

Infrared and Laser Raman Spectral Studies of 2-Cyanopyridine

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The infrared absorption ($4000\text{--}200\text{ cm}^{-1}$) and laser Raman Spectra ($3500\text{--}100\text{ cm}^{-1}$) of 2-cyanopyridine are reported. An assignment of fundamentals is proposed and its comparison with similar molecule is included.

INTRODUCTION

Infrared and Raman spectra of pyridine and its various mono-substituted derivatives have been studied by several investigators.¹⁻³ Since the study of these compounds is significant as they play an important role in nucleic acids, Mochizuki *et al.*⁴ have reported the systematic study of the electronic absorption and Raman spectra of pyridine and its derivatives. The electronic spectra have also been studied by various investigators to know the complete vibrational studies of aminopyridines.^{5,6}

In order to study the substituted pyridines, the present study has been done to observe the complete vibrational (infrared and Raman) study of 2-cyanopyridine which has not been reported earlier. The present study also includes the complete assignment and comparison with similar molecules.

EXPERIMENTAL

Spec-pure compound 2-cyanopyridine has been obtained from M/s Sigma Aldrich Foreign Holding Company (USA) and used as such without further purification. However, its purity has been confirmed by elemental analysis and melting point determination (m.pt. of 2-cyanopyridine is $24\text{--}27^\circ\text{C}$). Infrared spectra have been recorded on Hitachi-250-70 IR spectrophotometer in the region $4000\text{--}200\text{ cm}^{-1}$ using KBr pallet. Raman spectra has been recorded on Bruker IFS 66V FTIR instrument with FT Raman attachment (FRA 106 Raman Module) in the region $3500\text{--}100\text{ cm}^{-1}$.

RESULTS AND DISCUSSION

The structure, infrared and Raman spectra of 2-cyanopyridine have been shown in Fig. 1 and Fig. 2. The ring fundamentals has been compared with pyridine (Innes *et al.*⁷).

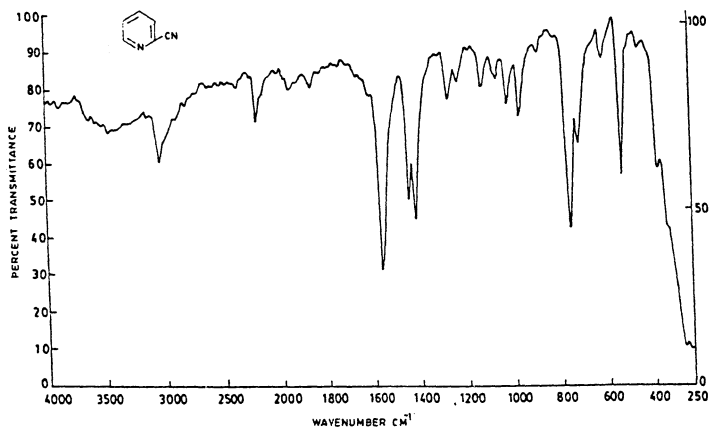


Fig. 1 Infrared spectrum of 2-cyanopyridine

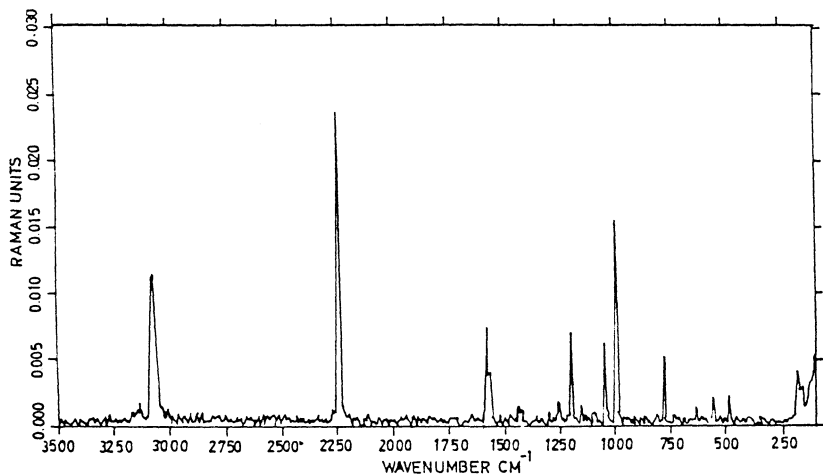


Fig. 2 Laser Raman spectrum of 2-cyanopyridine

The molecule 2-cyanopyridine belongs to C_{2v} point group symmetry and its 30 normal vibrations can be divided into various species as

