

Vibrational Analysis (Experimental & Ab initio Computation) of 2-ethylnaphthalene

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Abstract—The compound under investigation 2-ethylnaphthalene (2EN) has wide applications in the biological, pharmaceutical and industrial processes and hence a complete vibrational analysis of 2EN have been carried out using HF and DFT methods (B3LYP) with 6-311++G and 6-311+G (d, p) basis sets using Gaussian 09W program package. The room temperature Fourier transform IR and Raman spectra of title compound were experimentally recorded and all the observed vibrational frequencies were completely assigned based on the abinitio computational results and earlier assignments published on similar compounds and all the assignments agrees well with the literature values. The calculated frequencies were corrected for the assumptions made in the computational work by employing multiple scale factors. After scaling the simulated spectra obtained from calculation exhibits good similarity with the recorded spectra which validates the accuracy of the work. Along with complete vibrational analysis, thermo-dynamical properties and Mullikan charge distribution were also reported for the first time.

Keywords; FTIR, FT Raman, Gaussian09, 2-ethylnaphthalene, DFT, HF, Vibrational assignment, thermo-dynamical properties.

I. INTRODUCTION

Naphthalene and its derivatives are of diverse importance as intermediates for agriculture, construction, pharmaceutical, photographic, rubber, tanning and textile chemicals [1]. Among the derivatives of naphthalene, the study of 2-ethylnaphthalene (2EN) has received a great deal of attention because of its possible carcinogenic and mutagenic properties [2]. 2EN is a photo fluorescence substance which undergoes vigorous reaction with strong oxidizing agents, sometimes, amounting to explosions [3]. Since the density of this colorless liquid is high, its volatility and flammability are low; it is a good scintillator [4]. Its fluorescence decay-time measurement is used to study the intra-micelle properties [5]. Moreover, 2EN is a starting material for the preparation of number of organic compounds like 2-naphthalylacetonitrile, naphthalen-2-ethanol, 2-naphthylaceticacid, 2-acetonaphthone, and naphthalene sulfonates [3].

On account of its interesting properties and wide industrial applications, the study of vibrational spectra of 2EN is desirable which may be valuable in understanding structural characteristics and chemical properties. Many authors [6-10] have studied the vibrational analysis of substituted naphthalene compounds and in particular Andrea Alparone et al [11] reported the vibrational study of 1-ethylnaphthalene and 2-ethylnaphthalene to study their polluting nature and also to distinguish these isomers, but they have not used experimental spectra to validate their studies. Our literature survey reveals that combined computational and experimental studies have not been carried out so far for the title compound. Hence the goal of the present study is to record the vibrational spectra and carry out the quantum chemical computation of 2-ethyl naphthalene and give a complete description of the molecular geometry, geometrical parameters, normal modes of vibrations, dipole moment, rotational constants, atomic charges and thermodynamic parameters of the title molecule.

II. EXPERIMENTAL SECTION

The fine sample of 2-ethylnaphthalene, provided by the Sigma Aldrich Chemical Co. (USA), with a stated purity of greater than 98%, was used as such for the spectral measurements. The room temperature a Fourier transform IR spectrum of the title compound was measured in 3700-100 cm^{-1} region at a resolution of $\pm 2 \text{ cm}^{-1}$ using Bruker IFS -66V Fourier transform spectrometer. The FT-Raman spectrum of 2EP was recorded on the same instrument equipped with an FRA-106 FT-Raman accessory. The spectrum was recorded in the 3700-100 cm^{-1} with Nd: YAG laser operating at 200 mW power. The reported wave numbers are expected to be accurate within $\pm 2 \text{ cm}^{-1}$.

III. COMPUTATIONAL DETAILS

Using the version 8 of Gaussian 09W (revision B.01) program [12], the HF and DFT calculation of the title compound was carried out on Intel Core2Duo/2.20 GHz processor. The Becke-3-Lee-Yang-Parr (B3LYP) functional

[13, 14] were used to carry out both the HF and DFT analysis with the standard 6-311+G and 6-311+G (d,p) basis sets. The normal coordinate analysis of the title compound has been computed at the fully optimized geometry by assuming C_s point-group symmetry. The simulated IR and Raman spectra were drawn using pure Lorentzian band shapes with the band width of 10 cm^{-1} employing the Gabedit Version 2.32 [15]. The Gauss view 05 graphical interface [16] for Gaussian program was employed to visualize vibrational modes of the title compound and to check whether the mode was pure or mixed and hence for the proper assignment of the vibrations; bands of the title compound. The idea of using multiple scale factors found in the literature [17] and recent studies [18, 19] had been adopted for this study and it minimized the deviation between the computed and the experimental frequencies. Most of the scale factors were much closer to the unity in the case of DFT studies which implies that DFT-B3LYP computations yield results much closer to the experimental values and as expected, when compared to DFT, the scale factors to HF study deviate markedly from unity.

