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Vibrational spectroscopic study of 2, 6- and 2, 7-dimethylnaphthalenes by Density functional theory.

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ABSTRACT

Fourier transform infrared and Fourier transform Raman spectra of 2, 6- and 2, 7-dimethylnaphthalenes in solid phase, have been investigated. The theoretical calculations of the vibrations of 2, 6- and 2, 7-dimethylnaphthalenes were performed by using density functional theory (DFT)-Beck3–Lee–Yang–Parr (B3LYP) levels with 6-31G* and 6-311+G** basis sets. The complete assignments are performed on the basis of the potential energy distribution (PED) of the vibrational modes, calculated with scaled quantum mechanics method (SQM) by using MOLVIB program. The computational frequencies are in good agreement with the observed results. The comparisons between the observed and calculated frequencies are shown.

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Introduction:

Diesel fuels contain alkyl polycyclic aromatic hydrocarbons including methylnaphthalenes (MNs) and dimethylnaphthalenes (DMNs)[1,2]. These exhibit persistent toxicity and are carcinogenic and mutagenic pollutants due to their chemical stability and resistance to biodegradation process. It is well established that the carcinogenic activity of PAH's and their methyl derivatives is due to the products in sequence of oxidative metabolic reactions.

Theoretical infrared spectra of methyl substitution [3] have been reported. The infrared spectra of 1, 5- , 1, 6- , and 2, 6- dimethylnaphthalenes in the gas phase were reported by Prasanta Das et.al[4] but full normal mode analysis and assignment of frequencies with PED were not reported

As part of the research Programme in our laboratory, we have taken up the theoretical and experimental studies of a number of substituted naphthalenes using Infrared absorption and Raman scattering and the Gaussian Programme coupled with MOLVIB. The author investigated the vibrational spectra of one of the isomers 2, 3-, 2, 6- and 2, 7-dimethylnaphthalenes (theoretical and experimental) and assigned the experimental frequencies to the different modes ─ (author's private communication). The present paper reports the experimental and theoretical calculations of the vibrational frequencies of 2, 6- and 2, 7-dimethylnaphthalenes.

The FT-IR and FT-Raman spectra are recorded for the identification of the vibrational frequencies of 2, 6- and 2, 7-dimethylnaphthalenes. The theoretical prediction of all the vibrational frequencies based on the DFT calculation at B3LYP/6-31G* and B3LYP/6-311+G** is carried out. The frequencies which could not be identified from the spectral investigations could be well predicted and modes determined on the basis of DFT calculations coupled with MOLVIB program[5,6,7]. The experimental results, the calculated values and the final assignments of all the vibrational frequencies of the molecule are presented in detail.

Experimental:

The molecules 2, 6- and 2, 7-dimethylnaphthalenes (solid) were purchased from Sigma – Aldrich chemical company, USA and used as such without purification to get the spectral measurements. For the IR spectral measurements, the spectra were recorded over the range of 4000-450 cm^{-1} (fig-1) at a resolution of $1cm^{-1}$ using Perkin Elmer spectrum RX1 spectrometer equipped with He-Ne laser source, KBr beam splitter and $LiTaO_3$ detector .the sample for this measurement was finely grinded and mixed with KBr. This mixture was then pressed under vacuum at high pressure to obtain a transparent disc which was then placed in sample compartment of the spectrometer.

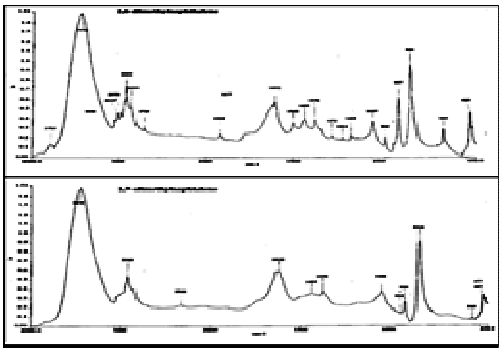

Fig1: FT-Infrared spectra of 2,6- and 2,7-dimethylnaphthalenes(experimental).

A Bruker IFS-66v FT-Raman model Interferometer equipped with FRA 106 Raman module was used as an accessory for the FT-Raman spectral recordings. The instrument with a resolution ~2-3cm^{-1} and multitasking OPUS software on a PC/AT 486 computer was used for processes of signal averaging, signal enhancement and also base line correction. An air cooled diode pumped Nd-YAG laser operated at 1064nm with the laser output maintained at 200mW was used for Raman spectral measurements. The Raman spectrum was recorded in the range 3500-100cm^{-1}(fig-2).

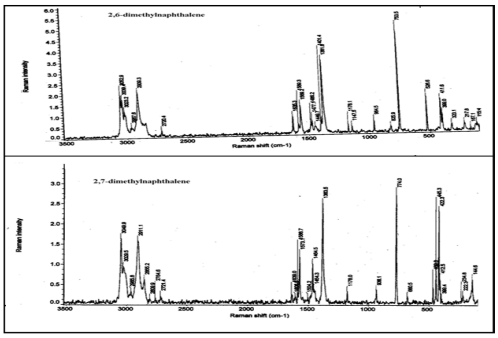

Fig2: FT-Raman spectra of 2,6- and 2,7-dimethylnaphthalenes(experimental).

The FT-Raman spectrum was recorded at CECRI, KaraiKudi, Tamil Nadu. And the FT-IR spectral measurements were carried out at Sophisticated Analytical instrumentation Facilities (SAIF), IIT, Chennai.

Computational details:

Computational calculations were performed at the DFT levels of theory using the two basis sets 6-31G* and 6-311+G**. The Geometry optimization calculations are carried out using the electronic structure package GAUSSIAN 03[8] on the personal computer. In these DFT calculations, we use B3LYP levels of theory where density functional theory the exchange functional -B3- corresponds to Beck-3- parameter and correlation functional – LYP – corresponds to Lee – Yang – Parr.

We have considered Cs symmetry for 2, 6- and 2, 7-dimethylnaphthalenes; this model was visualized using Gaussian View Programme[9]. The Cartesian representation of the theoretical force constants have been computed at optimized geometries by assuming Cs symmetry by using B3LYP combined with the standard basis sets 6-31G* and 6-311+G**. At the optimized structure of the examined species, no imaginary wave number modes were obtained, a true minimum on the potential surface was found.

In order to get the normal modes in a molecular coordinate system, a set of internal and local symmetry coordinates(shown in tables 5,6,7 and 8) for the 2, 6- and 2, 7-dimethylnaphthalenes were defined as recommended by Fogarasi and Pulay[10, 11]. Scaling of force field was performed according to the SQM procedure[12, 13] using selective scaling procedure in the natural internal coordinates representation[10,11], the calculation of the PED and prediction of IR intensities were done on our PC with MOLVIB program (Version 7.0-G77), written by Tom Sundius[5,6,7]. The Raman activity (S_i) calculated by Gaussian 03 and adjusted during scaling procedure with MOLVIB were converted to relative Raman intensity (I_i) using the following relation from the basic theory of Raman scattering[14, 15]

$$I_i = \frac{f(\nu_o - \nu_i)^4 S_i}{\nu_i[1 - \exp(-hc\nu_i/KT)]}$$

Here ν_o is the exciting frequency (in cm^{-1} units); ν_i is the vibrational wave number of the normal mode; h,c,k are the universal constants and f is suitably chosen common normalization factor for all the intensities.

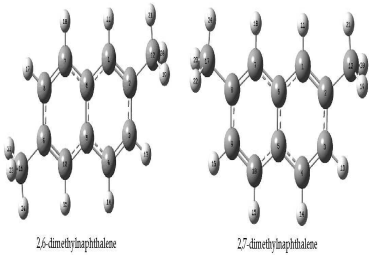

Fig3: Molecular structure and labeling of atoms of molecules.

The labeling of atoms of the molecules of 2, 6- and 2, 7-dimethylnaphthalenes are shown in fig-3. Finally the scaled and unscaled frequencies of 2, 6- and 2, 7-dimethylnaphthalenes are shown in table-8 and 9 respectively. The experimental values of the frequencies obtained in the Raman and infrared absorption spectra are thus compared with the assigned frequencies (see tables 10 and 11) and also the observed and calculated frequencies of 2, 6- and 2, 7-dimethylnaphthalenes are shown in table(tables-12 and 13).

Geometry optimization:

The molecules of 2, 6- and 2, 7-dimethylnaphthalenes consist of 24 atoms of each, and have 66 Fundamentals of vibrational modes. Their molecular structures have not been studied by any diffraction technique. We have taken into account one symmetry depending on the conformation of the CH_3 groups. On the basis of C_s symmetry, the 66 fundamental vibrations of 2, 6- and 2, 7-dimethylnaphthalenes of each can be distributed as $43A'+23A''$.The Calculated energies for 2, 6- and 2, 7-dimethylnaphthalenes, determined by DFT method at B3LYP/6-31G* and B3LYP/6-311+G** basis sets are presented in Table-1. The geometrical optimized parameters are presented table-2 and 3

Table1: Total energies of 2, 6- dimethylnaphthalene and 2, 7-dimethylnaphthalene (in hartrees).

