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Archives of Physics Research, 2010, 1 (4): 211-216
(http://scholarsresearchlibrary.com/archive.html)

ISSN 0976-0970
CODEN (USA): APRRC7

Vibrational Spectra and Analysis of Trans – decahydronaphthalene

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ABSTRACT

FTIR and FTR spectra of Trans-Decahydronaphthalene have been recorded in the regions 200 - 4000 cm^{-1} and 30- 4000 cm^{-1}. The vibrational analysis has been carried out by assuming C_s symmetry. The observed frequencies were assigned to various modes of vibrations on the basis of intensity, frequencies from allied molecules and the normal coordinate calculations. The potential energy distributions associated with normal modes are also reported here. The assignment of fundamental vibrational frequencies for Trans- Decahydronaphthalene agree with the calculated frequencies.

Keywords: Vibrational spectra, Normal coordinate calculation,Trans-Decahydronaphthalene

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INTRODUCTION

Tras-Decahydronaphthalene, derivative of naphthaelen is a colourless liquid with boiling point 185°C, flash point 52°C and melting point - 32°C. It is stable, combustible and incompatible with oxidizing agent. It may form explosive peroxides in storage. It is harmful if swallowed or inhaled. It has skin, eye and respiratory irritant. It is flammable liquid. It has other names called trans-decalin, perhydronaphthalene, and naphthane.This compound was widely investigated by the scientist Seyer and Walker. The Phase transformation in solutions of syndiotactic polystyrene in cis - decalin has been investigated by dynamic scanning calorimetry wide and small angle X-ray scattering and Fourier transformed IR spectroscopy [1]. The role of solvent molecules in the physical gelation of isotactic polystyrene was studied in cis and trans-decalin [2] .Lai, Wei-chuan, Song and Chunshan [3] reported the isomerization of cis-decahydronaphthalene to trans-decahydronapthalene in the presence of zeolite catalyst. Inspite of several reports for these compounds in the literature, no report is available on vibrational spectra and analysis of these compounds. Hence, an attempt has been made in the present work to record the FTIR and FTR spectra of these compounds and to study the complete vibrational analysis for first time.

MATERIALS AND METHODS

Experimental Details

The molecular structure of trans-Decahydronaphthalene is given in figure1. FTIR and FT Raman spectra of trans-Decahydronaphthalene were recorded on Brucker IFS 66V spectrometer in the region 4000 - 200 cm^{-1}. FT Raman Spectrum is recorded with FRA 106 Raman module equipped with Nd : YAG laser source operating at 1064 nm line with a scanning speed of 30 cm^{-1} min^{-1} of spectral width 20 cm^{-1}. The frequencies for all sharp bands were accurate to ±1 cm^{-1}. The recorded spectra are shown in figure2.