IV. RESULTS AND DISCUSSION

A. Molecular geometry

This molecule belongs to C_s point group with 66 modes as it has 24 atoms and the optimized molecular geometry of 2EN obtained by the DFT computational analysis is shown in Fig. 1. The optimized geometrical parameters of 2EN are presented in Table 1 and in the title compound C1–C2, C3–C4, C5–C6 and C7–C8 bond lengths are found to be about 1.36 \AA and this is also established by X-ray diffraction [13]. The C9–C10, C8–C9, C7–C6 and C10–C5 bond lengths are found to be 1.43, 1.42, 1.42 and 1.42 \AA and they are found to be consistent with values shown by David et al [14]. The calculated C–C bond lengths (in C2–C11 and in C11–C12) in this study are found to be 1.517 and 1.529 \AA respectively which are consistent with the values shown in the earlier literature [15]. The ring CH bonds lengths show little discrepancies with experimental data and moreover all the six CH bond lengths in ethyl group are found to be identical but X-ray diffraction study shows variation. These discrepancies may be mainly because ab initio computations are carried out for a isolated molecule. The inner bond angles [C1–C2–C11] is found to be 125° and outer bond angle [C3–C2–C11] are found to be 116° where the ethyl group is attached to the ring and show deviations from ideal 120° . This may be mainly due to the electron donating nature of ethyl group on the naphthalene ring and hence the hexagonal ring may be distorted [16]. However, the carbon–carbon bond length is not distorted because of any much deviation in their values both in IR and Raman.

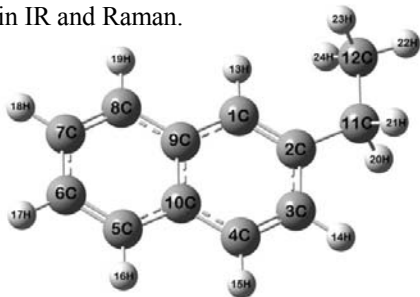


Figure 1. Structure of 2-ethylnaphthalene

B. Assignment of spectra

The FTIR and FT Raman spectra of 2-ethyl naphthalene are shown in Fig.2 and 3 respectively. Table 2 lists the wave numbers of the bands observed in FTIR and FT Raman spectra of the title compound, the scaled and unscaled theoretical frequencies and infrared and Raman intensities computed by DFT-B3LYP/6311+G (d, p) of the title compound.

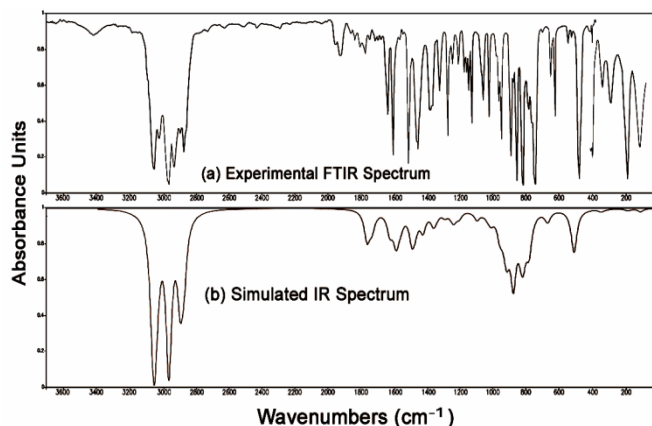


Figure 2. Comparison of observed and simulated Infrared spectra of 2-ethylnaphthalene.