Basis set	Total energy (in Hartees)	
	2,6-dimethylnaphthalene	2,7-dimethylnaphthalene
B3LYP/6-31G*	-464.326447	-464.326487
B3LYP/6-311+G**	-464.443367	-464.443466

Results & Discussion:

2,6 – dimethylnaphthalene and 2,7 – dimethylnaphthalene molecules of each are expected to have 6 CH stretching, 6 CH in plane bending(bCH), 6 CH out of plane bending(gCH), 2 CC in plane bending (bCC), 2 CC out of plane bending(gCC), 6 Ring in plane bending(deformation) , 11 CC stretching, 6 ring torsion vibrations(deformation),6 – CH_3 stretching (2-CH_3ss,2-CH_3ips,2- CH_3ops), 10 CH_3 bending (2- CH_3sb, 2-CH_3ipb,2- CH_3opb, 2- CH_3ipr, 2- CH_3opr), 2 CH_3 torsion (tCH3), 1 butterfly, 2 CC_{me} stretching vibrations(total of 66 modes).

1. Vibrational analysis of 2, 6 – dimethylnaphthalene:

Out of the 6 CH stretching frequencies three are fairly strong in Raman spectrum at 3052, 3039, and 3023cm-1, whereas two are observed in IR as 3050 and 3017 cm-1. These are agreeing well with the calculated and assigned frequencies. The sixth frequency at 3033 could be only predicted.

Table-2: The geometrical optimized parameters of 2, 6-dimethylnaphthalene

Parameter	B3LYP/6-31G*	B3LYP/6-311+G**
Bond lengths		
C1-C2	1.3791	1.3770
C2-C3	1.4349	1.4336
C3-C4	1.3791	1.3771
C4-C5	1.4197	1.4185
C5-C6	1.4298	1.4272
C6-C7	1.4202	1.4192
C7-C8	1.3774	1.3752
C8-C9	1.4165	1.4149
C5-C10	1.4202	1.4192
C1-H11	1.0886	1.0862
C2-C12	1.5101	1.5089
C3-H13	1.5102	1.5089
C4-H14	1.0886	1.0862
C10-H15	1.0878	1.0853
C9-C16	1.0868	1.0843
C8-H17	1.0868	1.0843
C7-H18	1.0878	1.0853
C12-H19	1.0978	1.0951
C12-H20	1.0978	1.0951
C12-H21	1.0941	1.0913
C16-H22	1.0978	1.0951
C16-H23	1.0978	1.0951
C16-H24	1.0941	1.0913
Bond angles		
C1-C2-C3	119.2184	119.2158
C2-C3-C4	119.2331	119.2276
C3-C4-C5	122.3427	122.3437
C4-C5-C6	118.4241	118.4333
C5-C6-C7	118.9612	118.9596
C6-C7-C8	120.7695	120.7692
C7-C8-C9	120.2713	120.2714
C6-C5-C10	118.9578	118.9556
C2-C1-H11	119.3739	119.3813
C3-C2-C12	120.3436	120.3576
C4-C3-H13	120.4455	120.4291
C3-C4-H14	119.3822	119.3877
C5-C10-H15	118.7919	118.8813
C8-C9-C16	119.6296	119.6196
C9-C8-H17	119.6282	119.6200
C6-C7-H18	118.7908	118.8783
C2-C12-H19	111.7567	111.6250
C2-C12-H20	111.7567	111.6250
C2-C12-H21	111.0474	110.9400
C9-C16-H22	111.7694	111.6164
C9-C16-H23	111.7694	111.6164
C9-C16-H24	111.016	110.9533

All the six CH in plane bending frequencies could be observed either from IR absorption or from Raman studies. All the Raman lines at 1147, 1178 and 1381 cm-1 are strong while the IR absorption at 1165, 1182, 1214, and 1245 cm-1 are weak. It is noticed that the calculated frequencies and assigned to these modes are 1147, 1164, 1191, 1209, 1261cm-1 are coupled with the CC stretching modes. There are two more frequencies 1303 and1377 which can be considered to represent bCH mode

on the basis of PED, while one of them at 1303 has got a combination with 20% of R1trid and 13% of CC. whereas the other at 1377 has next contribution as 20% of CC similar to the other bCH assigned vibrations. The frequency 1377 is assigned to CH in plane bending frequency which is observed in Raman spectrum at 1381.while 1303 frequency may be considered more for R1trid rather than bCH.This is only a probable suggestion.

Table-3: The geometrical optimized parameters of 2, 7-dimethylnaphthalene.

Parameter	B3LYP/6-31G*	B3LYP/6-311+G**
Bond lengths		
C1-C2	1.3800	1.3777
C2-C3	1.4234	1.4218
C3-C4	1.3750	1.3729
C4-C5	1.4203	1.4189
C5-C6	1.4301	1.4273
C6-C7	1.4211	1.4203
C7-C8	1.3799	1.3776
C8-C9	1.4235	1.4219
C5-C10	1.4204	1.4191
C1-H11	1.0886	1.0862
C2-C12	1.5099	1.5085
C3-H13	1.0879	1.0856
C4-H14	1.0879	1.0854
C10-H15	1.0879	1.0854
C9-H16	1.0879	1.0856
C8-C17	1.5099	1.5085
C7-H18	1.0886	1.0862
C12-H19	1.0977	1.0949
C12-H20	1.0977	1.0949
C12-H21	1.0945	1.0917
C17-H22	1.0977	1.0949
C17-H23	1.0977	1.0949
C17-H24	1.0945	1.0917
Bond angles		
C1-C2-C3	118.5475	118.5473
C2-C3-C4	121.2059	121.2136
C3-C4-C5	120.9056	120.9046
C4-C5-C6	118.5675	118.5653
C5-C6-C7	118.8775	118.8846
C6-C7-C8	121.8955	121.8840
C7-C8-C9	118.5480	118.5476
C6-C5-C10	118.5669	118.5647
C2-C1-H11	119.725	119.7304
C3-C2-C12	119.8164	119.7435
C4-C3-H13	119.8079	119.7478
C3-C4-H14	120.2678	120.2024
C5-C10-H15	118.8196	118.8857
C8-C9-H16	118.9788	119.0307
C9-C8-C17	119.8073	119.7342
C6-C7-H18	118.3749	118.3809
C2-C12-H19	111.3535	111.1587
C2-C12-H20	111.3535	111.1587
C2-C12-H21	111.47 00	111.4222
C8-C17-H22	111.3522	111.1574
C8-C17-H23	111.3522	111.1574
C8-C17-H24	111.4716	111.4237

Table-4: Description of internal coordinates of 2, 6-dimethylnaphthalene.

Symbol	Type	Definition
Stretching		
r_{1-6}	C-H(Aromatic)	C1-H11, C3-H13, C4-H14, C10-H15, C8-H17, C7-H18.
Q_{7-8}	C-C(Methyl)	C2-C12, C9-C16.
Q_{9-19}	C-C(Aromatic)	C1-C2,C2-C3,C3-C4,C4-C5,C5-C6,C6-C1, C6-C7, C7-C8, C8-C9, C9-C10, C10-C5.
r_{20-25}	C-H(Methyl)	C12-H19, C12-H20, C12-H21, C16-H22, C16-H23, C16-H24.
Bending		
β_{26-37}	C-C-H	C2-C1-H11,C6-C1-H11,C5-C4-H14, C4-C3-H13, C2-C3-H13, C3-C4-H14,C9-C10-H15,C5-C10-H15, C7-C8-H17, C9-C8-H17, C6-C7-H18, C8-C7-H18.
γ_{38-41}	C-C-C	C3-C2-C12, C1-C2-C12, C8-C9-C16, C10-C9-C16.
β_{42-47}	C-C-H	C2-C12-H19,C2-C12-H20,C2-C12-H21, C9-C16-H22, C9-C16-H23, C9-C16-H24.
α_{48-53}	H-C-H	H19-C12-H20,H19-C12-H21,H20-C12-H21, H22-C16-H23, H22-C16-H24, H23-C16-H24.
γ_{54-65}	C-C-C(Ring)	C1-C2-C3 , C2-C3-C4, C3-C4-C5 , C4-C5-C6 ,C5-C6-C1, C6-C1-C2, C9-C10-C5,C10-C5-C6, C5-C6-C7,C6-C7-C8, C7-C8-C9, C8-C9-C10.
Out of plane bending ω_{66-71}	H-C-C-C	H11-C1-C2-C6,H13-C3-C4-C2,H14-C4-C5-C3, H15-C10-C5-C9, H17-C8-C9-C7, H18-C7-C8-C6.
Φ_{72-73}	C-C-C-C	C12-C2-C3-C1, C16-C9-C10-C8.
τ_{74-85}	C-C-C-C(Ring)	C1-C2-C3-C4, C2-C3-C4-C5 ,C3-C4-C5-C6, C4-C5-C6-C1, C5-C6-C1-C2, C6-C1-C2-C3, C9-C10-C5-C6,C10-C5-C6-C7, C5-C6-C7-C8, C6-C7-C8-C9, C7-C8-C9-C10, C8-C9-C10-C5.
τ_{86-91}	$C-CH_3$	C3(C1)-C2-C12-H19 ,C3(C1)-C2-C12-H20, C3(C1)-C2-C12-H21, C8 (10)-C9-C16-H22, C8 (10)-C9-C16-H23, C8 (10)-C9-C16-H24.
τ_{92-93}	Butterfly	C4-C5-C6-C7 (C1), C10-C5-C6-C1 (C7).

Table5: Description of internal coordinates of 2, 7-dimethylnaphthalene.