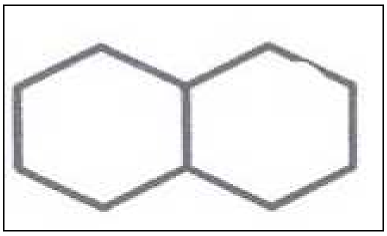

Fig.1. Structure of the compound

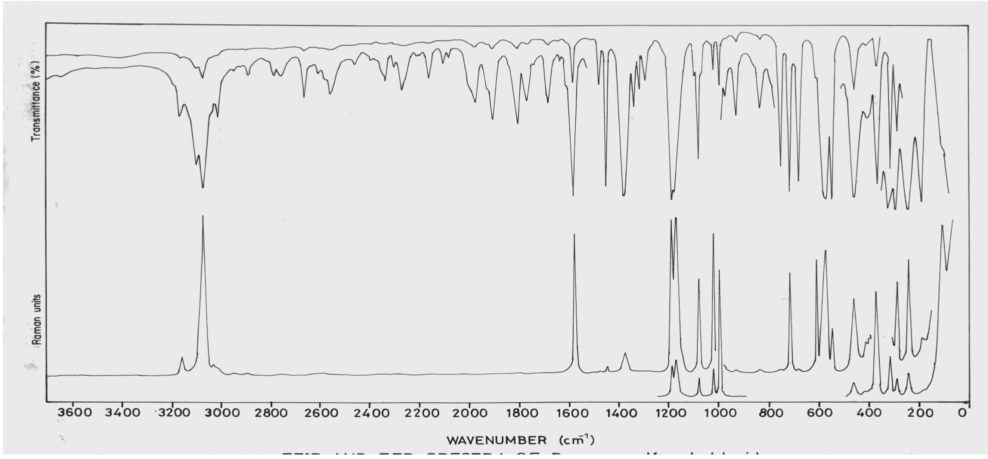

Fig.2.FTIR and FTR spectra of Trans – decahydronaphthalene

2.1 Theoretical Considerations

The effective use of vibrational spectroscopy for investigation on the polyatomic molecules is possible only with necessary conclusions from theoretical considerations. The symmetry possessed by a molecule helps to determine and classify the actual number of fundamental vibrations of the system. The observed spectra of Trans-decahydronaphthalene is explained on the basis of C_s point group symmetry which consists of 28 atoms and the 78 normal modes of vibrations span the irreducible representation as $\Gamma_{vib} = 54\ a'$ (in-plane) + $24\ a''$ (out-of-plane). All the modes are active in both Raman and infrared. The assignments have been made on the basis of relative intensities, magnitudes of the frequencies and polarisation of the Raman lines.

2.2 Normal Coordinate Analysis

In order to obtain a more complete description of the molecular motions involved in the normal modes of Trans-decahydronaphthalene, a normal coordinate analysis has been carried out. The method of normal coordinate analysis is necessary for a complete assignment of the vibrational frequencies of larger polyatomic molecules and for a quantitative description of the vibrations. In fact a normal coordinate analysis for an observed vibrational spectrum is a logical extension of any vibrational spectral study. Wilson's FG matrix method is used for the normal coordinate calculations. The structural parameters employed in the present work have been taken from allied molecules and Sutton table [4]. The computer program for normal coordinate calculations developed by Fuhrer *et al.,* [5] was suitably modified and used in the present work. The simple general valence force field has been adopted to analyse both in plane and out of plane vibrations. The initial set of force constants are taken from allied molecules. The predicted infrared intensities are used along with Raman data and depolarisation ratios to aid in the assignments of vibrational frequencies. The normal coordinate calculations have also yielded vibrational frequencies and the potential energy distribution for the various modes.

In the normal coordinate analysis, the potential energy distribution plays an important role for the characterisation of the relative contributions from each internal coordinates to the total potential energy associated with particular normal coordinate of the molecule.

2.3 Potential Energy Distributions

To check whether the chosen set of assignments contribute maximum to the potential energy associated with the normal co-ordinates of the molecules, the potential energy distribution (PED) has been calculated using the relation.

$$\mathrm{PED} = \frac{F_{ii}L^{2}_{ik}}{\lambda_k}$$

Where F_{ii} are the force constants defined by damped square technique, L_{ik} the normalised amplitude at the associated element (i,k) and λ_k the eigne value corresponding to the vibrational frequency of the element k. The PED contribution corresponding to each of the observed frequencies over 10% are alone listed in the present work.

RESULTS AND DISCUSSIONS

The observed infrared and Raman frequencies and the calculated frequencies along with the PED of various modes of vibrations of Trans-decahydronapthalene, has been presented in Table1. The assignment of frequencies is made as follows

Stretching vibration

C-H stretching vibration

The observed frequencies at 2631, 2656, 2663, 2681, 2690, 2700, 2713, 2750, 2794, 2810, 2838, 2856, 2875, 2888, 2900, 2913, 2935, and 3056 cm^{-1} are assigned to C-H stretching vibrations which agree well with the calculated frequencies and literature values [6]. All the C-H stretching frequencies are pure modes except at frequencies at 2888, 2856, 2810, 2713 and 2631 cm^{-1} where they are mixed mode of C-C stretching vibrations as per the PED calculation.

C – C stretching

Ten C-C stretching vibrations of Trans-dehydronapthalene have been assigned to 1038, 1050, 1063, 1075, 1088, 1125, 1138, 1150, 1162 and 1175 cm^{-1} which agree with the calculated values.