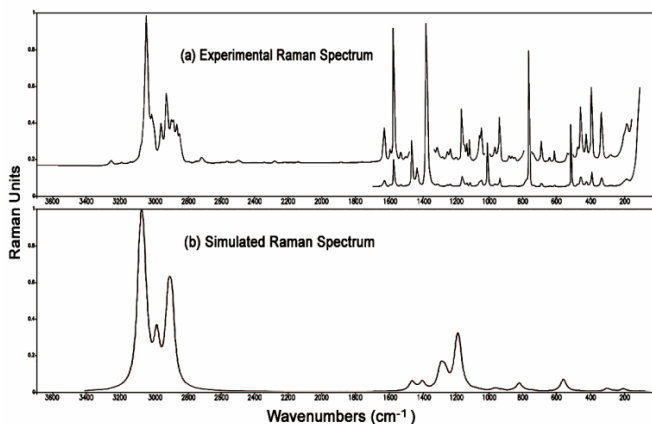


Figure 3. Comparison of observed and simulated Raman spectra of 2-ethylnaphthalene

TABLE I. OPTIMIZED GEOMETRICAL PARAMETERS OF 2EP OBTAINED BY DFT AND HF/6-311+G (d,p) BASIS SETS.

Parameters	HF	DFT (B3LYP)	Experimental Data (Ref)
	6-311+G(d,p)	6-311+G(d,p)	
Bond length (Å)			
C2 - C3	1.4268	1.4243	1.41
C1 - C2	1.3588	1.3764	1.377
C2 - C11	1.5163	1.5170	1.422
C3 - C4	1.3541	1.3708	
C3 - H14	1.0768	1.0860	1.098

C4 - C10	1.4223	1.4207	1.421	A(2,11,12)	116.5725	116.6226
C4 - H15	1.0762	1.0854	1.095	A(2,11,20)	107.9942	108.0890
C10 - C5	1.4177	1.4183		A(2,11,21)	107.9941	108.0890
C9 - C10	1.4048	1.4284		A(12,11,20)	108.9963	109.0981
C5 - C6	1.3599	1.3753		A(12,11,21)	108.9963	109.0982
C5 - H16	1.0762	1.0853		A(20,11,21)	105.7554	105.2479
C6 - C7	1.4145	1.4142		A(11,12,22)	109.8436	110.2026
C6 - H16	1.0754	1.0842		A(11,12,23)	111.6567	111.6747
C7 - C8	1.3601	1.3754		A(11,12,24)	111.6566	111.6748
C7 - H18	1.0755	1.0843		A(22,12,23)	107.6636	107.5732
C8 - C9	1.4186	1.4193		A(22,12,24)	107.6637	107.5732
C8 - H19	1.0761	1.0853		A(23,12,24)	108.1902	107.9591
C1 - C9	1.4246	1.4222				
C1 - H13	1.0745	1.0842				
C11 - C12	1.5256	1.5290				
C11 - H20	1.0883	1.0972				
C11 - H21	1.0883	1.0972				
C12 - H22	1.0855	1.0928				
C12 - H23	1.0858	1.0935				
C12 - H24	1.0858	1.0935				
Bond angle (°)						
A(1,2,3)	118.2627	118.2570				
A(3,2,11)	117.6561	118.1835				
A(1,2,11)	124.0812	123.5595				
A(2,3,4)	121.5441	121.5934				
A(2,3,14)	118.7909	118.7826				
A(4,3,14)	119.6650	119.6240				
A(3,4,10)	120.7824	120.8763				
A(3,4,15)	120.2189	120.2273				
A(10,4,15)	118.9986	118.8964				
A(4,10,5)	122.3593	122.6382				
A(4,10,9)	118.3392	118.2423				
A(5,10,9)	119.3015	119.1194				
A(10,5,6)	120.6922	120.7957				
A(10,5,16)	118.9606	118.8247				
A(6,5,16)	120.3472	120.3796				
A(5,6,7)	120.0855	120.1634				
A(5,6,17)	120.2818	120.1690				
A(7,6,17)	119.6327	119.6676				
A(6,7,8)	120.3186	120.3405				
A(6,7,18)	119.5454	119.6061				
A(8,7,18)	120.1361	120.0534				
A(7,8,9)	120.7691	120.8848				
A(7,8,19)	120.2592	120.2789				
A(9,8,19)	118.9717	118.8362				
A(10,9,8)	118.8330	118.6961				
A(10,9,1)	119.3872	119.1969				
A(1,2,11)	121.7797	122.1070				
A(1,2,9)	121.6844	121.8341				
A(2,1,13)	120.6645	120.4573				
A(9,1,13)	117.6510	117.7086				

It may be noted that the calculated vibrational frequencies are consistent with the experimental results after scaling and correlation graph between the scaled calculated and observed results for 2EN is shown in Fig.4.

