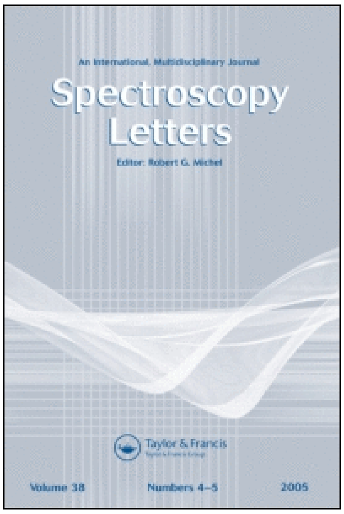

Spectroscopy Letters
Publication details, including instructions for authors and subscription information:
http://www.informaworld.com/smpp/title~content=t713597299

INFRARED SPECTROSCOPIC STUDIES OF POLYCYCLIC AROMATIC HYDROCARBONS IN SOLID WAX FILMS: ANTHRACENE AND PHENENTHRENE

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To cite this Article NaziruddinKhan, M. , Kumar, Pardeep , Garg, R. K. , Patel, B. S. and Zaidi, Z. H.(2002) 'INFRARED SPECTROSCOPIC STUDIES OF POLYCYCLIC AROMATIC HYDROCARBONS IN SOLID WAX FILMS: ANTHRACENE AND PHENENTHRENE', Spectroscopy Letters, 35: 4, 489 — 500

To link to this Article: DOI: 10.1081/SL-120013885

URL: http://dx.doi.org/10.1081/SL-120013885

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SPECTROSCOPY LETTERS, 35(4), 489–500 (2002)

INFRARED SPECTROSCOPIC STUDIES OF POLYCYCLIC AROMATIC HYDROCARBONS IN SOLID WAX FILMS: ANTHRACENE AND PHENENTHRENE

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ABSTRACT

Mid-infrared spectra of anthracene and phenanthrene from 2000–400 cm^{-1} are being investigated in wax films. Solid wax films technique is employed for vibrational study in infrared region for the first time. The harmonic frequency positions and relative intensities are compared with theoretical values obtained by Density Functional Theory (DFT) model and with gas-phase spectra. Excellent agreement in their spectral positions, strengths between the experiment and DFT calculations are observed. The effects on spectra due to change of

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matrix is also being discussed. Some additional bands in wax film are observed compared to gas-phase spectra, also supported by theoretical predicted values.

Key Words: Infrared spectroscopy; Polycyclic Aromatic Hydrocarbons; DFT

INTRODUCTION

The importance of including environmental issues in the traditional chemistry curriculum a growing as public concern for these issues heightens. Human population is exposed to large variety of natural and synthetic chemical compounds from various environmental sources such as air, water and food. Polycyclic aromatic hydrocarbons (PAHs), which comprise a major class of environmental contaminants, are predicted as potent carcinogens.[1] They are the dominant component of coals, coal derived liquids and an important by product of petroleum manufacture.[2] PAHs are also found in the burning of tobacco as well as during incomplete combustion of organic matter in wood and fossil fuels.[3,4] PAHs have been the subject of several classic investigations in molecular spectroscopy. Despite the considerable interest that attaches to the condensed aromatic hydrocarbons, the treatment of their molecular vibrations has been largely neglected. During the past decade evidences have been mounting that PAHs are important components of the interstellar medium.[5–7]

Recently, we have studied some PAHs by UV-Visible Spectroscopy[8–10] and Photoacoustic Spectroscopy,[11–12] which have explained non-radiative transitions in the UV–VIS region. Now, here an attempt is made to have a detailed mid-infrared spectroscopic analysis of anthracene and phenanthrene molecules in solid matrix (wax film). The infrared spectroscopic data for PAHs that are free from the perturbations of intermolecular interactions are very important. For this, a suitable matrix at low temperature is needed. Therefore, solid wax film is found excellent matrix for the infrared study and able to make at low temperature, which also can prepare easily. To properly address the astrophysical problem, a number of works of both theoretical and experimental effort has been brought over the last several years. No one has ever been used such matrix, we are using this technique for the first time and the task is found satisfactory. In this paper, we attempt to assign the observed bands in the solid wax films in comparison to gas-phase spectra and theoretical predicted values. The measurement is made in the range 2000–400 cm^{-1}. The study reveals some new bands. The experimental results are being compared with Density Functional

Theory (DFT) model. The importance of IR spectrometry as a tool of the practicing organic chemist is readily apparent from the number of literatures. Since IR spectrum of each molecular species is unique, IR is a powerful tool for the identification organic compounds. Infrared is also extremely useful in the elucidation of unknown structures and aid in the development of the polymer industry.