In plane and out of plane bendings

The observed frequencies at 1138, 1150, 1162, 1175, 1213, 1225, 1250, 1275, 1288, 1300, 1325, 1338, 1350, 1363, 1388, 1413, 1450 and 1463 cm^{-1} have been assigned to C-H in plane bending vibrations which agree with the calculated frequencies. Based on the PED, majority of these vibrations are mixed with other vibrational modes and the nature of all the vibrations can be identified from the Table 1.

CCC in plane bending vibrations is assigned to 400, 450, 492, 513, 525 and 563 cm^{-1} which agree with calculated frequencies. H out of plane bendings and CCC out of plane bendings are assigned to their respective observed frequencies as presented in the table. The CCC trigonal bending and CCC ring breathing are assigned to 1025 cm^{-1} and 850 cm^{-1}.

Table : 1 Observed, calculated frequencies (cm^{-1}), vibrational assignments and potential energy distribution of Trans-Decahydronaphthalene

Species	Observed frequency / Intensity		Calculated wavenumber	Assignment	% PED
	Infrared	Raman			
a′	3056 vw	-	3051	C-H stretching	$92\ \nu_{CH}$
a′	-	2935 s	2932	C-H stretching	$88\ \nu_{CH}$
a′	2913 vs	2913 m	2909	C-H stretching	$80\ \nu_{CH}$
a′	2900 m	-	2897	C-H stretching	$94\ \nu_{CH}$
a′	-	2888 w	2880	C-H stretching	$71\ \nu_{CH} + 15\ \nu_{CC}$
a′	2875 m	-	2869	C-H stretching	$82\ \nu_{CH}$
a′	-	2856 s	2851	C-H stretching	$70\ \nu_{CH} + 24\ \nu_{CC}$
a′	2838 s	-	2830	C-H stretching	$90\ \nu_{CH}$
a′	-	2810 s	2802	C-H stretching	$71\ \nu_{CH} + 21\ \nu_{CC}$
a′	2794 s	-	2791	C-H stretching	$86\ \nu_{CH}$
a′	2750 w	-	2742	C-H stretching	$85\ \nu_{CH}$
a′	2713 w	2713 w	2707	C-H stretching	$70\ \nu_{CH} + 19\ \nu_{CC}$
a′	2700 w	-	2691	C-H stretching	$92\ \nu_{CH}$
a′	-	2690 w	2681	C-H stretching	$86\ \nu_{CH}$
a′	2681 w	-	2672	C-H stretching	$91\ \nu_{CH}$
a′	2663 s	-	2654	C-H stretching	$89\ \nu_{CH}$
a′	-	2656 m	2651	C-H stretching	$82\ \nu_{CH}$
a′	2631 s	-	2622	C-H stretching	$74\ \nu_{CH} + 16\ \nu_{CC}$
-	2581 w	-	-	1350 + 1219	-
a′	1463 vs	-	1460	C-H in plane bending	$81\ \beta_{CH}$
a′	1450 vs	1450 vs	1441	C-H in plane bending	$88\ \beta_{CH}$
a′	1413 w	-	1408	C-H in plane bending	$79\ \beta_{CH} + 10\ \beta_{CC}$
a′	1388	-	1381	C-H in plane bending	$91\ \beta_{CH}$
a′	-	1363 vs	1358	C-H in plane bending	$96\ \beta_{CH}$
a′	1350 w	-	1342	C-H in plane bending	$80\ \beta_{CH} + 18\ \beta_{CC}$
a′	-	1338 m	1328	C-H in plane bending	$92\ \beta_{CH}$
a′	1325 m	-	1319	C-H in plane bending	$70\ \beta_{CH} + 22\ \beta_{CC}$
a′	1300 m	-	1288	C-H in plane bending	$88\ \beta_{CH}$
a′	1288 vw	1288 vw	1279	C-H in plane bending	$89\ \beta_{CH}$
a′	-	1275 vw	1271	C-H in plane bending	$90\ \beta_{CH}$
a′	1250 s	1250 w	1241	C-H in plane bending	$69\ \beta_{CH} + 21\ \beta_{CC} + 10\ \nu_{CC}$
a′	1225 m	1225 w	1220	C-H in plane bending	$92\ \beta_{CH}$
a′	-	1213 vw	1207	C-H in plane bending	$91\ \beta_{CH}$
a′	-	1175 vw	1170	C-H in plane bending	$61\ \beta_{CH} + 30\ \nu_{CC}$
a′	-	1175 vw		C-C stretching	
a′	-	1162 vw	1155	C-H in plane bending	$58\ \beta_{CH} + 29\ \nu_{CC}$
a′	-	1162 vw		CC stretching	
a′	1150 vw	-	1140	C-H in plane bending	$54\ \beta_{CH} + 26\ \nu_{CC}$
a′	1150 vw	-		C-C stretching	
a′	1138 m	1138 vw	1129	C-H in plane bending	$62\ \beta_{CH} + 24\ \nu_{CC}$