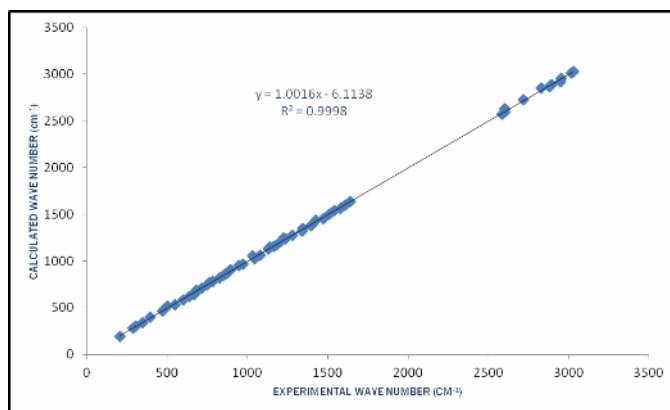


Figure 4: The correlation diagram for the calculated and the experimental frequencies of 2-ethylnaphthalene.

C. Ethyl Group Vibrations

In the title compound, ethyl group is present at the second position of the ring as a substituent, it is an alkane residue consisting of methyl and methylene groups, the general appearance of alkane residues in organic molecules may be seen in the infrared and Raman spectra and hence the vibrations due to both are discussed below.

D. Methyl Group Vibrations

The methyl group can exhibit the following types of vibrations: symmetric and asymmetric stretching, symmetric and asymmetric scissoring, twisting, wagging and rocking [24]. The CH stretching in CH₃ occurs at lower frequencies than those of aromatic ring (3100–300 cm⁻¹) [25]. In the title molecule the asymmetric stretching modes of CH₃ have been observed at 2850 and 2720 cm⁻¹ in FTR and in FTIR it is seen at 2726 cm⁻¹. The symmetrical stretching band of CH₃ is observed at 2628 cm⁻¹ and no corresponding peak is found in FTR. These assignments found support from the normal modes of animation option of Gauss view 05 which indicates theoretical three peaks at 2829, 2719 and 2603 cm⁻¹ as the corresponding frequencies. For methyl substituted aromatic

ring the asymmetric deformation of CH₃ is usually observed at around 1460 cm⁻¹ [26]. In line with the values reported in literature [27], a very strong asymmetric deformation band has been identified in 2EP at 1506 cm⁻¹ and the corresponding

TABLE II. EXPERIMENTAL AND CALCULATED FREQUENCIES, IR & RAMAN INTENSITIES AND ASSIGNMENTS FOR 2-ETHYLNAPHTHALENE.