Symbol	Type	Definition
Stretching		
r_{1-6}	C-H(Aromatic)	C1-H11, C3-H13, C4-H14, C10-H15, C9-H16, C7-H18.
Q_{7-8}	C-C(Methyl)	C2-C12, C8-C17.
Q_{9-19}	C-C(Aromatic)	C1-C2,C2-C3,C3-C4,C4-C5,C5-C6,C6-C1, C6-C7, C7-C8, C8-C9, C9-C10, C10-C5.
r_{20-25}	C-H(Methyl)	C12-H19, C12-H20, C12-H21, C17-H22, C17-H23, C17-H24.
Bending		
β_{26-37}	C-C-H	C2-C1-H11,C6-C1-H11,C5-C4-H14, C4-C3-H13, C2-C3-H13, C3-C4-H14,C9-C10-H15,C5-C10-H15, C8-C9-H16, C7-C9-H16, C6-C7-H18, C8-C7-H18.
γ_{38-41}	C-C-C	C3-C2-C12, C1-C2-C12, C7-C8-C17, C9-C8-C17.
β_{42-47}	C-C-H	C2-C12-H19,C2-C12-H20,C2-C12-H21, C8-C17-H22, C8-C17-H23, C8-C17-H24.
α_{48-53}	H-C-H	H19-C12-H20,H19-C12-H21,H20-C12-H21, H22-C17-H23, H22-C17-H24, H23-C17-H24.
γ_{54-65}	C-C-C(Ring)	C1-C2-C3 , C2-C3-C4, C3-C4-C5 , C4-C5-C6 ,C5-C6-C1, C6-C1-C2, C9-C10-C5,C10-C5-C6, C5-C6-C7,C6-C7-C8, C7-C8-C9, C8-C9-C10.
Out of plane bending		
ω_{66-71}	H-C-C-C	H11-C1-C2-C6,H13-C3-C4-C2,H14-C4-C5-C3, H15-C10-C5-C9, H16-C9-C10-C8, H18-C7-C8-C6.
Φ_{72-73}	C-C-C-C	C12-C2-C3-C1, C17-C8-C9-C7.
τ_{74-85}	C-C-C-C(Ring)	C1-C2-C3-C4, C2-C3-C4-C5 ,C3-C4-C5-C6, C4-C5-C6-C1, C5-C6-C1-C2, C6-C1-C2-C3, C9-C10-C5-C6,C10-C5-C6-C7, C5-C6-C7-C8, C6-C7-C8-C9, C7-C8-C9-C10, C8-C9-C10-C5.
τ_{86-91}	C-CH_3	C3(C1)-C2-C12-H19 ,C3(C1)-C2-C12-H20, C3(C1)-C2-C12-H21, C7 (9)-C8-C17-H22, C7 (9)-C8-C17-H23, C7 (9)-C8-C17-H24.
τ_{92-93}	Butterfly	C4-C5-C6-C7 (C1), C10-C5-C6-C1 (C7).

Table 6: Local symmetry coordinates of 2, 6-dimethylnaphthalene

S.NO	Symbol	Definition
1-6	CH	r_1,r_2,r_3,r_4,r_5,r_6.
7-8	CCme	Q_7,Q_8.
9-19	CC	$q_9,q_{10},q_{11},q_{12},q_{13},q_{14},q_{15},q_{16},q_{17},q_{18},q_{19}$.
20-21	CH3ss	$\frac{1}{\sqrt{3}}(r_{20}+r_{21}+r_{22})$, $\frac{1}{\sqrt{3}}(r_{23}+r_{24}+r_{25})$
22-23	CH3ips	$\frac{1}{\sqrt{6}}(2r_{22}-r_{20}-r_{21})$, $\frac{1}{\sqrt{6}}(2r_{25}-r_{23}-r_{24})$.
24-25	CH3ops	$\frac{1}{\sqrt{2}}(r_{20}-r_{21})$, $\frac{1}{\sqrt{2}}(r_{23}-r_{24})$.
26-31	bCH	$\frac{1}{\sqrt{2}}(\beta_{26}-\beta_{27})$, $\frac{1}{\sqrt{2}}(\beta_{28}-\beta_{29})$, $\frac{1}{\sqrt{2}}(\beta_{30}-\beta_{31})$, $\frac{1}{\sqrt{2}}(\beta_{32}-\beta_{33})$, $\frac{1}{\sqrt{2}}(\beta_{34}-\beta_{35})$, $\frac{1}{\sqrt{2}}(\beta_{36}-\beta_{37})$.
32-33	bCC	$\frac{1}{\sqrt{2}}(\gamma_{38}-\gamma_{39})$, $\frac{1}{\sqrt{2}}(\gamma_{40}-\gamma_{41})$.
34-35	CH3sb	$\frac{1}{\sqrt{6}}(-\beta_{42}-\beta_{43}-\beta_{44}+\alpha_{48}+\alpha_{49}+\alpha_{50})$, $\frac{1}{\sqrt{6}}(-\beta_{45}-\beta_{46}-\beta_{47}+\alpha_{51}+\alpha_{52}+\alpha_{53})$.
36-37	CH3ipb	$\frac{1}{\sqrt{6}}(-\alpha_{48}-\alpha_{49}+2\alpha_{50})$, $\frac{1}{\sqrt{6}}(-\alpha_{51}-\alpha_{52}+2\alpha_{53})$.
38-39	CH3opb	$\frac{1}{\sqrt{2}}(\alpha_{48}-\alpha_{49})$, $\frac{1}{\sqrt{2}}(\alpha_{51}-\alpha_{52})$.
40-41	CH3ipr	
42-43	CH3opr	
44-45	Rtrid	$\frac{1}{\sqrt{6}}(-\beta_{42}-\beta_{43}+2\beta_{44})$, $\frac{1}{\sqrt{6}}(-\beta_{45}-\beta_{46}+2\beta_{47})$.
46-47	Rsymd	$\frac{1}{\sqrt{2}}(\beta_{42}-\beta_{43})$, $\frac{1}{\sqrt{2}}(\beta_{45}-\beta_{46})$.
48-49	Rasyd	$\frac{1}{\sqrt{6}}(\gamma_{54}-\gamma_{55}+\gamma_{56}-\gamma_{57}+\gamma_{58}-\gamma_{59})$, $\frac{1}{\sqrt{6}}(\gamma_{60}-\gamma_{61}+\gamma_{62}-\gamma_{63}+\gamma_{64}-\gamma_{65})$.
50-55	gCH	$\frac{1}{\sqrt{6}}(2\gamma_{54}-\gamma_{55}-\gamma_{56}+2\gamma_{57}-\gamma_{58}-\gamma_{59})$, $\frac{1}{\sqrt{6}}(2\gamma_{60}-\gamma_{61}-\gamma_{62}+2\gamma_{63}-\gamma_{64}-\gamma_{65})$.
56-57	gCC	
58-59	tRtrid	$\frac{1}{2}(\gamma_{55}-\gamma_{56}+\gamma_{58}-\gamma_{59})$, $\frac{1}{2}(\gamma_{61}-\gamma_{62}+\gamma_{64}-\gamma_{65})$.
60-61	tRsym	$\omega_{66},\omega_{67},\omega_{68},\omega_{69},\omega_{70},\omega_{71}$.
62-63	tRasy	Φ_{72}, Φ_{73}.
64-65	tCH3	$\frac{1}{\sqrt{6}}(\tau_{74}-\tau_{75}+\tau_{76}-\tau_{77}+\tau_{78}-\tau_{79})$, $\frac{1}{\sqrt{6}}(\tau_{80}-\tau_{81}+\tau_{82}-\tau_{83}+\tau_{84}-\tau_{85})$.
66	tbuterfly	$\frac{1}{\sqrt{6}}(\tau_{74}-\tau_{76}+\tau_{77}-\tau_{79})$, $\frac{1}{\sqrt{6}}(\tau_{80}-\tau_{82}+\tau_{83}-\tau_{85})$. $\frac{1}{\sqrt{6}}(-\tau_{74}+2\tau_{75}-\tau_{76}-\tau_{77}+2\tau_{78}-\tau_{79})$, $\frac{1}{\sqrt{6}}(-\tau_{80}+2\tau_{81}-\tau_{82}-\tau_{83}+2\tau_{84}-\tau_{85})$ $\frac{1}{\sqrt{3}}(\tau_{86}+\tau_{87}+\tau_{88})$, $\frac{1}{\sqrt{3}}(\tau_{89}+\tau_{90}+\tau_{91})$ $\frac{1}{\sqrt{2}}(\tau_{92}-\tau_{93})$.

Table7: Local symmetry coordinates of 2,7-dimethylnaphthalene.