In earlier works, infrared spectroscopic of organic molecule studied in crystal and solution. S.Califano[13] investigated the infrared spectra of anthracene in the gas phase, in solution, in KBr pellets and in single crystals with polarized radiation. E.P. Krainov[14] carried out a calculation of frequencies and forms of the vibrations of the anthracene. Further, D.J. Evans and D.B. Scully[15] extensively carried out a normal co-ordinate treatment of the vibrations using a valence force field transferred from benzene. A. Bree and R.A. Kydd[16] reported the infrared spectrum of anthracene crystals. Latter, B.N. Cyvin and S.J. Cyvin[17] performed the spectroscopic analysis of the molecular vibrations of anthracene and calculated the mean amplitudes of vibration for some of its isotopic compounds. Arvid Bakke and coworkers[18] further investigated the five-parameter approximation of the in-plane force field of molecular vibrations of condensed aromatics including anthracene which compared the results from the celebrated method of Califano and Neto with collaborators.[19–22] An attempt had been made to completely assign the fundamental vibrational spectra of phenanthrene, including the analysis of the crystal spectrum in polarized light and normal coordinate treatment.[21] Later, some workers[23] reported a more detail of vibrational assignments of phenanthrene molecule for the ground and excited states. Further, vibrational spectrum of fully deuterated phenanthrene using the same method described in[24] was extensively investigated. The polarized infrared and Raman spectra of single crystals of phenanthrene and deuterated phenanthrene were re-investigated by some workers.[25] The Scaled Quantum Mechanical (SQM) force field at the MNDO level for the determining normal vibration of PAHs was also carried out.[26] Szczpanski et al.[27] investigated experimental studies in Argon (Ar) matrix and theoretical calculations of anthracene using RHF/3-21G and ROHF/3-21G with Gaussian 88 computer codes.[28] Stephen R. Langhoff[29] extensively determined the harmonic frequencies and intensities of the neutral molecules using density functional theory (Gaussian 92/DFT computer codes)

In addition to this, Jan M. L. Martin and co-workers[30] also studied the structure and vibrational spectrum of some PAHs including anthracene and phenanthrene by DFT (Gaussian 94 package). Recently, Douglas M. Hudgins groups[31] employed the matrix isolation technique to isolate individual PAH molecules in an argon matrix. Comparisons with the experimental data indicate that DFT does an excellent job of describing the majority of the infrared active fundamentals of the PAHs.

METHOD

Melvin E. Peterkin[32] developed a simple technique for far-IR studies of powders. He employed the technique of cold pressing and finely divided samples in a wax matrix having high melting point. This matrix does not have any absorption in the far-IR spectral range (40–400 cm^{-1}).

About 10 g of wax or equivalent is placed in a 2 oz covered can. The whole is emerged in liquid nitrogen for several minutes, and then removed using an insulating material and vigorously hand – shaken for 20 sec. The resulting powder is then shifted through a 20-mesh screen (or finer if desired) and kept at moderate to cool temperature until used. An appropriate amount of sample is placed in a stoppered vial along with sufficient powdered wax to give the required thickness of final disk. The mixture should be well shaken to obtain a uniform sample. The die may be any suitable vacuum die. The bottom face should be covered with a precut disk of thin polyethylene film. The sample wax mixture is poured in a smooth out to an even thickness. Another polyethylene film disk is placed on the top of the sample. After evacuation, the die is held at about 600 psi for about 30 m sec and then removed. The polyethylene films adhering to the sample may be removed or left in place as situation demands.

EXPERIMENTAL

By adopting the above technique, we have extended the study for paraffin wax in IR spectral region. The wax matrix is almost transparent over the 400–2000 cm^{-1} spectral region. A weighed quantity of solid wax and PAH was taken into a mortar for fine grinding and the mixture was transferred in a crucible. The fine mixture was heated into a furnace up to 70°C at which temperature it melted. After 15–20 min the PAH was homogeneously dissolved in the wax and the molten mixture was quickly cast between the two glass plates spaced about 0.1 mm apart. After cooling to the room temperature, the wax formed a very thin transparent film and was removed from the glass plates. Anthracene and phenanthrene were obtained from M/S Fluka AG (Switzerland) and solid wax was obtained from M/S Central Drug House (P) Ltd (India). An FT-IR spectrometer (Nicolet Instrument Corporation. U.S.A. Model 410-IMPACT) was used to record the spectra of the samples. Mid-Infrared spectra (4000–400 cm^{-1})

were collected using a DTGS detector/KBr beam splitter combination. All spectra reported here were measured at $1\,\mathrm{cm}^{-1}$ resolution.