Mode of Vibration	Experimental Frequency ^a		Calculated frequency(cm ⁻¹) B3LYP-6-311+G(d,p)				Vibrational Assignment ^b		
	IR	Raman	Unscaled	Scaled	IR Intensity	Raman Activity			
1	3030	vs	3038	vs	3187	3028	21.83	351.08	v _s CH
2	3015	s	3015	m	3176	3018	18.56	80.42	v _s CH
3	2955	vs	2960	m	3174	2952	23.25	94.96	v _{as} CH
4	2922	vs	2928	s	3169	2947	20.73	165.29	v _{as} CH
5	2890	s	2896	m	3161	2892	0.02	101.62	v _s CH
6			2884	m	3156	2888	3.05	7.44	v _{as} CH
7	2864	vs	2864	m	3149	2882	6.78	64.58	v _{as} CH
8			2850	m	3092	2829	40.45	146.15	v _{as} CH (CH ₃)
9	2726	w	2720	w	3090	2719	33.38	24.98	v _{as} CH (CH ₃)
10	2628	w			3027	2603	23.38	158.44	v _s CH (CH ₃)
11			2591	w	3024	2601	11.83	111.64	v _{as} CH (CH ₂)
12	2569	w	2571		3005	2584	25.24	259.41	v _s CH (CH ₂)
13	1634	s	1633	m	1671	1638	13.84	34.54	v CC
14	1602	vs	1596	m	1643	1610	8.06	3.21	v CC
15	1566	w	1578	vs	1610	1578	0.35	31.97	v CC
16	1544	w	1532	w	1541	1541	9.58	0.61	v CC
17	1506	vs	1507	w	1509	1509	6.62	12.43	δ _{as} CH ₃ + vCC
18	1456	vs	1468	m	1502	1472	0.23	57.07	v CC
19			1434	m	1501	1426	8.53	9.25	δ _{as} CH ₂
20			1395	vs	1480	1406	4.54	47.95	δ _s CH ₃
21	1378	s	1384	vs	1468	1394	0.70	16.47	δ _s CH ₂
22	1351	s			1415	1344	10.10	2.67	β CH + δ _s CH ₃
23	1322	m	1315	m	1409	1339	4.00	120.56	β CH
24	1275	s	1285	w	1398	1279	2.26	20.09	β CH + δ _s CH ₂ + δ _s CH ₃
25	1244	m	1253	w	1393	1226	3.31	107.19	β CH
26			1235	m	1351	1237	9.02	3.73	v C- CH ₂ + β CH
27	1207	m	1203	w	1300	1209	0.05	4.01	β CH
28	1175	m	1171	m	1291	1181	6.35	0.14	β CH
29	1156	m			1272	1164	1.74	1.97	β CH
30	1148	m	1141	m	1226	1140	2.60	0.71	γ CH
31	1127	s	1123	m	1188	1129	1.32	6.48	γ CH + C-CH ₃
32	1059	m	1061	m	1177	1077	2.73	1.28	γ CH + β CC
33			1054	m	1171	1031	2.02	3.36	γ CH + β CC
34	1022	s	1020	m	1143	1046	3.14	3.78	ρ CH ₃ +βCC
35	964	m	972	m	1106	973	0.01	0.25	□CH ₂ + □CH ₃
36	949	s	944	m	1078	948	0.18	2.31	□CH ₂ + □CH ₃
37	904	vs			1042	896	4.06	29.73	γ CH + β CC
38			891	w	1007	886	0.34	3.23	v CCC
39	879	m			997	877	0.00	0.13	γ CH+βCC
40			863	w	983	865	1.57	0.17	R asymd
41	847	vs	849	w	967	851	1.62	1.37	γ CH
42	817	vs			960	825	3.12	2.05	R symd
43	784	s			911	783	9.76	0.79	γ CH
44			765	vs	888	764	3.17	0.15	v CCC
45	746	vs			872	750	17.82	0.37	R symd
46	709	w			833	717	31.60	0.16	γ CH
47			688	m	791	680	9.79	0.24	t CH ₂ + t CH ₃
48	659	m			783	673	0.02	45.86	R asymd
49			640	w	777	668	16.91	0.02	R symd

50	622	s	620	w	744	640	16.99	1.10	R symd
51	584	w			696	599	0.06	2.17	γ CCC
52	532	w			640	550	1.66	0.03	ω CH ₂ + ω CH ₃
53			516	m	636	500	3.64	0.72	t Rasym
54	477	vs	478	m	526	481	0.03	11.54	t Rasym
55			462	m	516	472	0.09	0.05	γ CH+□CC
56					486		0.09	2.53	γ C-CH ₂ -CH ₃
57			427	m	486	427	20.74	0.01	γ C-CH ₂ -CH ₃
58	397	w	400	s	431	394	0.07	9.78	δ C-CH ₃
59	337	m	341	m	403	347	0.21	1.27	ρ CH ₃
60	301	m			331	303	1.35	2.06	γ CCC
61			283	w	302	287	0.25	0.03	t CH ₃
62	189	m	188	m	241	208	0.00	0.08	t CH ₃
63	115	m			180		0.85	0.01	t Rasym
64					169		0.25	1.03	t Rasym
65					106		1.61	1.40	t Et
66					37		0.02	1.81	t Et

a vs – very strong; s – strong; m – medium; w – weak;

b ν_{as} – asymmetric stretching; ν_s – symmetric stretching; δ – scissoring; ρ – rocking; τ – torsion; t – twisting; β – in-plane bending; γ – out-of-plane bending;

symd – symmetric deformation, Et – ethyl group

theoretical value is 1509 cm⁻¹ and very strong symmetric deformation peak is found at 1395 cm⁻¹ in FTIR and the DFT counterpart is found to be at 1406 cm⁻¹. The strong peaks found at 1022 and 337 cm⁻¹ in FTIR and peaks at 1020 and 341 cm⁻¹ in FT Raman are assigned to CH₃ in-plane rocking modes. The bands at 964 and 949 cm⁻¹ are assigned to CH₃ out-of-plane bending vibrations while the frequencies at 283 and 189 cm⁻¹ are assigned to CH₃ twisting modes and the torsion modes of CH₃ have been identified at 169 and 106 cm⁻¹ with the help of Gauss view. The C-CH₃ stretching mode is identified at 1127 cm⁻¹ which is consistent with the identification made in the literature [28].