S.NO	Symbol	Definition
1-6	CH	r_1,r_2,r_3,r_4,r_5,r_6.
7-8	CCme	Q_7,Q_8.
9-19	CC	$q_9,q_{10},q_{11},q_{12},q_{13},q_{14},q_{15},q_{16},q_{17},q_{18},q_{19}$.
20-21	CH3ss	$\frac{1}{\sqrt{3}}(r_{20}+r_{21}+r_{22})$, $\frac{1}{\sqrt{3}}(r_{23}+r_{24}+r_{25})$
22-23	CH3ips	$\frac{1}{\sqrt{6}}(2r_{22}-r_{20}-r_{21})$, $\frac{1}{\sqrt{6}}(2r_{25}-r_{23}-r_{24})$.
24-25	CH3ops	$\frac{1}{\sqrt{2}}(r_{20}-r_{21})$, $\frac{1}{\sqrt{2}}(r_{23}-r_{24})$.
26-31	bCH	$\frac{1}{\sqrt{2}}(\beta_{26}-\beta_{27})$, $\frac{1}{\sqrt{2}}(\beta_{28}-\beta_{29})$, $\frac{1}{\sqrt{2}}(\beta_{30}-\beta_{31})$, $\frac{1}{\sqrt{2}}(\beta_{32}-\beta_{33})$, $\frac{1}{\sqrt{2}}(\beta_{34}-\beta_{35})$, $\frac{1}{\sqrt{2}}(\beta_{36}-\beta_{37})$.
32-33	bCC	$\frac{1}{\sqrt{2}}(\gamma_{38}-\gamma_{39})$, $\frac{1}{\sqrt{2}}(\gamma_{40}-\gamma_{41})$.
34-35	CH3sb	$\frac{1}{\sqrt{6}}(-\beta_{42}-\beta_{43}-\beta_{44}+\alpha_{48}+\alpha_{49}+\alpha_{50})$, $\frac{1}{\sqrt{6}}(-\beta_{45}-\beta_{46}-\beta_{47}+\alpha_{51}+\alpha_{52}+\alpha_{53})$.
36-37	CH3ipb	$\frac{1}{\sqrt{6}}(-\alpha_{48}-\alpha_{49}+2\alpha_{50})$, $\frac{1}{\sqrt{6}}(-\alpha_{51}-\alpha_{52}+2\alpha_{53})$.
38-39	CH3opb	$\frac{1}{\sqrt{2}}(\alpha_{48}-\alpha_{49})$, $\frac{1}{\sqrt{2}}(\alpha_{51}-\alpha_{52})$.
40-41	CH3ipr	
42-43	CH3opr	
44-45	Rtrid	$\frac{1}{\sqrt{6}}(-\beta_{42}-\beta_{43}+2\beta_{44})$, $\frac{1}{\sqrt{6}}(-\beta_{45}-\beta_{46}+2\beta_{47})$.
46-47	Rsymd	$\frac{1}{\sqrt{2}}(\beta_{42}-\beta_{43})$, $\frac{1}{\sqrt{2}}(\beta_{45}-\beta_{46})$.
48-49	Rasyd	$\frac{1}{\sqrt{6}}(\gamma_{54}-\gamma_{55}+\gamma_{56}-\gamma_{57}+\gamma_{58}-\gamma_{59})$, $\frac{1}{\sqrt{6}}(\gamma_{60}-\gamma_{61}+\gamma_{62}-\gamma_{63}+\gamma_{64}-\gamma_{65})$.
50-55	gCH	$\frac{1}{\sqrt{6}}(2\gamma_{54}-\gamma_{55}-\gamma_{56}+2\gamma_{57}-\gamma_{58}-\gamma_{59})$, $\frac{1}{\sqrt{6}}(2\gamma_{60}-\gamma_{61}-\gamma_{62}+2\gamma_{63}-\gamma_{64}-\gamma_{65})$.
56-57	gCC	
58-59	tRtrid	$\frac{1}{2}(\gamma_{55}-\gamma_{56}+\gamma_{58}-\gamma_{59})$, $\frac{1}{2}(\gamma_{61}-\gamma_{62}+\gamma_{64}-\gamma_{65})$.
60-61	tRsym	$\omega_{66},\omega_{67},\omega_{68},\omega_{69},\omega_{70},\omega_{71}$.
62-63	tRasy	Φ_{72}, Φ_{73}.
64-65	tCH3	$\frac{1}{\sqrt{6}}(\tau_{74}-\tau_{75}+\tau_{76}-\tau_{77}+\tau_{78}-\tau_{79})$, $\frac{1}{\sqrt{6}}(\tau_{80}-\tau_{81}+\tau_{82}-\tau_{83}+\tau_{84}-\tau_{85})$.
66	tbuterfly	$\frac{1}{\sqrt{6}}(\tau_{74}-\tau_{76}+\tau_{77}-\tau_{79})$, $\frac{1}{\sqrt{6}}(\tau_{80}-\tau_{82}+\tau_{83}-\tau_{85})$. $\frac{1}{\sqrt{6}}(-\tau_{74}+2\tau_{75}-\tau_{76}-\tau_{77}+2\tau_{78}-\tau_{79})$, $\frac{1}{\sqrt{6}}(-\tau_{80}+2\tau_{81}-\tau_{82}-\tau_{83}+2\tau_{84}-\tau_{85})$ $\frac{1}{\sqrt{3}}(\tau_{86}+\tau_{87}+\tau_{88})$, $\frac{1}{\sqrt{3}}(\tau_{89}+\tau_{90}+\tau_{91})$ $\frac{1}{\sqrt{2}}(\tau_{92}-\tau_{93})$.

Table-8: Calculated frequencies (in cm-1) of 2, 6-dimethylnaphthalene

	B3LYP/6-31G*				B3LYP/6-311+G**			
Species	**unscaled**	**scaled**	**IR Intensity**	**Raman Intensity**	**unscaled**	**scaled**	**IR Intensity**	**Raman Intensity**
A"	84	84	1.2229	0	81	83	1.6097	0
A"	98	104	0	0.6711	95	103	0	0.6836
A"	102	107	0	0.0001	100	107	0.0418	0.0001
A"	186	176	0.3925	0	181	170	0.8398	0
A"	207	200	0	2.3857	203	199	0	1.8538
A'	221	215	0.8877	0	222	213	1.1671	0
A'	322	331	0	0.73	323	331	0	1.3256
A"	343	345	2.8968	0	342	347	4.3285	0
A"	407	397	0	3.1192	406	398	0	1.4678
A'	413	406	0	15.506	413	407	0	17.9074
A'	442	441	2.3023	0	444	443	2.4025	0
A"	497	482	5.8984	0	492	483	13.66	0
A'	536	517	0	11.829	536	516	0	12.0439
A"	540	554	0	0.7843	538	553	0	0.6089
A'	591	594	1.2129	0	590	594	1.3026	0
A"	650	632	3.4148	0	650	635	7.4525	0
A'	686	678	1.3694	0	685	676	0.9527	0
A'	768	747	0	33.751	765	745	0	41.626
A"	778	772	0	6.2364	778	774	0	0.0242
A"	812	806	0	4.4252	811	803	0	0.0938
A"	834	827	31.41	0	828	819	40.957	0
A'	843	845	0	3.9505	840	845	0	4.2278
A"	900	892	22.349	0	897	889	30.053	0
A"	910	906	50	5.393	906	899	0.0004	0.465
A'	936	927	0.9745	0	930	928	1.3551	0
A"	967	962	0.9856	0.0002	977	972	0	1.2984
A"	967	972	0.0002	0.7542	979	979	0	12.9781
A'	984	982	0	7.9928	982	983	2.1979	0
A'	1032	1039	0	5.7372	1019	1039	0	2.526
A'	1040	1053	13.829	0	1028	1052	14.429	0
A"	1077	1081	8.5922	0	1063	1080	5.9604	0.0001
A"	1078	1082	0.0004	0.7364	1063	1084	0.0019	0.3389

Table-8(contd..)

	B3LYP/6-31G*				B3LYP/6-311+G**			
Species	**unscaled**	**scaled**	**IR Intensity**	**Raman Intensity**	**unscaled**	**scaled**	**IR Intensity**	**Raman Intensity**
A'	1164	1147	1.846	0	1154	1148	2.8554	0
A'	1184	1164	0	4.4095	1173	1168	0	6.0001
A'	1203	1191	3.9165	0.0001	1187	1190	3.9725	0.0001
A'	1213	1209	0	20.146	1199	1208	0	18.0535
A'	1254	1261	1.0245	0.0003	1239	1260	1.2926	0.0004
A'	1294	1273	0	1.7838	1284	1273	0	1.0063
A'	1302	1303	5.2769	0	1291	1303	4.4926	0
A'	1386	1377	1.7318	0.0001	1370	1376	2.1606	0.0001
A'	1421	1400	0.0018	182.08	1401	1400	0.0011	231.2234
A'	1425	1402	5.5008	0.0563	1405	1402	4.3708	0.0487
A'	1444	1422	1.4759	0.001	1416	1422	0.0006	76.4632
A'	1445	1427	0	136.16	1416	1426	1.1218	0.0486
A'	1451	1467	0	36.531	1432	1466	0	63.3389
A"	1514	1507	10.851	0.0051	1485	1507	14.188	0.0058
A"	1514	1508	40.001	47.153	1485	1508	0.0043	19.082
A'	1517	1525	111.1	0.0004	1488	1525	16.322	0.0001
A'	1527	1530	0	103.07	1499	1530	0	61.2947
A'	1536	1542	0.0003	36.976	1517	1543	0.0004	62.731
A'	1560	1564	11.667	0.0009	1540	1564	15.461	0.0017
A'	1626	1626	0	29.144	1607	1627	0	30.0277
A'	1672	1647	26.048	0.0009	1651	1648	30.923	0.0009
A'	1694	1698	0.0003	70.976	1674	1698	0.0005	60.9136
A'	3039	2722	86.7	0.02	3019	2722	85.937	0.0355
A'	3039	2845	0.003	583.17	3019	2845	0.004	759.2165
A"	3088	2859	1.7225	254.29	3066	2859	1.577	231.5657
A"	3088	2909	43.048	10.168	3066	2909	34.299	10.6393
A'	3125	2967	13.252	79.522	3101	2967	15.821	74.9702
A'	3125	2970	20.072	52.48	3101	2970	18.348	64.6313
A'	3170	3030	12.768	0.244	3150	3030	10.003	0.1691
A'	3170	3031	0.0319	54.226	3151	3031	0.0178	73.2031
A'	3172	3032	40.255	4.1144	3153	3032	3.9543	183.9083
A'	3173	3033	0.907	191.66	3153	3033	33.314	22.0784
A'	3190	3050	62.559	0.0305	3170	3050	48.572	0.0986
A'	3191	3051	0.0046	375.62	3171	3051	0.0108	407.257