RESULTS AND DISCUSSION

Anthracene

The anthracene molecule belongs to the symmetry point group D_{2h}, and its 66 normal vibrations are distributed in the following way among the symmetry types:

$$\Gamma = 12A_{1g} + 5A_{1u} + 11B_{1g} + 6B_{1u} + 4B_{2g} + 11B_{2u} + 6B_{3g} + 11B_{3u}$$

For the free molecule (gaseous state) only the normal modes belonging to the species B_{1u}, B_{2u} and B_{3u} are active in infrared. Vibrations of types A_u is completely forbidden both in infrared and in Raman spectra, while those of species A_{1g}, B_{1g}, B_{2g} and B_{3g} are allowed only in the Raman spectrum.[14] Figures 1 and 2 show the 2000–400 cm^{-1} spectrum of solid matrix isolated anthracene. The frequency positions and strengths of the absorption bands

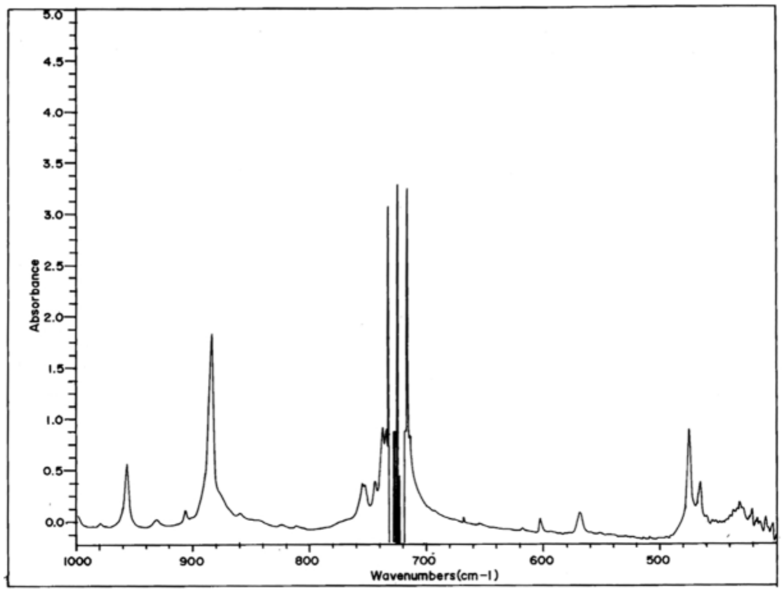

Figure 1. Infrared spectrum of neutral anthracene in solid wax films in 1000–400 cm^{-1}.

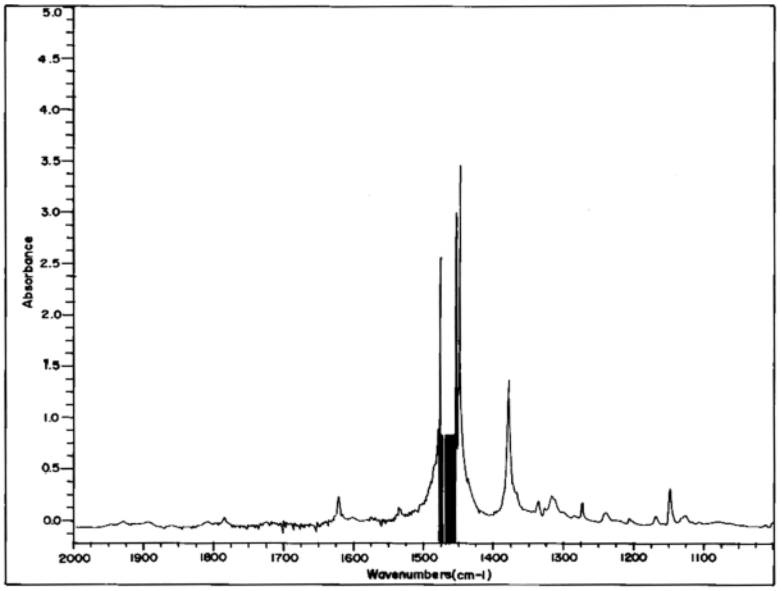

Figure 2. Infrared spectrum of neutral anthracene in solid wax films in 2000–1000 cm^{-1}.

are listed in Table 1, together with their DFT calculated values[29] and experimental data of Hudgins et al.[31] and Szczepanski et al.[27]

DFT calculations predict 17 fundamental bands out of which 6, 7 and 4 bands are of B_{1u}, B_{2u} and B_{3u} symmetry groups respectively.

