



## Vibrational Spectral and Analysis of *cis*-Decahydronaphthalene

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FTIR and FTR spectra of *cis*-decahydronaphthalene have been recorded in the regions 4000-200 and 4000-30  $\text{cm}^{-1}$ . The vibrational analysis has carried out by assuming Cs 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 *cis*-decahydronaphthalene agrees with the calculated frequencies.

**Key Words:** Vibrational spectra, Normal coordinate calculation, *cis*-Decahydronaphthalene.

### INTRODUCTION

*cis*-Decahydronaphthalene derivative of naphthalene is colourless liquid with boiling point 193 °C, melting point 43 °C and flash point 58 °C. It is stable and incompatible with oxidizing agents. It may form explosive peroxides. Heat and light accelerate peroxide formation. It is harmful if inhaled, swallowed or absorbed through skin.

This compound was widely investigated by Seyer and Walker<sup>1</sup>. Dynamic scanning calorimetry wide and small angle X-ray scattering have investigated the phase transformations in solutions of syndiotactic polystyrene in *cis*-decalin and Fourier transformed IR spectroscopy<sup>2</sup>. The role of solvent molecules in the physical gelation of isotactic polystyrene was studied in *cis* and *trans*-decalin<sup>3</sup>. Lai and Song<sup>4</sup> had reported the isomerization of *cis*-decahydronaphthalene to *trans*-decahydronaphthalene in the presence of zeolite catalyst.

In spite of several reports for this compound in the literature, no report is available on vibrational spectra and analysis of this compound. Hence, an attempt has been made in the present work to record the FTIR and FTR spectra of this compound and to study the complete vibrational analysis for first time.

### EXPERIMENTAL

The molecular structure of *cis*-decahydronaphthalene is given in Fig. 1. The FTIR and FT Raman spectra of *cis*-decahydronaphthalene were recorded on Bruker IFS 66V

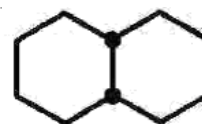


Fig. 1. Structure of the compound

spectrometer in the region 4000-200  $\text{cm}^{-1}$ . 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  $\text{cm}^{-1} \text{min}^{-1}$  of spectral width 20  $\text{cm}^{-1}$ . The frequencies for all sharp bands were accurate to  $\pm 1 \text{ cm}^{-1}$ . The recorded spectra are shown in Fig. 2.

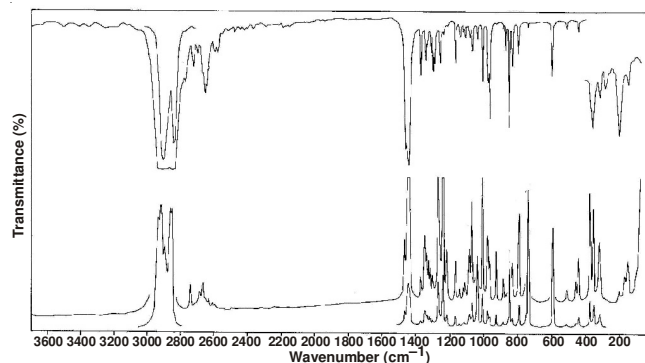


Fig. 2. FTIR and FTR spectra of *cis*-decahydronaphthalene

**Theoretical considerations:** The effective use of vibrational spectroscopy for investigation on the polyatomic molecules is possible only with necessary conclusions from

TABLE-1  
OBSERVED, CALCULATED FREQUENCIES ( $\text{cm}^{-1}$ ), VIBRATIONAL ASSIGNMENTS AND  
POTENTIAL ENERGY DISTRIBUTION OF *CIS*-DECAHYDRONAPHTHALENE