Table-9: Calculated frequencies (in cm-1) of 2, 7-dimethylnaphthalene

	B3LYP/6-31G*				B3LYP/6-311+G**			
Species	**unscaled**	**scaled**	**IR Intensity**	**Raman Intensity**	**unscaled**	**scaled**	**IR Intensity**	**Raman Intensity**
A"	89	81	0.012	1.1650	86	81	1.3663	0.0040
A"	97.5	104	0.2464	0.0000	93.4	103	0.0001	0.3550
A"	119.9	115	2.2300	0.5640	117.9	116	1.1619	1.4394
A"	132.8	136	1.6381	0.0000	129.3	138	0.0000	1.1011
A'	218	217	0.5944	0.6020	218.6	215	0.8180	0.7628
A"	282.1	245	0.2265	0.5492	278.1	247	0.5157	0.2359
A"	285.7	273	0.0290	0.0000	281.6	269	0.0000	0.1288
A'	28.8	330	0.0488	1.2663	330.1	326	1.3066	0.1126
A"	418.9	412	3.1490	0.0000	416.1	411	0.0000	1.8391
A'	426.2	416	12.0248	0.8545	425.5	417	0.8059	15.3235
A'	448.5	447	6.5806	0.2268	449.9	447	0.3227	5.6987
A'	472.7	477	7.0410	0.0014	473.7	478	0.0639	7.2673
A"	492.7	495	0.2505	8.8505	485.7	498	19.4731	0.0157
A"	554.4	562	0.5338	3.1616	557.9	562	5.1599	0.0007
A"	645.3	651	0.0760	0.0000	642.4	645	0.0000	0.3569
A'	650.6	660	0.6572	2.0561	649.3	656	1.9762	0.5711
A'	690	690	2.5456	0.7821	688.7	697	0.5541	2.2540
A'	780	778	0.0543	0.0045	777.1	777	0.0549	0.1197
A"	780.3	785	4.9367	1.4111	778.1	785	1.3104	0.0659
A'	790.9	788	37.1534	0.0993	787.4	790	0.0446	46.4644
A"	799	790	4.9974	0.0000	794.6	816	0.0000	0.0270
A"	855.2	836	1.5964	43.0448	850.5	830	59.0301	0.2001
A"	877.3	867	0.2927	0.0000	873.9	858	0.0000	0.2508
A"	921.1	910	4.0043	9.5139	917.1	903	11.7262	0.1273
A'	959.2	940	5.9561	0.1807	951.7	934	0.062	11.7277
A"	960.1	944	0.2436	0.0000	970.5	946	3.0037	0.0184
A"	970	956	0.2433	0.5863	971.2	964	0.0000	1.3124
A'	973.4	986	0.0058	2.2519	983.6	981	1.9259	0.1677
A'	1023.4	1021	0.0697	11.0334	1009.7	1021	10.7663	0.6173
A'	1053.6	1043	8.3633	0.1140	1041.8	1043	0.4279	5.1734
A"	1076.2	1053	0.2731	0.0000	1061.4	1050	0.0000	0.2697
A"	1077.8	1070	0.5992	8.8434	1063.2	1073	6.1175	0.1363
A'	1167.6	1164	4.5802	1.1693	1158	1163	1.7793	6.5152

Table-9 (contd..)

	B3LYP/6-31G*				B3LYP/6-311+G**			
Species	**unscaled**	**scaled**	**IR Intensity**	**Raman Intensity**	**unscaled**	**scaled**	**IR Intensity**	**Raman Intensity**
A'	1187.3	1178	4.0956	1.4282	1173.7	1166	2.0839	2.1748
A'	1207.3	1209	6.1335	3.3555	1195.6	1197	4.2561	8.1389
A'	1210.3	1217	6.1142	1.3656	1196.4	1227	1.5001	4.1035
A'	1243.9	1233	0.6959	0.2361	1228.7	1237	0.0491	0.6092
A'	1290.1	1273	1.4278	0.1122	1279.7	1260	0.0542	0.7332
A'	1302.9	1323	0.1395	4.1455	1291.9	1334	3.1901	0.0309
A'	1383.4	1381	0.2331	0.7910	1366.9	1384	0.7919	1.0703
A'	1421.8	1399	191.7817	0.0343	1402.2	1396	0.0602	240.9676
A'	1423.1	1407	0.7515	5.4439	1403.3	1405	4.7852	1.5222
A'	1443.5	1444	15.2690	1.2587	1415.1	1444	0.3705	4.6119
A'	1444.5	1446	114.0387	0.2369	1415.9	1447	0.7752	87.6255
A'	1466.2	1463	0.0359	0.4717	1446.2	1482	1.5337	0.0120
A'	1506.4	1500	42.9083	6.5896	1483.4	1491	13.4956	34.2850
A"	1513.5	1525	17.9460	0.0052	1485.2	1524	0.0069	8.3258
A"	1513.6	1526	27.8972	10.8414	1485.3	1526	14.2460	10.2433
A'	1527	1552	106.9697	5.4753	1501.1	1552	3.3331	116.0190
A'	1530.3	1575	8.3462	0.2003	1503.8	1577	0.9383	2.2528
A'	1567.7	1584	0.0075	14.8573	1547.8	1585	19.6125	0.2047
A'	1625.1	1607	26.9749	0.0157	1606.6	1616	0.0322	27.6599
A'	1672.3	1650	15.8516	9.8325	1651.4	1641	8.2132	14.0618
A'	1693.2	1692	25.2763	21.9708	1672.5	1689	32.9503	28.0871
A'	3039.1	2856	11.2499	76.5641	3019.4	2856	74.8066	18.0422
A'	3039.4	2868	547.4794	6.5915	3019.7	2868	7.2340	715.0810
A"	3088.7	2910	258.6455	0.4014	3065.8	2910	0.3400	236.8021
A"	3088.7	2933	2.7938	43.8799	3065.9	2933	34.9822	2.4193
A'	3125.3	2965	7.9762	1.5629	3101.6	2965	1.1133	10.5997
A'	3125.3	2978	119.8021	31.4449	3101.7	2978	32.7163	124.8646
A'	3169.2	3038	10.3961	1.4243	3149.8	3038	0.9752	12.8150
A'	3170.8	3039	14.6497	9.7479	3151.2	3040	9.6337	17.1384
A'	3172.4	3041	103.8219	2.3314	3152.5	3041	0.4439	118.5943
A'	3173.6	3042	115.4654	40.7381	3154	3042	36.2056	127.6226
A'	3189.1	3057	68.0044	24.8524	3169.4	3057	17.7136	61.5887
A'	3191.7	3060	318.2322	35.6598	3171.8	3060	29.0081	350.1187

Table-10: Observed and calculated frequencies of 2, 6-dimethylnaphthalene with PED

Experiment		B3LYP/6-31G* (scaled)	PED(%)
IR (cm^{-1})	Raman (cm^{-1})		
-	-	84	Butrfl (19), tR1sym (18), gCH (16), tR2asy (12), tCH3 (12), tR2sym (11)
-	-	104	tCH3 (85), gCC (9)
-	115	107	tCH3 (75), Butrfl (6), tR2asy (5)
-	167	176	tR2asy (29), tR1asy (28), Butrfl (14), gCH (10), tR1sym (8)
-	207	200	R2symd (63), bCC (18), CC (11)
-	217	215	tR1sym (23), gCH (22), gCC (22), tR2asy (8), tR2sym (7), tR2tri (6)
-	323	331	bCC (37), R2symd (25), R1asyd (17), CC (11)
-	343	345	gCC (36), tR1tri (18), tR2tri (16), gCH (12)
-	411	397	tR1asy (49), tR2sym (22), gCH (17)
-	399	406	bCC (62), R1symd (9), R2symd (9), CH3opr (6), CC (5)
457	-	441	R2asyd (31), bCC (22), CC (21), R1asyd (11), CCme (5)
483	-	482	tR2sym (50), Butrfl (23), tR1asy (12), gCH (8)
526	526	517	R1symd (46), CC (17), bCC (16), R1asyd (9), R2symd (5)
548	-	554	gCC (43), tR1sym (23), tR2asy (18), gCH (5)
598	-	594	R1asyd (33), R2asyd (21), R2trid (14), CCme (13), CC (10)
648	-	632	tR1tri (30), gCC (28), tR2tri (21), gCH (9)
670	-	678	R2asyd (30), R1symd (21), R2trid (17), CC (15), bCC (6), CCme (5)
736	-	747	tR2tri (45), tR1tri (37), gCH (7), gCC (5)
-	753	772	CC (51), R1symd (10), CCme (9), R1asyd (7), R2asyd (7), R1trid (7)
816	-	806	gCH (83)
-	825	827	gCH (90)
855	-	845	CC (30), R2trid (29), R1trid (18), CCme (12)
887	-	892	gCH (84)
915	-	906	gCH (80), tR1tri (8), tR2tri (5)
934	-	927	CC (48), CCme (20), R2trid (10), CH3opr (6), bCH (6)
962	-	962	gCH (88), tR2tri (7)
-	964	972	gCH (88), tR1tri (6)
982	-	982	CC (38), R1trid (17), CH3opr (11), R2trid (9), bCH (9)
1037	-	1039	CH3opr (41), CH3ipr (27), CC (17)
1064	-	1053	CH3ipr (26), CH3opr (25), CC (19), R1trid (10), bCH (6)
1073	-	1081	CH3ipr (38), CH3opr (29), gCC (10), gCH (9)
1085	-	1082	CH3ipr (40), CH3opr (26), gCC (11), gCH (10)
-	1147	1147	bCH (54), CC (31), R1trid (8)

Table-10(contd..)