In the experimental spectrum, we have observed 19 bands. The strongest band predicted at 730.2 cm^{-1} is correlated with the observed band 724.3 cm^{-1}. All the observed bands are in accordance with the theoretical values except the predicted band at 1157 cm^{-1}, which is, absent in experiment. The average difference in frequencies of predicted and observed bands is about 4 cm^{-1}. Hudgins[31] observed 33 bands of anthracene in Ar matrix out of which 18 matches with the predicted bands. Szczepanski reported 22 bands, which are in accordance with theoretical values.

When we compare our results with the work reported by Hudgins and Szczepanski et al, we find that our assignments of some bands are in better agreement with the theoretical calculations. For an instance, the relative strength of feature at 997.8 cm^{-1} directly corresponds to the theory at 1000.7 cm^{-1}, which was in discrepancy earlier.

Our observations indicate that the band assignments for the 1316.3 and 1335.5 cm^{-1} features are in better agreement with the predicted

Table 1. Infrared Frequencies and Relative Intensities for Neutral Anthracene

DFT Freq. (int) cm^{-1}	Hudgins Freq. (int) cm^{-1}	Szczepanski Freq. (int) cm^{-1}	Present Work Freq. (int) cm^{-1}
			465.2(0.10)
471.3(0.23)	468.0(0.20)	468.0,470(0.29)	473.9(0.23)
			568.4(0.06)
612.7(0.10)	602.9(0.09)	603(0.14)	602.0(0.03)
			715.8(0.53)
730.2(1.00)	725.6,729.6(1.00)	726,729(1.00)	724.3(1.00)
885.3(0.84)	878.3(0.77)	878.5(0.68)	883.4(0.50)
908.0(0.02)	906.8,908.5(0.01)	908(0.02)	905.6(0.02)
962.0(0.11)	954.9(0.07)	955,958(0.07)	956.4(0.12)
1000.7(0.04)	1000.9(0.08)	1001(0.07)	997.8(0.04)
1156.2(0.06)	1149.2(0.07)	1149,1151(0.04)	1147.4(0.08)
1157.7(0.04)			
1169.3(0.01)	1166.9(0.05)	1167,1169(0.03)	1167.2(0.01)
1274.6(0.13)	1272.5(0.06)	1272(0.05)	1272.0(0.04)
1311.2(0.03)	1318.1(0.10)	1318(0.12)	1316.3(0.06)
1342.6(0.05)	1345.6,1346.4(0.02)	1346(0.01)	1335.5(0.03)
1455.3(0.05)	1450.5(0.04)	1450(0.05)	1447.3(0.46)
1456.1(0.03)	1460.0(0.03)	1460(0.04)	1452.7(0.46)
1533.7(0.06)	1542.0(0.08)	1540,1542(0.04)	1534.3(0.02)
1620.0(0.10)	1610.5(0.02)	1627(0.12)	1620.3(0.06)
	1783.0(0.01)		

intensities than Hudgin and Szczepanski et al. reports. The experimentally observed 1147.4 and 1167.2 cm^{-1} bands (relative intensities 0.08 and .0.01 respectively) are related to the theoretically predicted bands at 1156.2, 1157.7 and 1169.3 cm^{-1} (0.06, 0.04, and 0.01 respectively). So far as the assignment of the observed band at 1620.3 cm^{-1} is concerned, it is in agreement directly with the predicted 1620.0 cm^{-1}, as H_2O contaminant falls in the 1630–1590 cm^{-1}. However, the possibility of H_2O contaminant is very less in wax film since it is not hygroscopic. Thus, the band 1620.3 cm^{-1} may assign to fundamental mode of molecule. We observe two new bands at 465.2 and 568.4 cm^{-1} for the first time.

Theoretical calculations do not give such frequencies in this region, but the relative strengths in experimental results are favorably strong as compared with other bands in the spectrum. No such bands have been observed in earlier matrix isolation studies of anthracene. Moreover, observed band at 465.2 cm^{-1} is in accordance with the anthracene crystal band at 456 cm^{-1} reported by A. Bree et al[16]assigned to symmetry type B_{3u}.

These experimentally observed bands are not being obtained theoretically due to limitations in the DFT model.

