	0.8490	2.8191	b CH
A'	-	1192(vs)	985	1190	8.2636	4.7258	33.7176	b CH
A'	1150(w)	-	965	1153	11.0609	6.0664	92.7770	b CH
A'	-	1155(vs)	945	1157	1.5758	0.8325	19.7553	b CH
A'	1089(w)	1088(vw)	918	1088	6.4733	3.2171	19.8840	R_1 trigd
A'	-	1048(s)	884	1047	1.5242	0.7013	0.0520	R_1 symd
A'	997(w)	997(m)	869	997	5.9934	2.6668	30.0872	R_1 asymd
A'	-	961(vw)	778	963	3.2887	1.1722	8.2527	R_2 trigd
A'	-	926(ms)	752	923	3.7771	1.2575	18.2160	R_2 symd
A'	911(ms)	-	752	908	6.4745	2.1546	8.1375	R_2 asymd
A'	-	842(ms)	726	840	2.9455	0.9140	41.9310	b CN
A'	836(w)	-	711	831	9.1221	2.7141	98.2158	b CN
A'	-	799(vs)	705	800	4.9839	1.4588	0.1869	NO_2 sciss
A'	759(s)	-	686	754	10.1026	2.8031	9.7151	NO_2 sciss
A'	-	735(vw)	668	730	4.3052	1.1304	8.2566	b CO
A'	-	729(s)	647	721	6.0231	1.4861	0.0910	NO_2 rock
A'	-	705(vw)	627	710	10.4130	2.4129	2.3227	NO_2 rock
A"	-	779(vw)	613	773	8.6205	1.9115	4.1075	ω CH
A"	705(vw)	705(w)	582	707	2.9528	0.5883	9.5177	ω CH
A"	688(w)	-	506	695	8.4264	1.2694	14.2347	ω CH
A"	-	654(m)	470	650	3.3633	0.4381	1.1650	ω CH
A"	-	648(vw)	446	649	9.6516	1.1309	5.6315	ω CH
A"	-	640(vw)	422	645	8.7582	0.9183	9.6979	NO_2 wag

A"	625(vw)	-	413	624	2.9952	0.3014	0.9753	NO₂ wag
A"	-	559(m)	405	562	9.1876	0.8891	6.9293	t R₁ trigd
A"	553(w)	-	389	550	11.3741	1.0138	4.0932	t R₁ symd
A"	-	540(vw)	383	547	7.7552	0.6707	0.0948	t R₁ asymd
A"	-	526(vw)	334	524	1.5842	0.1039	92.7760	t R₂ trigd
A"	504(vw)	-	323	500	10.2525	0.6312	0.2072	t R₂ symd
A"	-	480(vw)	279	486	6.5621	0.3014	5.8757	t R₂ asymd
A"	460(vw)	460(vs)	235	462	4.5789	0.1494	8.8618	ω CN
A"	-	430(w)	211	425	12.1565	0.3203	3.9246	ω CN
A"	416(vw)	414(ms)	196	415	10.6853	0.2425	1.0934	ω CO
A"	-	359(vs)	191	356	8.0191	0.1717	14.1284	ω OH
A"	-	331(s)	152	330	4.2527	0.0576	6.4911	NO₂ twist
A"	-	286(w)	-104	288	3.6520	0.0231	33.7774	NO₂ twist
A"	-	184(vw)	-161	180	4.1943	0.0644	8.6364	Butter fly

O-H vibrations

The précised position of the O-H bond is dependent on the strength of the hydrogen bond. In same samples, intra molecular hydrogen bonding may occur, the resulting hydroxyl group band which appears at 3590 – 3400 cm⁻¹ being sharp and unaffected by concentration changes [9]. Accordingly in 2,4-dinitro-1-naphthol, the IR band observed at 3448 cm⁻¹ is assigned to O-H stretching vibration.

C-H vibrations

The heteroaromatic structure shows the presence of C-H stretching vibrations in the region 3000 – 3100 cm⁻¹which is the characteristic region for the ready identification of C-H stretching vibrations [10]. Accordingly in the present study the C-H vibrations of the title compound are observed at 2995 and 2975 cm⁻¹ in the FTIR spectrum and 3085, 3059 cm⁻¹ in the FT Raman spectrum.

C-C vibrations

The carbon-carbon stretching vibrations [11,12] of the 2,4-Dinitro-1-naphthol are observed at 1721, 1629, 1583, 1528 and 1479 cm⁻¹ in FTIR and 1624, 1595, 1588, 1545, 1523, and 1498 cm⁻¹ in FT Raman. The in-plane and out-of plane bending vibrations of carbon-carbon group are presented in table 4. These assignments are good agreement with the literature [13, 14].

C-N vibrations

The identification of C-N stretching frequency is a very difficult task, since the mixing of bands is possible in this region. Hence the FTIR bands observed at 1394cm⁻¹ and the Raman bands at 1361cm⁻¹ in 2,4-dinitro-1-naphthol are assigned to C-N stretching modes of vibrations are presented in table 4.

Nitro group vibrations

For molecules with an NO₂ group, the NO₂ asymmetric stretching vibration band range is 1625-1540cm⁻¹ and that of the symmetric stretching vibration is 1400-1360cm⁻¹ [15]. The FT-Raman bands observed at 1413 and 1399cm⁻¹ have been assigned to NO₂ asymmetric stretching vibrations. The IR and Raman bands observed at 1338 and 1298cm⁻¹ have been assigned to NO₂ symmetric stretching vibrations respectively.

Conclusion

The vibrational properties of have been 2,4 dinitro-1-naphthal investigated by FTIR and FT-Raman spectroscopic analysis were performed according to the SQM force field method based on DFT calculations at B3LYP/6-31+G level. The assignments of the most of the fundamentals of 2,4-dinitro-1-naphthal provided in this work are quit comparable and unambiguous. The results confirm the ability of the methodology applied for interpretation of the vibrational spectra of the 2,4-dinitro-1-naphthal.

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