Experiment		B3LYP/6-31G* (scaled)	PED(%)
IR(cm^{-1})	Raman(cm^{-1})		
1165	1178	1164	bCH (76), CC (20)
1182	-	1191	bCH (54), CC (35), CCme (9)
1214	-	1209	bCH (59), CC (18), CCme (16)
1245	-	1261	bCH (51), CC (24), R2trid (11), CCme (10)
1272	-	1273	CC (58), CCme (19), bCH (10)
1295	-	1303	bCH (51), R1trid (20), CC (13), CCme (9)
1400	-	1377	bCH (54), CC (24), R1trid (6), bCC (6)
-	1401	1400	CH3sb (71), CC (16), CCme (6)
1435	-	1402	CH3sb (78), CCme (10), CC (7)
1441	1449	1422	CC (85), bCH (7)
-	1477	1427	CC (63), bCH (13), CCme (11), CH3sb (9)
1502	1486	1467	CC (51), bCH (21), bCC (9), CH3opb (5)
-	1514	1507	CH3ipb (90), CH3ipr (6)
1522	-	1508	CH3ipb (86), CH3ipr (7)
1534	-	1525	CC (38), bCH (30), CCme (13), CH3opb (10)
1541	-	1530	CH3opb (68), CC (18), bCH (8)
1559	1569	1542	CH3opb (70), CC (12), CH3opr (6)
1628	-	1564	CC (47), CH3opb (19), bCH (18), CH3opr (6)
-	1635	1626	CC (73), bCH (7), R2asyd (6)
1695	-	1647	CC (71), bCH (14)
-	1381	1698	CC (66), bCH (14), R1asyd (11)
2722	2720	2722	CH31ss (99)
2855	-	2845	CH32ss (98)
2859	-	2859	CH31ip (98)
2909	2909	2909	CH32ip (92), CH32op (7)
-	2967	2967	CH32op (92), CH32ip (6)
2970	-	2970	CH31op (98)
3017	-	3030	CH (99)
-	3023	3031	CH (99)
-	3039	3032	CH (99)
-	-	3033	CH (99)
3050	-	3050	CH (99)
-	3052	3051	CH (99)

Table-11: Observed and calculated frequencies of 2, 7dimethylnaphthalene with PED

Experiment		B3LYP/6-31G* (scaled)	PED(%)
IR(cm^{-1})	Raman(cm^{-1})		
-	-	81	Butrfl (33), gCC (21), tCH3 (16), gCH (13), tR1sym (7), tR2sym (5)
-	-	104	tCH3 (79), gCC (17)
-	120	115	tCH3 (72), Butrfl (18), gCH (6)
-	144	136	tR1sym (42), tR2asy (16), gCC (13), tR1asy (9), gCH (7)
-	222	217	bCC (54), CC (19), R1asyd (13)
-	234	245	gCC (49), tR1asy (14), Butrfl (14), gCH (7), tR1sym (5)
-	286	273	gCC (36), tR2asy (16), tR1asy (8), tR1sym (8), tR1tri (8), gCH (7)
-	329	330	bCC (73), R1symd (7), CH3opr (5)
-	412	412	tR1asy (49), tR1sym (15), gCH (12), gCC (11), tR2sym (8)
-	422	416	R1asyd (52), CC (22), bCC (12), CCme (6)
-	445	447	bCC (28), R1symd (23), R2asyd (15), CC (15), R1asyd (6)
477	469	477	tR2sym (66), Butrfl (10), gCH (10), gCC (5), tR1asy (5)
495	-	495	R2symd (49), R1asyd (14), CC (12), bCC (9), CCme (6)
558	-	562	tR1tri (24), tR2asy (20), gCC (19), tR1sym (12), tR1asy (11), gCH (11)
650	-	651	R1symd (46), R2asyd (36), CC (8)
663	-	660	tR2tri (47), gCC (14), gCH (14), tR2asy (13), tR1tri (10)
695	680	690	R1trid (30), CC (18), CCme (14), R2symd (14), R2asyd (11), R1symd (5)
764	-	778	CC (69), R2asyd (14)
-	774	785	gCH (82), tR2tri (9)
786	-	788	tR1tri (40), gCH (29), tR2tri (21)
-	799	790	CCme (31), CC (30), R2trid (17), R1trid (13)
832	-	836	gCH (70), tR1tri (8), tR2asy (7)
875	-	867	gCH (93)
910	-	910	gCH (72), tR1tri (12), tR2tri (5)
936	-	940	CC (39), R1trid (25), CCme (14), bCH (7)
938	938	944	gCH (87), tR2tri (10)
968	-	956	gCH (86), tR1tri (9)
-	973	986	CC (35), R2trid (19), CH3opr (11), R1trid (10), CH3ipr (8), R2symd (8)
1029	-	1021	CH3ipr (50), CH3opr (20), CC (17)
1038	-	1043	CH3ipr (68)
1055	-	1053	CH3opr (48), CH3ipr (28)
1068	-	1070	CH3opr (63), CC (11), bCH (6), R2trid (6)
-	1168	1164	bCH (48), CC (32), R2trid (8), R1trid (5)

Table-11(contd..)

Experiment		B3LYP/6-31G* (scaled)	PED(%)
IR(cm^{-1})	Raman(cm^{-1})		
1178	1178	1178	bCH (58), CC (40)
-	1207	1209	bCH (54), CC (26), CCme (15)
-	1210	1217	CCme (32), CC (31), bCH (30)
-	1230	1233	CC (65), CCme (13), bCH (12)
1277	-	1273	bCH (43), CC (29), R1trid (14), CCme (10)
-	1328	1323	bCH (51), R2trid (25), CC (16)
1375	1383	1381	bCH (55), CC (23), bCC (6), R2trid (6)
1402	-	1399	CC (88)
1418	-	1407	CC (68), bCH (24)
1437	-	1444	CH3sb (82), CCme (7), CC (6)
-	1454	1446	CH3sb (87), CCme (9)
-	1464	1463	CC (46), bCH (13), CH3sb (9), R2trid (8)
-	1504	1500	bCH (52), CC (34)
1514	-	1525	CH3ipb (90), CH3ipr (6)
1537	-	1526	CH3ipb (89), CH3ipr (6)
1546	-	1552	CC (47), bCH (38), CCme (5)
-	1573	1575	CH3opb (75), CC (13), bCH (5)
-	1588	1584	CH3opb (84), CH3opr (7)
1616	1606	1607	CC (62), CH3opb (11), bCH (10), R2asyd (7)
-	1639	1650	CC (62), bCH (19), R1asyd (6)
1695	-	1692	CC (61), bCH (17), R2symd (14)
2856	2856	2856	CH32ss (94), CH32op (5)
-	2868	2868	CH31ip (97)
2910	2911	2910	CH32op (90), CH32ip (5)
2933	-	2933	CH31ss (71), CH31op (29)
-	2965	2965	CH31op (69), CH31ss (28)
2978	-	2978	CH32ip (94)
3011	-	3038	CH (99)
-	3029	3039	CH (99)
3044	-	3041	CH (99)
-	3049	3042	CH (99)
3067	-	3057	CH (99)
-	3078	3060	CH (99)

Table12: observed and calculated frequencies of 2, 6-dimethylnaphthalene with mode of vibration

Mode of vibration	calculated(scaled)		observed	
	6-31G* (cm^{-1})	6-311+G** (cm^{-1})	IR (cm^{-1})	Raman (cm^{-1})
CH Stretching	3030	3030	-	3052
	3031	3031	3050	-
	3032	3032	-	-
	3033	3033	-	3039
	3050	3050	-	3023
	3051	3051	3017	-
CH3 stretching	2722	2722	2722	2720
	2845	2845	2855	-
CH3 in plane stretching	2859	2859	2859	-
	2909	2909	2909	2909
CH3 out of plane stretching	2967	2967	-	2967
	2970	2970	2970	-
CH in plane bending (bCH)	1147	1148	-	1147
	1164	1168	1165	1178
	1191	1190	1182	-
	1209	1208	1214	-
	1261	1260	1245	-
	1303	1303	1295	-
	1377	1376	-	1381
CH out of plane bending (gCH)	806	803	816	-
	827	819	-	825
	892	889	887	-
	906	899	915	-
	962	972	962	-
	972	979	-	964
CC in plane bending (bCC)	331	331	-	323
	406	407	-	411
CC out of plane bending (gCC)	345	347	-	343
	554	553	548	-
Ring in plane bending (b Ring)	200	199	-	207
	441	443	457	-
	517	516	526	526
	594	594	598	-
	678	676	670	-
CCme Stretching	772	774	-	753
	845	845	855	-

Table12 (contd...)