a′	1138 m	1138 vw		C-C stretching	
a′	-	1125 vw	1123	C-C stretching	94 ν_{CC}
a′	-	1088 vw	1079	C-C stretching	86 ν_{CC}
a′	-	1075 vw	1069	C-C stretching	89 ν_{CC}
a′	1063 m	-	1061	C-C stretching	74 ν_{CC}
a′	-	1050 w	1047	C-C stretching	91 ν_{CC}
a′	-	1038 w	1030	C-C stretching	88 ν_{CC}
a′	1025 m	-	1019	CCC trigonal bending	92 β_{CC}
a″	990 m	990m	986	C-H out of plane bending	72 η_{CH}
a″	975 s	-	971	C-H out of plane bending	81 η_{CH}
a″	925 s	-	919	C-H out of plane bending	70 η_{CH} + 15 η_{CC}
a″	-	912 vw	906	C-H out of plane bending	81 η_{CH}
a″	-	900 vw	891	C-H out of plane bending	74 η_{CH} + 16 η_{CC}
a″	-	875 w	868	C-H out of plane bending	69 η_{CH} + 21 η_{CC}
a″	863 vw	-	861	C-H out of plane bending	84 η_{CH}
a′	-	850 w	842	CCC ring breathing	91 β_{CCC}
a″	838 s	-	827	C-H out of plane bending	72 η_{CH}
a″	825 s	-	818	C-H out of plane bending	86 η_{CH}
a″	800 vw	-	791	C-H out plane bending	70 η_{CH} + 20 η_{CC}
a″	-	763 vw	758	CH out of plane bending	85 η_{CH}
a″	-	763 vw		CH out of plane bending	
a″	-	743 m	740	CH out of plane bending	87 η_{CH}
a″	-	743 m		CH out of plane bending	
a″	-	731 vw	721	CH out of plane bending	91 η_{CH}
a″	-	731 vw		CH out of plane bending	
a″	-	695 vw	690	C-H out of plane bending	86 η_{CH}
a″	-	695 vw		C-H out of plane bending	
a′	-	563 vw	554	CCC in plane bending	88 β_{CH}
a′	525 w	-	519	CCC in plane bending	72 β_{CC} + 21 β_{CH}
a′	-	513 vw	503	CCC in plane bending	86 β_{CCC}
a′	-	492 s	480	CCC in plane bending	72 β_{CCC} + 22 β_{CH}
a′	450 vw	-	439	CCC in plane bending	86 β_{CCC}
a′	400 s	-	388	CCC in plane bending	81 β_{CCC}
a″	-	363 vw	352	CCC out of plane bending	71 η_{CCC} + 10 η_{CH}
a″	-	363 vw		CCC out of plane bending	
a″	341s	-	330	CCC out of plane bending	69 η_{CCC} + 19 η_{CH}
a″	341s	-		CCC out of plane bending	
a″	300 m	300 m	288	CCC out of plane bending	64 η_{CCC} + 22 η_{CH}
a″	300 m	300 m		CCC out of plane bending	

a′- in-plane vibrations, *a″- out-of plane vibrations.*
abbreviations used : w - weak; *m - medium; s - strong; vw - very weak; vs - very strong.*

CONCLUSION

A complete vibrational spectra and analysis is reported in the present work for the first time for Trans - decahydronaphthalene. The close agreements between the observed and calculated frequencies confirm the validity of the present assignment.

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