$$11a_1 + 10b_2 + 3a_2 + 6b_1$$

The C—H stretching vibrations are very much prominent in the spectrum of benzene and its substituted derivatives and are highly characteristic of the aromatic ring itself. In the present study, one C—H stretching vibration is well assigned in the region $3100\text{--}3000\text{ cm}^{-1}$. This is well co-related with assignment

given by the investigator in the various substituted pyridines^{1,7}. The frequency has been well assigned in the Raman mode at 3067 cm^{-1} .

TABLE-1
ASSIGNMENTS OF VIBRATIONAL FREQUENCIES OF
2-CYANOPYRIDINE (ALL VALUES IN cm^{-1})

IR		Raman	Assignments
2-Cyanopyridine	Pyridine	2-Cyanopyridine	
3460 w	—	—	$\nu(\text{C—H})$
3040 s	3054	3067 ms	$\nu(\text{C—H})$
2830 sh	—	—	—
2200 s	—	2237 vs	$\nu(\text{C—CN})$
1960 mw	—	—	ν ring
1618 sh	—	—	ν ring
1560 vvs	1583	1581 vs	ν ring
1440 vs	1439	1433 vvw	$\nu(\text{C—C}), \text{CN}$
1415 vs	1381	—	$\nu(\text{C—C}), \text{CN}$
1270 ms	1276	1253 w	$\beta(\text{C—C})$
1240 ms	—	—	ring vibration
1135 s	—	—	$\beta(\text{C—N})$
1070 s	1030	1045 w	ring vibration
1020 s	—	—	$\beta(\text{C—N})$
970 vs	992	992 ms	ring breathing
885 w	886	—	$\gamma(\text{C—H})$
740 vvs	—	778 w	trigonal bending
720 mb	700	—	$\gamma(\text{C—C})$
610 ms	—	633 vw	$\gamma(\text{C—C})$
540 vs	—	—	$\beta(\text{C—C})$
—	—	479 w	$\gamma(\text{C—C})$
460 s	429	—	$\gamma(\text{C—C})$
—	—	176 mw	$\beta(\text{C—CN})$

ν —stretching, β —in-plane bending, γ —out-of-plane bending, s—strong, vs—very strong, vvs—ver very strong, ms—medium strong, w—weak, vw—very weak, vvw—very very weak, sh—shoulder

In all substituted benzenes, four bands are usually observed in the region 1650–1400 cm^{-1} . In pyridine these bands are usually observed in the region 1600–1400 cm^{-1} as suggested by Bellamy². Consequently four bands corresponding to ν_{19b} , ν_{19a} , ν_{8a} and ν_{8b} have been assigned to ring CC and CN stretching mode. These vibrations are well assigned and correlated with the study of Pyridine⁷.

Hussain *et al.*⁸ assigned ring breathing mode at 994 cm^{-1} in 2-chloropyridine. Recently Salik *et al.*⁹ assigned this frequency at 820 cm^{-1} in substituted pyrimidines. Considering these facts, this frequency has been assigned at 970 cm^{-1} in infrared spectra and Raman value at 992 cm^{-1} has been well correlated in the present study. Green and Harrison¹⁰ assigned the Raman lines at 172 cm^{-1} to the CN in-plane bending mode^{10, 11}. In the present study, a Raman value at 176 cm^{-1} has been assigned to this mode. All other assignments to modes are given in Table-1 and are well assigned.

ACKNOWLEDGEMENT

One of the authors, M. Isaq is thankful to UGC, New Delhi for financial assistance.

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(Received: 27 March 1998; Accepted: 9 June 1998)

AJC-1511