Mode of vibration	calculated(scaled)		observed	
	6-31G* (cm^{-1})	6-311+G** (cm^{-1})	IR (cm^{-1})	Raman (cm^{-1})
CC Stretching	927	928	934	-
	982	983	982	-
	1273	1273	1272	-
	1422	1422	1435	-
	1427	1426	1441	1449
	1467	1466	-	1477
	1525	1528	1522	-
	1564	1564	1559	1569
	1626	1627	1628	-
	1647	1648	-	1635
	1698	1698	1695	-
Ring torsion bending	176	170	-	167
	215	213	-	217
	397	392	-	399
	482	483	483	-
	632	-	648	-
	747	745	736	-
CH3 symmetric bending (CH3ss)	1400	1400	1400	-
	1402	1402	-	1401
CH3 in plane bending (CH3ipb)	1507	1507	1502	1486
	1508	1508	-	1514
CH3 out of plane bending (CH3opb)	1530	1530	1534	-
	1542	1543	1541	-
CH3 in plane rocking (CH3ipr)	1081	1080	1073	-
	1082	1084	1085	-
CH3 out of plane rocking (CH3opr)	1039	1039	1037	-
	1053	1052	1064	-
Methyl torsion (tCH3)	104	103	-	-
	107	107	-	115
Butterfly	84	83	-	-

Table13: observed and calculated frequencies of 2, 7-dimethylnaphthalene with mode of vibration

Type of mode	6-31G* (scaled)	6-311+G** (scaled)	IR (cm^{-1})	Raman (cm^{-1})
CH Stretching	3038	3038	3011	-
	3039	3040	-	3029
	3041	3041	3044	-
	3042	3042	-	3049
	3057	3057	3067	-
	3060	3060	-	3078
CH3 symmetric stretching	2856	2856	2856	2855
	2933	2933	2933	-
CH3 in plane stretching	2868	2868	-	2868
	2978	2978	2978	-
CH3 out of plane stretching	2901	2910	2910	2911
	2965	2965	-	2965
CH in plane bending (bCH)	1164	1163	-	1168
	1178	1166	1178	1178
	1209	1197	-	1207
	1273	1260	1277	-
	1381	1384	1375	1383
	1500	1491	-	1504
CH out of plane bending (gCH)	785	777	-	774
	836	830	832	-
	867	858	875	-
	910	903	910	-
	944	946	938	938
	956	964	968	-
CC in plane bending (bCC)	217	215	-	222
	330	326	-	329
CC out of plane bending (gCC)	245	247	-	234
	273	269	-	286
Ring in plane bending (b Ring)	416	417	-	422
	447	447	-	445
	495	498	495	-
	651	645	650	-
	690	697	695	680
	1323	1334	-	1328

Table13: (contd..)

Type of mode	6-31G* (scaled)	6-311+G** (scaled)	IR (cm^{-1})	Raman (cm^{-1})
CC Stretching	778	790	764	-
	940	934	936	-
	986	981	-	973
	1233	1237	1230	-
	1399	1396	1402	-
	1407	1405	1418	-
	1463	1482	-	1464
	1552	1552	1546	-
	1607	1616	1616	1606
	1650	1641	-	1639
	1692	1689	1695	-
Ring torsional bending	136	138	-	144
	412	411	-	412
	477	478	477	469
	562	562	558	-
	660	656	663	-
	788	785	786	-
CH3 symmetric bending(CH3ss)	1444	1444	1437	-
	1446	1447	-	1454
CH3 in plane bending (CH3ipb)	1525	1524	1514	-
	1526	1526	1537	-
CH3 out of plane bending (CH3opb)	1575	1577	-	1573
	1584	1585	-	1588
CH3 in plane rocking(CH3ipr)	1021	1021	1029	-
	1043	1043	1038	-
CH3 out of plane rocking(CH3opr)	1053	1050	1055	-
	1070	1073	1068	-
Methyl torsion (tCH3)	104	103	-	-
	115	116	-	120
C-CH3 Stretching (CCme)	790	816	-	799
	1217	1227	-	1210
Butterfly	81	81	-	-

Table14: Observed frequencies and assignment of the three isomeric methylnaphthalenes

Type of mode	2,3-dimethylnaphthalene		2,6-dimethylnaphthalene		2,7-dimethylnaphthalene	
	Infrared	Raman	Infrared	Raman	Infrared	Raman
CH Stretching	3009	3009	3017	-	3011	-
	-	3015	-	3023	-	3029
	-	-	-	3039	3044	-
	3049	3049	-	-	-	3049
	-	-	3050	-	3067	-
	-	3070	-	3052	-	3078
CH3 symmetric stretching	2725	-	2722	2720	2856	2855
	-	2844	2855	-	2933	-
CH3 in plane stretching	2978	-	2859	-	-	2868
	-	2983	2909	2909	2978	-
CH3 out of plane stretching	2918	2918	-	2967	2910	2911
	2932	-	2970	-	-	2965
CH in plane bending (bCH)	1128	-	-	1147	-	1168
	1150	1145	1165	1178	1178	1178
	1174	-	1182	-	-	1207
	1233	-	1214	-	1277	-
	1251	-	1245	-	1375	1383
	1275	-	-	1381	-	1504
CH out of plane bending (gCH)	741	-	816	-	-	774
	803	-	-	825	832	-
	816	815	887	-	875	-
	832	-	915	-	910	-
	921	-	962	-	938	938
	948	-	-	964	968	-
CC in plane bending (bCC)	-	270	-	323	-	222
	-	-	-	411	-	329
CC out of plane bending (gCC)	-	448	-	343	-	234
	686	-	548	-	-	286
Ring in plane bending (bRing)	-	414	-	207	-	422
	455	-	457	-	-	445
	-	518	526	526	495	-
	659	-	598	-	650	-
	672	-	670	-	695	680
	-	1017	1295	-	-	1328

Table 14 (Contd…)

Type of mode	2,3-dimethylnaphthalene		2,6-dimethylnaphthalene		2,7-dimethylnaphthalene	
	Infrared	Raman	Infrared	Raman	Infrared	Raman
CC Stretching	-	1063	934	-	764	-
	-	1105	982	-	936	-
	-	1332	1272	-	-	973
	-	1354	1435	-	1230	-
	1381	1381	1441	1449	1402	-
	-	1470	-	1477	1418	-
	-	1481	1522	-	-	1464
	-	1541	1559	1569	1546	-
	-	1599	1628	-	1616	1606
	1633	1632	-	1635	-	1639
	-	1685	1695	-	1695	-
Ring torsional bending	120	-	-	167	-	144
	240	-	-	217	-	412
	296	-	-	399	477	469
	-	482	483	-	558	-
	-	532	648	-	663	-
	768	-	736	-	786	-
CH3 symmetric bending(CH3ss)	-	-	1400	-	1437	-
	-	-	-	1401	-	1454
CH3 in plane bending (CH3ipb)	-	1428	1502	1486	1514	-
	1437	-	-	1514	1537	-
CH3 out of plane bending (CH3opb)	-	1448	1534	-	-	1573
	1465	-	1541	-	-	1588
CH3 in plane rocking(CH3ipr)	-	970	1064	-	1029	-
	-	1022	1073	-	1038	-
			1085	-		
CH3 out of plane rocking(CH3opr)	-	982			1055	-
	-	1000	1037	-	1068	-
Methyl torsion (tCH3)	149	-	-	-	-	-
	180	-	-	115	-	120
Butterfly	100	-	-	-	-	-
C-CH3 Stretching(CCme)	-	777	-	753	-	799
	-	874	855	-	-	1210

All the six out of plane CH bending vibrations could be recorded either in Raman spectrum or in IR absorption spectrum. They are observed at 825 w, 964(s) in Raman and at 816 (vw) 887 (vvs) 915(w), 962s in IR absorption spectrum. The calculated frequencies of this mode are 806, 827, 892, 906, 962, and 972cm-1 are agreeing well with the observed frequencies.

The PED determination indicates that there are 13 CC ring stretching vibrations. But from the structure of molecule there should be only 11 CC stretching frequencies. All the 11 CC stretching frequencies could be observed either from IR absorption or from Raman spectrum. While the Raman lines are strong, the IR absorption bands are weak. They are observed at 1635s, 1569s, 1477w, 1449vs in Raman spectrum and 1695vvw, 1628w, 1559vvw, 1522vvw, 1441vvw, 1435w, 1272ms, 982w, 934vvw in IR absorption spectrum. These are well agreeing with the calculated frequencies at 1698, 1647, 1626, 1564, 1525, 1467, 1427, 1422, 1273, 982, 927cm^{-1}. PED contribution shows two more frequencies 772(51%), 845(30%) as comparable with the other CC stretching frequencies. In general the order of CC frequencies of condensed ring system lies above 900 cm-1. Besides, It is also that the CCme stretching frequency has shown the values of this range in some of the methyl substituted molecules ━ 3- chloro- 4 – methyl aniline a value at 697[16], in 2 – chloro – 4 – methyl aniline at 772[17], 3 – bromo – 5-hydroxy – 2, 6 – dimethyl pyridine is 711 and 719, 3-chloro – 5-hydroxy, 2, 6 – dimethyl pyridine is 805, 814[18]. Hence the author prefers to assign the two frequencies 772 and 845 as the CCme stretching frequencies

The calculated Ring in plane bending vibrations (deformations) as per the PED contribution are clearly five and they are 200, 441, 517, 594, 678 cm-1. The sixth one is generally having higher value in the range 1000-1350. The calculated value at 1303 has a component contribution of 20% of Ring deformation. Between two frequencies 1303 and 1377 both showing the maximum contribution of CH in plane bending but the next in order being different as shown in table in view of these the author suggests 1303 as due to ring bending mode more than the additional CH in plane bending mode. Now all the six ring bending frequencies are in good agreement with experimental values as shown in table. The frequency 1377 is already discussed in the section on CH inplane bending modes.