Species	Observed frequency/intensity		Calculated wave number	Assignment	PED (%)
	Infrared	Raman			
a'	2975 vw	—	2970	C-H stretching	96 $\nu_{\text{CH}}$
a'	—	2938 s	2935	C-H stretching	87 $\nu_{\text{CH}}$
a'	—	2919 s	2911	C-H stretching	81 $\nu_{\text{CH}}$
a'	2912 s	—	2902	C-H stretching	90 $\nu_{\text{CH}}$
a'	—	2900 m	2986	C-H stretching	74 $\nu_{\text{CH}}$ + 12 $\nu_{\text{CC}}$
a'	—	2863 s	2861	C-H stretching	86 $\nu_{\text{CH}}$
a'	—	2850 s	2851	C-H stretching	71 $\nu_{\text{CH}}$ + 21 $\nu_{\text{CC}}$
a'	2838 vs	—	2829	C-H stretching	91 $\nu_{\text{CH}}$
a'	2781 m	—	2778	C-H stretching	70 $\nu_{\text{CH}}$ + 18 $\nu_{\text{CC}}$
a'	2770 vw	—	2761	C-H stretching	88 $\nu_{\text{CH}}$
a'	2750 vw	—	2742	C-H stretching	84 $\nu_{\text{CH}}$
a'	—	2738 w	2731	C-H stretching	75 $\nu_{\text{CH}}$ + 11 $\nu_{\text{CC}}$
a'	2731 w	—	2721	C-H stretching	90 $\nu_{\text{CH}}$
a'	2706 w	—	2694	C-H stretching	89 $\nu_{\text{CH}}$
a'	2675 w	—	2671	C-H stretching	95 $\nu_{\text{CH}}$
a'	2663 m	2663 m	2658	C-H stretching	91 $\nu_{\text{CH}}$
a'	2644 w	—	2638	C-H stretching	81 $\nu_{\text{CH}}$
a'	—	2631 vw	2625	C-H stretching	74 $\nu_{\text{CH}}$ + 10 $\nu_{\text{CC}}$
a'	1463 vs	1463 vs	1460	C-H in plane bending	88 $\beta_{\text{CH}}$
a'	—	1450 vs	1442	C-H in plane bending	92 $\beta_{\text{CH}}$
a'	1437 vs	—	1429	C-H in plane bending	85 $\beta_{\text{CH}}$ + 10 $\beta_{\text{CC}}$
a'	1381 w	—	1376	C-H in plane bending	74 $\beta_{\text{CH}}$ + 16 $\beta_{\text{CC}}$
a'	—	1368 w	1359	C-H in plane bending	90 $\beta_{\text{CH}}$
a'	1350 w	1350 s	1341	C-H in plane bending	94 $\beta_{\text{CH}}$
a'	—	1338 m	1331	C-H in plane bending	81 $\beta_{\text{CH}}$ + 11 $\beta_{\text{CC}}$
a'	—	1325 m	1319	C-H in plane bending	94 $\beta_{\text{CH}}$
a'	1319 w	1313 w	1307	C-H in plane bending	96 $\beta_{\text{CH}}$
a'	1305 w	1303 w	1300	C-H in plane bending	72 $\beta_{\text{CH}}$ + 19 $\beta_{\text{CC}}$
a'	—	1275 vs	1268	C-H in plane bending	86 $\beta_{\text{CH}}$
a'	1263 w	—	1255	C-H in plane bending	89 $\beta_{\text{CH}}$
a'	—	1245 vs	1239	C-H in plane bending	70 $\beta_{\text{CH}}$ + 12 $\beta_{\text{CC}}$ + 10 $\nu_{\text{CC}}$
a'	1234 vw	—	1228	C-H in plane bending	90 $\beta_{\text{CH}}$
a'	1219 vw	1219 m	1216	C-H in plane bending	67 $\beta_{\text{CH}}$ + 34 $\nu_{\text{CC}}$
a'	1219 vw	1219 vw	—	C-C stretching	—
a'	1175 w	—	1170	C-H in plane bending	54 $\beta_{\text{CH}}$ + 44 $\nu_{\text{CC}}$
a'	1175 w	—	—	C-C stretching	—
a'	—	1163 m	1151	C-H in plane bending	51 $\beta_{\text{CH}}$ + 46 $\nu_{\text{CC}}$
a'	—	1163 m	—	C-C stretching	—
a'	1150 vw	1150 vw	1147	C-H in plane bending	55 $\beta_{\text{CH}}$ + 38 $\nu_{\text{CC}}$
a'	1150 vw	1150 vw	—	C-C stretching	—
a'	—	1125 vw	1118	C-C stretching	89 $\nu_{\text{CC}}$
a'	1114 vw	—	1107	C-C stretching	79 $\nu_{\text{CC}}$
a'	1088 vw	1084 m	1077	C-C stretching	69 $\nu_{\text{CC}}$ + 24 $\nu_{\text{CH}}$
a'	1075 w	1075 vs	1067	C-C stretching	88 $\nu_{\text{CH}}$
a'	1050 w	—	1041	C-C stretching	91 $\nu_{\text{CC}}$
a'	—	1037 m	1031	C-C stretching	89 $\nu_{\text{CC}}$
a'	1012 m	1012 vs	1007	CCC trigonal bending	87 $\beta_{\text{CCC}}$
a''	981 m	975 s	977	C-H out of plane bending	74 $\eta_{\text{CH}}$
a''	981 m	975 s	—	C-H out of plane bending	—
a''	963 s	—	961	C-H out of plane bending	82 $\eta_{\text{CH}}$
a''	963 s	—	—	C-H out of plane bending	—
a''	938 vw	—	927	C-H out of plane bending	76 $\eta_{\text{CH}}$ + 12 $\eta_{\text{CC}}$
a''	—	925 m	919	CH out of plane bending	84 $\eta_{\text{CH}}$
a''	—	925 m	—	C-H out of plane bending	—
a''	895 vw	895 w	890	C-H out of plane bending	78 $\eta_{\text{CH}}$ + 16 $\eta_{\text{CC}}$
a''	881 w	875 w	878	C-H out of plane bending	71 $\eta_{\text{CH}}$ + 20 $\eta_{\text{CH}}$
a'	850 m	850 m	847	CCC ring breathing	89 $\beta_{\text{CC}}$

