Proc. Indian natn. Sci. Acad., **57**, A, No. 2, 1991, pp. 151-154.
© Printed in India.

VIBRATIONAL SPECTRA OF *META*-NITROBENZOPHENONE

S MOHAN AND N SUNDARAGANESAN

Raman School of Physics, Pondicherry University, JIPMER Campus, Pondicherry 605 006, *India*

(*Received* 13 *August* 1990; *Revised* 10 *January* 1991; *Accepted* 18 *March* 1991)

The infrared and Raman spectra of *m*-nitrobenzophenone were recorded on a Perkin-Elmer IR 983 double beam grating spectrophotometer with Ar^+ laser source. The observed frequencies have been assigned to various modes of vibrations in terms of fundamentals, overtones, combinations, asssuming C_s point group symmetry.

Key Words: Laser Excited Raman Spectrum; Infrared Spectrum; *Meta*-Nitrobenzophenone Vibrational Analysis

Introduction

The characteristic frequencies of diphenyl group were first reported by Cannon and Sutherland[1]. The infrared and laser Raman spectra of diphenyl molecule have been reported by Geiss and Sandroni[2] and Malligarjuna Rao and Narayanaswamy[3]. There is no report in the literature on the frequencies of *meta*-nitrobenzophenone. Hence, the present investigation has been undertaken to study the vibrational spectra of *m*-nitrobenzophenone. The assignments are made on the basis of C_s point group symmetry and they are accurate to ± 1 cm^{-1}. As all the normal vibrations could not be identified in the IR and Laser Raman spectra, it is not possible to carry out the normal coordinate analysis for this molecule in the present work.

Experimental

Spectroscopically pure chemicals were obtained from Tokyo Kasei Kogyo Co. Ltd., Japan and were used as such.

The infrared spectra of *m*-nitrobenzophenone in a KBr disc was recorded on a Perkin-Elmer IR 983 double beam grating spectrophotometer in the region 4000-200 cm^{-1}. The laser Raman spectrum was obtained from a powder sample using a Cary Model 82 grating spectrophotometer and 488 nm radiation from an argon ion laser excitation, operating at 4 W. The spectral width was 2 cm^{-1} and the scanning speed was 30 cm^{-1} min^{-1}. The observed infrared and Raman spectra are shown in Figs 1 and 2. The frequencies for all the sharp bands are accurate to ± 1 cm^{-1}.

Results and Discussion

The observed frequencies of *m*-nitrobenzophenone and the relative intensities and probable assignments are given in Table I. The observed spectra are explained on the basis of C_s point group symmetry for the molecule under consideration. Since there are 26 atoms, 72 vibrational fundamental frequencies are classified as:

$$\Gamma_{vib} = 49\ a'\ (\text{planar}) + 23\ a''\ (\text{non-planar})$$

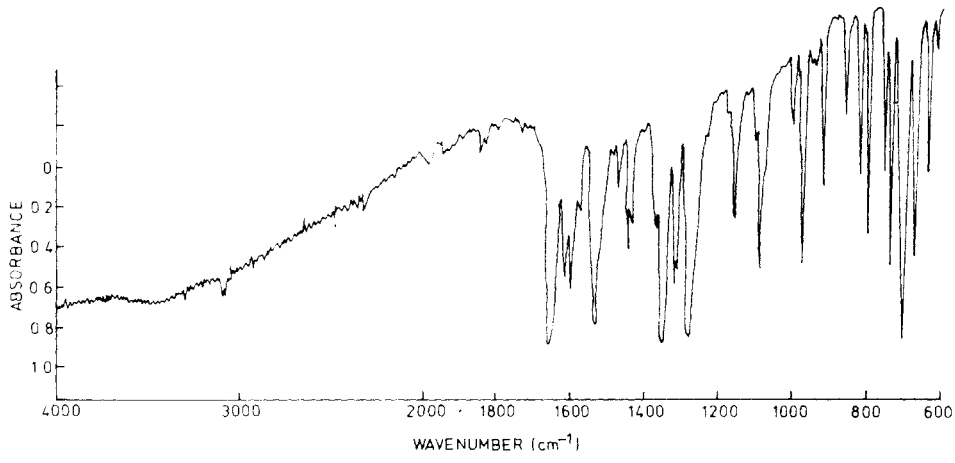

Fig 1 IR spectrum of *meta*-Nitrobenzophenone

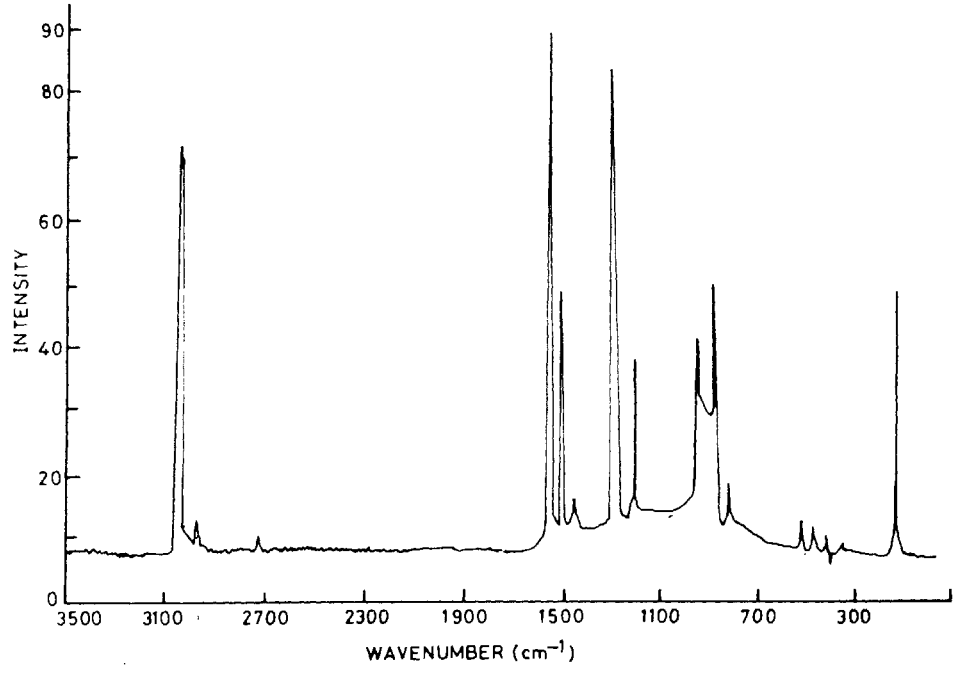

Fig 2 Raman spectrum of *meta*-Nitrobenzophenone

All the vibrations are active in both the infrared and raman spectra. Assignments have been made on the basis of similar assignments in spectra of molecules of similar structure[4-8]. These assignments are in good agreement with literature values reported by Stephenson *et al.*[9] and Brown *et al.*[10]

Table I

Assignments of vibrational frequencies (in cm^{-1}) of meta-nitrobenzophenone

Species	IR frequency and intensity	Laser Raman frequency and intensity	Assignment
1	2	3	4
	3302 W		2 × 1655
a'	3100 W	3090 S	C – H aromatic stretching
a'	3080 W	3062 W	C – H aromatic stretching
a'	—	2740 W	C – H stretching in Ketone group
	2480 VW	—	(1315 + 1158)
	2325 W		2 × 1158
	1975 VW		(1086 + 919)
	1950 W		(1100 + 859)
	1850 VW		(1086 + 751)
	1801 W		(998 + 800)
a'	1736 VW		C = O stretching
a'	1655 VW		C = O stretching
a'	1610 VS		C = C stretching
a'	1595 S	1585 VS(P)	C = C stretching
a'	1532 W		N = O asymmetric stretching
a'	1489 VS	1576 M(P)	C = C stretching
a'	1471 W		C = C stretching
a'	1445 W		C = C stretching
a'	1370 W	1360 VS	C = C stretching
a'	1354 VS		C = C stretching
a'	1321 VS		N = O symmetric stretching
a'	1315 W	1325 W	C – H in plane bending
a'	1309 M		C – NO_2 stretching
a'	1282 VS		C – H in plane bending
a'		1258 M	C – H in plane bending
a'	1158 S		C – H in plane bending
a'	1100 W		C – H in plane bending
a'	1086 VS		C – H in plane bending
a'	1011 S		C – C – C trigonal bending
a''	998 S		C – H out of plane bending
a''	985 S		C – H out of plane bending
a''	919 VS	937 M	C – H out of plane bending
a''	859 VS	867 M	C – NO_2 in plane bending
a'	815 W		C – C ring breathing vibrations

Contd.

(*Table* 1 *contd.*)

1	2	3	4
a″	800 VS		C – H out of plane bending
a″	751 VS		C – H out of plane bending
a″	738 VS	747 W	C – H out of plane bending
a′	706 VS		C – C – C in plane bending
a″	673 VS		C – C – C out of plane bending
a″	638 VS		C – C – C out of plane bending
a′	616 S		C – C – C in plane bending
a″		571 W	C – NO_2 out of plane bending
a′		457 W	C – C – C in plane bending
a″		420 W	C – C – C out of plane bending
a″		398 W	C – C – C out of plane bending
a″		260 M	C – C – C out of plane bending

VS—Very strong; S—Strong; M—Medium; W—Weak; VW—Very weak, P—Polarised.

Further, it is interesting to note that the fundamental vibrations assigned in the Raman spectrum agree favourably well with the infrared spectrum of the compound.

References

1 G G Cannon and G B B M Sutherland *Spectrochim Acta* **4** (1951) 373
2 F Geiss and S Sandroni *Spectrochim Acta* **22** (1966) 242
3 K Mallikarjuna Rao and C K Narayanaswamy *Indian J pure appl Phys* **8** (1970) 100
4 L J Bellamy *The Infrared Spectra of Complex Molecules* New York: John Wiley
5 D F Eggers and W E Lingren *Anal Chem* **28** (1956) 1328
6 J H S Green *Spectrochim Acta* **18** (1962) 39
7 W D Mross and G Zundel *Spectrochim Acta* **26A** (1970) 1097
8 H G Silver and J L Wood *Trans Farad Soc* **60** (1964) 5
9 C V Stephenson, W C Coburn and W S Wilcon *Spectrochim Acta* **17** (1961) 933
10 J F Brown *J Am chem Soc* 77 (1955) 6341