Phenanthrene

The infrared spectrum of phenanthrene in solid wax film is shown in Figs. 3 and 4. The frequency positions and relative values from 2000–400 cm^{-1} is presented in Table 2 and are compared to experimental gas phase spectra and theoretical values calculated using DFT. The results of solid phase spectra are in close agreement with theoretical values. Average difference in observed band positions and predicted match lies within 2.5 cm^{-1}. A few new bands are observed in solid phase spectra but these are in accordance with theoretical values. In Table 2, the observed bands are compared with DFT method and gas phase bands.

The position of observed bands at 430.2 and 441.6 cm^{-1} corresponds to the predicted values at 430.2 and 440 cm^{-1}. Due to involve-

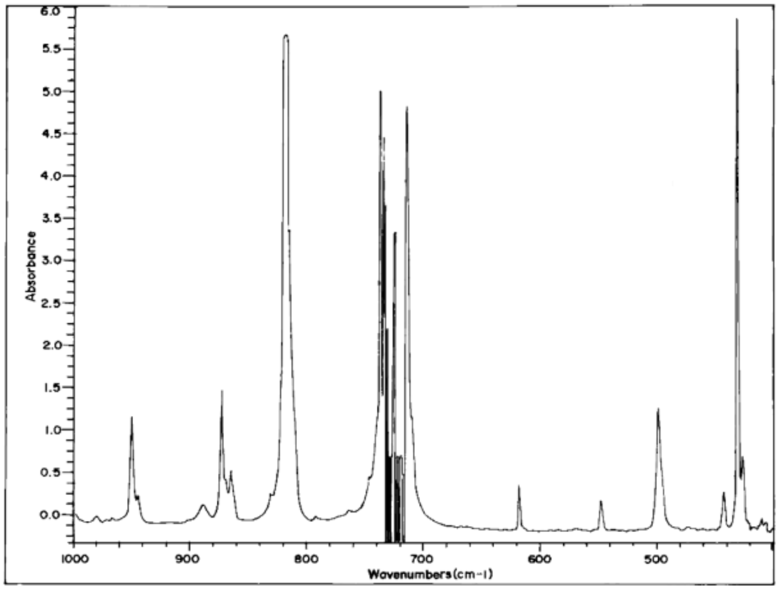

Figure 3. Infrared spectrum of neutral phenanthrene in solid wax films in 1000–400 cm^{-1}.

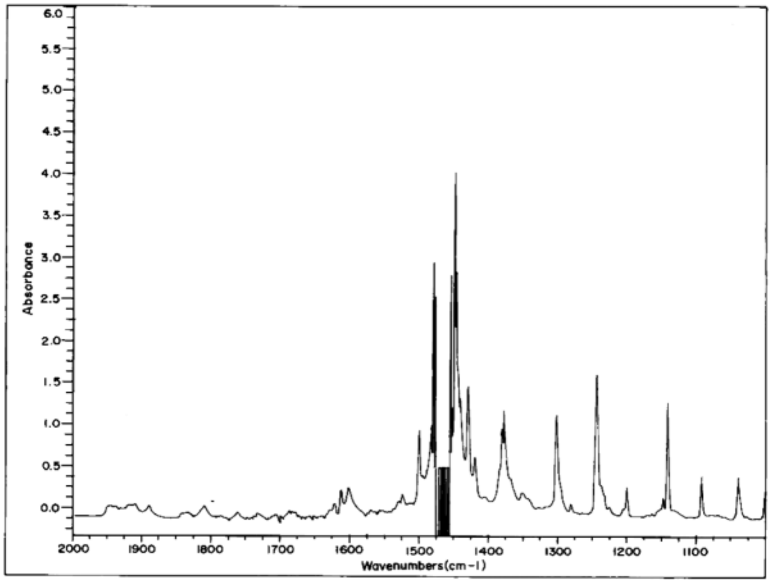

Figure 4. Infrared spectrum of neutral phenanthrene in solid wax films in 2000–1000 cm^{-1}.