E. Methylene Group Vibrations

For the assignments of CH₂ group frequencies, basically six fundamentals can be associated, namely, symmetric stretch, anti-symmetric stretch, scissoring and rocking which belongs to in-plane vibrations and in addition to that, wagging and twisting modes of CH₂ groups would be expected for out-of-plane symmetry species [25]. According to the literature [29] CH₂ asymmetric and symmetric vibrations are usually observed between 2850-3000 cm⁻¹ and in line with the literature the CH₂ asymmetric vibrations are observed in Raman spectra at 2591 cm⁻¹. The symmetric stretching modes have been identified at 2569 cm⁻¹ in FTIR and 2571 cm⁻¹ in FTR. These values are less than expected but correctness of these assignments have been ascertained by Gauss view and supported by the DFT computation values at 2601 and 2584 cm⁻¹. The scissoring band in the spectra of hydrocarbons occurs at nearly constant positions near 1465 cm⁻¹ [7] and in the title molecule it is established at 1434 cm⁻¹ and the rocking vibration is seen in FTIR and FTR at 1384 and 1378 cm⁻¹ respectively. The methylene twisting and wagging vibrations are observed at 688 and 532 cm⁻¹ in Raman and IR respectively. These bands are generally appreciably weaker than those resulting from methylene scissoring [25, 30].

F. C-C Vibrations

The C-C aromatic stretching vibrations give rise to characteristic bands in both the IR and Raman spectra, covering the spectral range from 1600–1400 cm⁻¹ [31]. The IR bands at 1634, 1602, 1566, 1544 and 1456 cm⁻¹ and the corresponding Raman bands at 1633, 1596, 1578, 1532 and 1468 cm⁻¹ are assigned to C-C stretching vibrations. Among these bands, 1634, 1602 and 1566 cm⁻¹ in IR and 1578 cm⁻¹ in Raman are characteristically strong. The corresponding computed peaks observed at 1638, 1610, 1578, 1541 and 1472 cm⁻¹ are in excellent agreement with experimental values. The C-C-C in-plane bending vibrations have given rise to weak bands across the low frequency region, that is to say, below 1000 cm⁻¹ [32] and in line with this, the IR bands at 1059, 1022, 904 and 879 cm⁻¹ and Raman band at 1054 cm⁻¹ in 2EN have been assigned to C-C in-plane bending vibrations [33,34]. The out-of-plane bending vibrations are observed at 584, 462 and 283 cm⁻¹.

G. C-H Vibrations

There are seven hydrogen atoms that are attached to the ring carbons. The C-H stretching modes usually appear with the strong Raman intensity and are highly polarized [25]. The C-H stretching vibrations of benzene derivatives generally appear in the region 3100-3000 cm⁻¹ and they give rise to multiple bands [35]. The very strong peaks observed at 3038, 3015 and 2896 cm⁻¹ in FTIR and the Raman bands at 3038, 3015 and 2896 cm⁻¹ are assigned to CH symmetric stretching vibrations. The corresponding DFT values are at 3028, 3018 and 2892 cm⁻¹. The asymmetric stretching vibrations are observed at 2955, 2922 and 2864 cm⁻¹ in FTIR and FTRaman bands are seen at 2960, 2928, 2884 and 2864 cm⁻¹. The scaled DFT values are 2952, 2947, 2888 and 2882 cm⁻¹. Both the above assignments are in excellent agreement with experimental values. The bands due to CH in-plane deformation occurs in the region 1300-1000 cm⁻¹ and it is found that the bands are sharp but are weak-medium intensity in the FTIR and they are observed at 1351, 1322, 1275, 1244, 1207, 1175 and 1156 cm⁻¹. The frequencies of CH out-of-plane

deformation vibrations are not very much affected by the nature of the substituent and they are generally seen in the region 1000 - 650 cm^{-1} [36] which is identified at 1059,904,879,847,784 and 709 cm^{-1} in the IR spectrum. The frequencies at 1061, 1054, 849 and 462 cm^{-1} are assigned to the Raman bands. The scaled vibrational frequencies due to the DFT calculations are established at 1077, 1031, 896, 877, 851,783 and 717 cm^{-1} and these assignments find support from the literature [11, 37].