There are two CC in plane bending (Pertaining to the methyl substitution) and two CC out of plane bending vibrations observed from IR and Raman spectrum. The two strong lines at 323, 411 in Raman spectrum are assigned to the CC inplane bending modes in agreement with the theoretical and assigned value at 331 and 406. Similarly the weak Raman line at 343 and weak IR absorption band at 548 are assigned to the two CC out of plane bending modes in fair agreement with the calculated values at 345 and 554 respectively.

All the 6 calculated frequencies 176, 215, 397, 482, 632,747cm-1 of ring torsion could be well compared with the experimental values which show two strong Raman lines at 217, 399 and one very strong IR absorption at 483, the remaining 167(R),648(IR),and 736(IR) as weak.

Methyl Group vibrations:

There are two methyl substitutions in the molecule. These give rise to 6 CH3 stretching frequencies ─ two each ,of symmetrical, in plane, and out of plane stretching modes. Similarly there are two symmetrical bending, two in plane bending, and two out of plane bending modes of CH3. There are also two in plane rocking and out of plane rocking, and two torsion bendings of CH3 groups.

Two CCme stretching frequencies at 772 and 845 have been already discussed earlier in connection with the description and fixation of CC stretching frequencies. Out of all the CH3 stretching frequencies, two are CH3 symmetric stretching, two are CH3 in plane stretching, and two are CH3 out of plane stretching of the methyl group. All of them could be observed and well compared with the theoretical assignments at 2722, 2845, 2859, 2909, 2967, 2970. The strong Raman lines at 2720, 2909 and very strong IR absorption bands at 2909, 2970 are significant and others observed at 2967 (Raman), 2722(IR), 2855(IR),2859(IR) are weak.

The 6 CH3 bending frequencies of the two methyl groups are two CH3 symmetric bending, two CH3 in plane bending and two CH3 out of plane bending modes. The calculated frequencies 1400, 1402 are assigned to CH3 symmetric bending modes, 1507, 1508 to CH3 in plane bending and 1530, 1542 to CH3 out of plane bending modes. The experimental values are in fair agreement with the calculated values. A very strong Raman line at 1486and medium strong IR absorption band at 1502 are prominent while others are weak.

Regarding CH3 in plane rocking, one should expect only two frequencies. PED contribution shows prominently two values at 1081(38%) and 1082(40%),while at 1053 there is almost equal probability of in plane rocking and out of plane rocking as well, but much less than that of 1081 or1082.

The author suggests the probability of 1053 as the CH3 out of plane rocking in preference to the in plane rocking mode, thus the two assigned CH3 out of plane rocking frequencies calculated to be at 1039 and 1053.

The in plane rocking mode frequencies are in good agreement with experimental value 1073 and 1085.

The two out of plane rocking mode frequencies are 1039 and 1053 which are in good agreement with the strong IR absorption band at 1037 and very weak absorption band at 1064.

The two CH3 torsion frequencies are assigned to 104 and 107 out of which only one is observed as weak Raman line at 115. The second torsion frequency is only predicted at 104. Similarly the butterfly frequency at 83 is predicted.

2. Vibrational Analysis of 2, 7 – dimethylnaphthalene:

Six frequencies of this molecule occurring in the region 3000-3100cm-1are assigned to CH stretching modes. From the calculations these are 3038, 3039, 3041, 3042, 3057, 3060cm-1. Two very strong Raman lines at 3029,3049, and weak Raman line at 3078, very weak infrared absorption bands at 3067, 3044, and 3011cm-1 are in agreement with the calculated frequencies.

For this molecule there are 6 CH in plane bending frequencies. The PED shows a prominence in 7 frequencies and they are 1164, 1178, 1208, 1273, 1323, 1381, and 1500cm-1. From the structure of the molecule, one expects only six CH inplane bending frequency. It is noticed that all other six excepting the frequency at 1323 have a combination with CC stretching vibration comparable with that of the in plane CH bending. But, for 1323 it is having a 25% combination with ring deformation and only 16% combination with CC stretching. This data suggests a probability that 1323 may be considered for ring deformation rather than the CH in plane bending mode. Two very strong Raman lines at 1178,1383(1375 in IR) and 3 weak Raman lines at 1168,1207,1504 cm-1 together with the two weak IR absorption band at 1178,1277 are in good agreement with the CH in plane bending frequencies calculated as 1164,1178,1209,1273,1381 and 1500cm-1.

Six CH out of plane bending frequencies 785,836,867,910,944,956cm-1 are in good agreement with the experimental values, the two strong Raman lines at 774,938cm-1 and the strong IR bands at 832,910cm-1 and weak IR absorption bands at 875,938,968cm-1.

The 11 calculated CC stretching frequencies 778, 940, 986, 1233, 1399, 1407, 1463, 1552, 1607, 1650, and 1692cm-1 are well in agreement with the experimental values. The two strong Raman lines at 1464 and 1639, medium strong infrared absorption band found at 936 and the remaining frequencies 764, 1230, 1402, 1418, 1546, 1616, 1695, are either weak or very weak in the infrared absorption spectrum.

The calculated values of CCme stretching on the basis of PED are assigned to 790 and 1217,these values are agreeable with the experimental values 799 and 1210 in Raman spectrum, thus confirming the assignments of experimental values.

The two CC(methyl substitution) in plane bending frequencies are assigned to strong Raman lines at 222 and weak Raman line at 329.These two are in good agreement with the calculated value at 217(54%) and 330(73%).

Actually the structure has only two CC (methyl substitution) in plane bending modes, calculations show one more CC (methyl substitution) in plane bending at 447(28%) which is in combination with almost equal percentage 23% of ring deformation. This is preferred to be more a ring symmetric deformation than the CC in plane bending mode. This is by way of suggestion.

The two weak Raman line at 234 and 286 are assigned to the two out of plane bending modes with the calculated values at 245 and 270.

There should be 6 ring bending modes. The calculations on the basis of PED give prominently four frequencies at 416,495,651and 690cm-1 which agree well with strong Raman line at 422 and two weak infrared absorption bands at 495,650 and strong Raman line at 680. The remaining two may be considered as 447 and 1323; the first one is already discussed with analysis of CC (methyl substitution) in plane bending mode frequencies as above; and the second is also earlier in assigning the CH in plane bending modes. While 447 agrees well with very strong Raman line at 445 , 1323 agrees with the weak Raman line at 1328.

The six ring torsion frequencies 136,412,477,562,660,788cm-1 assigned by calculation are in quite good agreement with the strong Raman lines at 144,412,469 and strong infrared band 477 and weak infrared absorptions at 556, 663,786 cm-1 respectively.

Methyl group vibrations:

There are two methyl substitutions in the molecule. These give rise to 6 CH_3 stretching frequencies ─ two each ,of symmetrical, in plane, and out of plane stretching modes. Similarly there are two symmetrical bending, two in plane bending, and two out of plane bending modes of CH_3. There are also two in plane rocking and out of plane rocking, and two torsion bendings of CH_3 groups.

The CH symmetrical (stretching of $CH_{3)}$ vibrations could be observed one in the Raman spectrum as strong line at 2855 cm^{-1}(in the IR as very weak band at

2856) and the other in IR absorption at 2933cm^{-1} as very weak band. These are well agreeing with the theoretical values at 2856 and 2933. The two CH_3 in plane stretching frequencies also could be obtained ─ one from Raman spectrum as a very weak line at 2863 and the other as a very weak absorption band at 2978 in the IR both agreeing very well with the theoretical values at 2868 and 2978. The CH_3 out of stretching frequencies are observed one as both in Raman and IR absorption at 2911 as strong line (2910 in IR as very strong band) and the other as Raman line at 2965. These two also agree exactly with the theoretical values at 2910 and 2965.

The two symmetrical bendings of CH_3 could be observed in IR absorption spectrum at 1437 as weak band and in Raman spectrum at 1454 as weak line. These agree well with the theoretical values at 1444 and 1446. The two in plane bending of CH_3 are observed as weak IR absorption bands at 1514 and 1537.These are well agreeable with the theoretically deducted values at 1525 and 1526.The two out of plane bending frequencies of CH_3 are noticed to be one as strong Raman line at 1573, and the other as weak Raman line at 1588. Both the frequencies agree very well with the theoretical values at 1575, 1584 cm^{-1}.The two in plane rocking frequencies of CH_3 are observed both in IR spectrum one as a very weak band at 1029 and the other as strong band at 1038,well compared with the calculated frequencies at 1021 and 1043 cm^{-1}.The two out of plane rocking mode frequencies of CH_3 are observed as weak in IR absorption at 1055and 1068. The calculated values for these frequencies are at 1053 and 1073.The CH_3 torsion frequencies are calculated to be at 104, 115. Only one frequency is observed in Raman spectrum as weak line at 120. The other is predicted to be 104cm^{-1}. Theoretical value of the butterfly frequency is predicted to be at 89 cm^{-1}.

1.2. Conclusions

There is good agreement between calculated and experimental values confirming the assignments for the observed vibrational frequencies. In case of any variations the author has taken into consideration the PED contribution of other modes of the frequency to suggest the most probable assignment, which is also based on the total number of frequencies of each mode and probable range of the frequencies of a particular mode. A comparison of the vibrational frequencies observed and assigned of all the three isomers is consolidated in table-14.

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