ment of much overtone/combination bands in the region, the intensity of the most intense band probably is enhanced. These bands are not being observed in Ar matrix. The observed bands at 441.6 cm^{-1} and 498.7 cm^{-1} are in accordance with the predicted values at 440.0 cm^{-1} and 498.4 cm^{-1}. The strongest band in experimental is appeared at 819.8 cm^{-1} which agree with theoretically predicted value at 736.6 cm^{-1} and observed band at 736.9(0.86) cm^{-1} matches with the theory value at 817.0 (0.80). All of these bands are observed in C-H out-of-plane bending and C–C in plane banding region in both experimental results. The intensities of few features at 869.3, 872.6 cm^{-1} are correlated with theory value 871.4 cm^{-1}. The experimental bands 943.8, 949.7 cm^{-1} are in agreement with the predicted value at 950.3 cm^{-1}. All the observed bands in cm^{-1} at 1147.0, 1199.7, 1243.5 and 1302.2 match with the calculated values at 1148.3, 1203.0, 1250.3 and 1298.8 respectively. The feature at 1377.3 cm^{-1} (0.11) and 1379.7 cm^{-1} (0.08) is observed only in this matrix. Both bands are attributable to C–C stretching in molecule. As in the anthracene spectrum, the 800–700 cm^{-1} bands appear overlap with overtone/combination bands and few more bands in the 1400–1500 cm^{-1} region show same situation.

Table 2. Infrared Frequencies and Relative Intensities for Neutral Phenanthrene

Hudgins Ar Matrix cm^{-1}	DFT Method cm^{-1}	Wax Film Solid Matrix cm^{-1}
		425.6(0.14)
	430.5(0.07)	430.2(0.74)
	440.0(0.02)	441.6(0.06)
494.0(0.04)	498.4(0.05)	498.0(0.24)
	546.7(0.04)	
617.5,618.8(0.06)	627.8(0.06)	617.3(0.08)
710.2,714.5(0.04)		713.7(0.84)
735.0(1.00)	736.6(1.00)	736.9(0.86)
812.8(0.69)	817.0(0.80)	819.8(1.00)
833.0(0.02)		830.7(0.04)
864.9(0.12)	870.2(0.02)	864.7(0.09)
877.6(0.02)	871.4(0.15)	869.3,872.6(0.25)
948.2(0.03)	950.3(0.06)	943.9,949.7(0.20)
1000.5,1003.7(0.02)	999.0(0.02)	999.7(0.04)
1039.9,1044.3(0.06)	1038.3(0.06)	1038.6(0.08)
1094.5,1095.9(0.02)	1093.0(0.01)	1091.5(0.07)
1144.1(0.03)	1148.3(0.02)	1147.0(0.02)
1202.7(0.03)	1203.0(0.03)	1199.7(0.04)
1245.8,1250.6(0.11)	1250.3(0.13)	1243.5(0.26)
1302.9(0.04)	1298.8(0.02)	1302.2(0.19)
1351.4(0.01)		
1419.0(0.01)	1417.8(0.01)	1418.3(0.07)
1460.4(0.14)	1461.7(0.19)	1447.5(0.63)
1504.7,1505.9(0.09)	1497.3(0.10)	1499.1(0.13)
1530.1,1531.8(0.02)	1521.9(0.02)	1522.9(0.01)
1597.9(0.01)	1595.1(0.06)	1600.7(0.05)
1602.8(0.004)	1610.5(0.01)	1612.7(0.04)

Numerous complex bands are not considered in the assignment because those bands are not predicted by theory, which may be failure in calculation. As compared to anthracene spectra, phenanthrene has more number of bands in the C–C stretch and C–H in plane band region and relative strengths also much greater. All the fundamental frequencies observed in solid wax matrix are in good agreement with theoretical values and spectra in gases phase. Newly observed features at 430.2 and 441.6 cm^{-1} may also be assigned as fundamental vibration due to the C–C out-of-plane bending. Moreover, the interaction in inert matrix and molecule is stronger than the inert matrix in gases phase.

CONCLUSION

Mid infrared spectra of neutral anthracene and phenanthrene are measured in solid wax films in 2000–400 cm^{-1}. Wax film is found excellent solid matrix for the infrared study of PAHs in the 2000–400 cm^{-1} spectral region and can provide unique spectral information of such compounds.

The experimental results are in good agreement with the theoretical predicted values. The observed spectra in this film are more distinguished than the other phase spectra and those additional bands in this film are supported by theoretical values.

The number of band features in the solid wax matrix are more observed than the number of bands appeared in gases phase matrix of anthracene and phenanthrene and the theoretical results predicted by DFT are in better agreement with our experimental result than the Hudgin and Szczepanski results.

ACKNOWLEDGEMENTS

The authors gratefully acknowledge the UGC and AICTE for financial support. The authors are also thankful to Dr. M. Husain, Jamia Millia Islamia, New Delhi for useful discussions and suggestions.

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Received January 3, 2002
Accepted May 13, 2002