V. MULLIKEN CHARGES

The calculation of partial atomic charges is helpful for qualitative understanding of the structure and reactivity of molecules. The electron distribution in 2EP is compared in two different quantum mechanical methods and the sensitivity of the calculated charges to change with the choice of methods is reported. The calculated Mulliken charges at different levels are listed in Table 3.

TABLE III. MULLIKEN ATOMIC CHARGES OF 2-ETHYLNAPHTHALENE FOR DFT AND HF WITH 6-311+G(d,p) BASIS SET

Atom with IUPAC Numbering	DFT 6-311+G(d,p)	HF 6-311+G(d,p)
C1	-0.722161	-0.571384
C2	0.970879	0.777607
C3	-0.164621	-0.101337
C4	-0.044151	-0.00511
C5	-0.099327	-0.133609
C6	-0.313551	-0.26314
C7	-0.326685	-0.31022
C8	-0.198025	-0.236681
C9	-0.289615	-0.25057
C10	0.657165	0.548061
C11	-0.534627	-0.501071
C12	-0.537781	-0.555046
H13	0.128564	0.118678
H14	0.126739	0.119677
H15	0.125825	0.117517
H16	0.124999	0.11705
H17	0.131261	0.124082
H18	0.131318	0.124032
H19	0.123627	0.115813
H20	0.156432	0.166463
H21	0.156431	0.166468
H22	0.135061	0.145716
H23	0.131121	0.143504
H24	0.131122	0.143502

VI. THERMODYNAMIC PROPERTIES

On the basis of vibrational analysis at B3LYP/ 6311+G (d, p) and HF/6311+G (d,p) methods, several thermodynamic parameters are calculated and are presented in Table 4. The total energy, zero point vibration energy (ZPVE), entropy, rotational constants, thermal energy and molar heat capacity are calculated to the extent of accuracy and the vibrations in ZPVE seem to be insignificant. The total energy and the change in the total entropy at room temperature at different methods do have notable change. As expected, computations made by DFT/B3LYP method yield a low value of -464.6394865au whereas the HF computations yield a higher value of -461.5270241au. This difference may be mainly attributed to the more approximations that are implemented in the HF than in DFT calculations. From Table 4, it is clear that

as the rotational temperature increases, there is a change in rotational constant values. The total energies are found to decrease with the increase of the basis set dimension. The rotational constant and rotational temperature values are very high when calculated in HF than in B3LYP.

TABLE IV. THEORETICALLY COMPUTED DIPOLE MOMENT (DEBYE), ENERGY(AU), ZERO POINT VIBRATIONAL ENERGY (KCAL MOL⁻¹), ENTROPY (CAL MOL⁻¹K⁻¹), ROTATIONAL TEMPERATURE (KELVIN), ROTATIONAL CONSTANT (GHZ), THERMAL ENERGY (KCAL/MOL) AND MOLAR CAPACITY AT CONSTANT VOLUME (CAL/MOL-KELVIN) OF 2-ETHYLNAPHTHALENE.

Parameters	B3LYP-6-311+G(d,p)	HF-6-311+G(d,p)
Dipole moment	0.6833	0.6378
Total energy	-64.6394865	-461.5270241
Zero point energy	127.21907	135.57638
Entropy		
Total	97.871	94.774
Translational	41.045	41.045
Rotational	30.577	30.551
Vibrational	26.248	23.178
Rotational temperature		
Total	0.10708	0.10842
Translational	0.0292	0.02939
Rotational	0.02308	0.02326
Vibrational		
Rotational constants		
Total	2.23114	2.25917
Translational	0.60842	0.61244
Rotational	0.48088	0.48466
Vibrational		
Thermal Energy		
Total	133.405	141.337
Translational	0.889	0.889
Rotational	0.889	0.889
Vibrational	131.628	139.56
Molar capacity at constant volume		
Total	39.777	36.69
Translational	2.981	2.981
Rotational	2.981	2.981
Vibrational	33.815	30.729

The tables for the frequencies calculated by all methods (DFT and HF) and basis sets [6311++G and 6311+G(d,p)] are not presented but are available on request from the authors.

VII. CONCLUSION

Comparison of the wave numbers calculated with the DFT method using 6-311+G (d, p) basis set with experimental values reveals that the B3LYP method shows very good agreement with experimental observation due to inclusion of electron correlation in this method. The assignment of fundamental modes of the title compound were carried out by comparison between calculated and experimental results using modeling programs like Gauss view and Gabedit animation. The observed and simulated spectra are found to be well comparable.

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