a''	–	843 m	840	C-H out of plane bending	79 $\eta_{\text{CH}}$
a''	–	843 m	–	CH out of plane bending	–
a''	830 w	–	822	C-H out of plane bending	64 $\eta_{\text{CH}}$ + 26 $\eta_{\text{CC}}$
a''	800 vw	800 vw	786	C-H out of plane bending	74 $\eta_{\text{CH}}$
a''	800 vw	800 vw	–	C-H out of plane bending	–
a''	–	768 w	761	C-H out of plane bending	76 $\eta_{\text{CH}}$
a''	–	768 w	–	CH out of plane bending	–
a''	743 vw	738 vs	739	CH out of plane bending	80 $\eta_{\text{CH}}$
a''	743 vw	738 vs	–	CH out of plane bending	–
a'	600 w	600 w	592	CCC in plane bending	74 $\beta_{\text{CCC}}$ + 20 $\beta_{\text{CH}}$
a'	600 w	600 w	–	CCC in plane bending	–
a'	512 w	512 w	502	CCC in plane bending	88 $\beta_{\text{CCC}}$
a'	512 w	512 w	–	CCC in plane bending	–
a'	444 vw	450 w	437	CCC in plane bending	71 $\beta_{\text{CC}}$ + 23 $\beta_{\text{CH}}$
a'	–	438 w	431	CCC in plane bending	81 $\beta_{\text{CC}}$
a'	–	381 vs	372	CCC out of plane bending	72 $\eta_{\text{CC}}$ + 14 $\eta_{\text{CH}}$
a''	–	356 s	360	CCC out of plane bending	81 $\eta_{\text{CC}}$
a''	–	356 s	–	CCC out of plane bending	–
a''	–	321 m	320	CCC out of plane bending	76 $\eta_{\text{CCC}}$ + 20 $\eta_{\text{CH}}$
a''	–	290 m	279	CCC out of plane bending	68 $\eta_{\text{CCC}}$ + 26 $\eta_{\text{CH}}$
a''	–	250 m	236	CCC out of plane bending	61 $\eta_{\text{CCC}}$ + 32 $\eta_{\text{CH}}$

a' : In-plane vibrations, a'' : out-of plane vibrations, abbreviations used.

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 *cis*-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  $\Gamma_{\text{vib}} = 54 a' (\text{in-plane}) + 24 a'' (\text{out-of-plane})$ . 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 polarization of the Raman lines.

**Normal coordinate analysis:** In order to obtain a more complete description of the molecular motions involved in the normal modes of *cis*-decahydronaphthalene, a normal coordinate analysis has been carried out. 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<sup>5</sup>. The computer program for normal coordinate calculations developed by Fuhrer *et al.*<sup>6</sup>, 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 depolarization 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<sup>7</sup>.

**Potential energy distribution:** 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.

$$\text{PED} = \frac{F_{ii} L_{ik}^2}{\lambda_k}$$

where  $F_{ii}$  are the force constants defined by damped square technique,  $L_{ik}$  the normalized amplitude at the associated

element (i, k) and  $\lambda_k$  the eigen 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 DISCUSSION

The observed infrared and Raman frequencies and the calculated frequencies along with the PED of various modes of vibrations of *trans*-decahydronaphthalene and *cis*-decahydronaphthalene have been presented in Table-1. The assignment of frequencies is made as follows.

**C-H stretching:** The observed frequencies at 2631, 2644, 2663, 2675, 2706, 2731, 2738, 2750, 2770, 2781, 2838, 2850, 2863, 2900, 2912, 2919, 2938 and 2975  $\text{cm}^{-1}$  have been assigned to C-H stretching vibrations which agree with calculated frequencies. The PED calculation indicates that C-H stretching vibrational frequencies at 2631, 2738, 2781, 2850 and 2900  $\text{cm}^{-1}$  are mixed mode and there are little contributions from C-C stretchings also.

**C-C stretching:** The bands appear in the region 1200-900  $\text{cm}^{-1}$  are associated to C-C skeletal stretching modes. In the present work, the observed frequencies at 1037, 1050, 1075, 1084, 1114, 1125, 1150, 1163, 1175 and 1219  $\text{cm}^{-1}$  have been assigned to C-C stretching modes which agree with the calculated frequencies and also available literature<sup>8</sup>.

**In plane and out of plane bendings:** The observed frequencies at 1150, 1163, 1175, 1219, 1234, 1245, 1263, 1275, 1305, 1319, 1325, 1338, 1350, 1368, 1381, 1437, 1450 and 1463  $\text{cm}^{-1}$  are assigned to C-H in plane bendings which agree with calculated frequencies. The most of C-H in plane bending modes are not pure. The calculated frequencies at 1147, 1151, 1216, 1239, 1300 and 1331 of C-H in plane bendings are mixed mode and little contribution from C-C in plane bendings. CCC in plane bendings is assigned with the observed frequencies at 438, 450, 512 and 592  $\text{cm}^{-1}$ . They all agree with the calculated frequencies<sup>9-11</sup>.

The C-H out of plane bending vibrations occur between 1000 and 800  $\text{cm}^{-1}$ . The observed frequencies at 738, 768, 800, 830, 843, 881, 895, 938 and 963  $\text{cm}^{-1}$  have been assigned to C-H out of plane bendings, which agree with the calculated frequencies. The normal coordinate analysis shows that these modes are partially mixed with CCC out of plane bending vibrations. CCC out of plane bending vibrations are assigned to 250, 290, 319, 356 and 381  $\text{cm}^{-1}$  of observed frequencies which agree with the calculated frequencies. The PED calculation indicates that majority of these modes are mixed with CH out of plane bendings<sup>9-17</sup>.

### Conclusion

A complete vibrational spectra and analysis is reported in the present work for the first time for *cis*-decahydronaphthalene. The close agreement between the observed and calculated frequencies confirms the validity of the present assignment.

### REFERENCES

1. W.F Sayer and B.D. Walker, *J. Am. Chem. Soc.*, **60**, 2125 (1938).
2. T. Roels, S. Rastogi, J. De Rudder and H. Berghmann, *Macromolecules*, **30**, 7939 (1997).
3. H. Itagaki and Y. Nakatani, *Macromolecules*, **30**, 7793 (1997).
4. W.-C. Lai and C.S. Song, *J. Am. Chem. Soc.*, **40**, 1018 (1995).
5. L.E. Sutton, *The Interatomic Bond Distances and Bond Angles in Molecules and Ions*, London Chem., Soc., London (1983).
6. H. Fuhrer, V.B. Kartha K.G. Kidd, P.J. Krueger and H.H. Matsch, *Computer Program for Infrared Spectrometry, Normal Coordinate Analysis*, Ottawa, National Research Council, Canada, p. 5 (1976).
7. G. Varsanyi, *Assignments for Vibrational Spectra of Seven Hundred Benzene Derivatives Volume No. 7*, Adam Hilger, London (1974).
8. G. Socrates, *Infrared and Raman Characteristic Group Frequencies Tables and Charts*, John Wiley & Sons Ltd., edn. 3 (2001).
9. S. Mohan and R. Murugan, *Indian J. Pure Appl. Phys.*, **30**, 283 (1992).
10. S.R. Salman, *Spectrochim. Acta A*, **42**, 409 (1986).
11. N.B. Colthup, L.H. Daly and S.E. Wiberley, *Introduction to Infrared and Raman Spectroscopy*, Academic press, New York, edn. 2 (1975).
12. N.L. Alpert, W.E. Keiser and H.A. Szymanski, *IR Theory and Practice of Infrared Spectroscopy*, Plenum Press, New York (1970).
13. M. Avram and Gh. D. Mateescu, *Infrared Spectroscopy-Applications in Organic Chemistry*, Wiley-Interscience, New York (1970).
14. W. Kemp, *Organic Spectroscopy*, ELBS-McMillan, London (1979).
15. J.R. Dyer, *Applications of Absorption Spectroscopy of Organic Compounds*, Prentice Hall, Eagle wood Cliffs, N.J. (1965).
16. K. Nakanishi, *Infra-Red Absorption Spectroscopy-Practical*, Holden Day, San Francisco, California, USA (1962).
17. J.R. Durig, *Chemical, Biological and Industrial Applications of Infrared Spectra*, New York: Wiley (1985).