

Vibrational Analysis of 6-Methyl 2-Pyridyl Formamide

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The infrared spectrum of 6-methyl 2-pyridyl formamide has been recorded in the region $4000\text{--}200\text{ cm}^{-1}$, using KBr pellet. Probable assignments to the observed bands are made on the basis of magnitude and relative intensities of the recorded spectrum. The assignments made in the present study are in good agreement with the earlier assignments proposed by several investigators on some similar type of molecules.

INTRODUCTION

Pyridine and its derivatives are of considerable importance, because of their biological and pharmaceutical applications¹. The vibrational assignments of pyridine were first reported by Wilmfurst and Bernstan² and later modified by Green *et al*³. The present investigation is undertaken in order to extend the study of 2-pyridyl formamide reported earlier⁴, by adding methyl group in the 6th position of the pyridyl ring. The observed frequency shifts in the spectrum of the title compound are due to the addition of methyl group, with 2-pyridyl formamide. In general pyridine derivatives belong to C_{2v} point group symmetry, but in this compound the substituents of formamide in the second position and the methyl group in the sixth position of the pyridine ring have made the molecule asymmetrical. Moreover, the compound is newly synthesized and hence reliable X-ray reports are not available to fix the point group for vibrational analysis of species, which are required for normal coordinate analysis. Therefore, no attempt for a normal coordinate analysis could be made.

EXPERIMENTAL

Spectroscopically pure solid sample of 6-methyl 2-pyridyl formamide was obtained as gift and it was used as such. The infrared spectrum of the molecule was recorded on Perkin-Elmer model 599 spectrometer, using KBr pellet technique, in the region $4000\text{--}200\text{ cm}^{-1}$. The frequencies for all sharp bands are accurate to $\pm 1\text{ cm}^{-1}$.

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RESULTS AND DISCUSSION

The molecular structure of the title compound has been shown in Fig 1. The observed frequencies of 6-methyl 2-pyridyl formamide with their probable

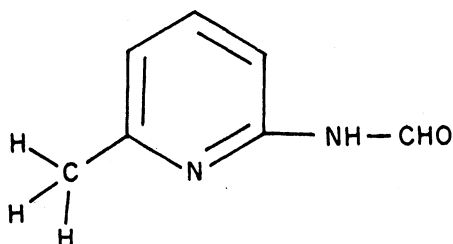
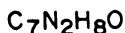


Fig. 1. 6-Methyl-2-pyridyl formamide

assignments are presented in Table-1. Assignments to the observed bands are made in analogy with the assignments proposed by the earlier investigators. The vibrational analyses are discussed in the following paragraphs.

N—H vibrations: In all the primary aromatic amines the N—H stretching vibrations⁵⁻⁷ occur in the region 3500–3300 cm^{-1} . Hence, in the present study, the medium band observed at 3315 cm^{-1} has been assigned to N—H stretching vibrations.

C—H vibrations: The heterocyclic aromatic compound shows the presence of C—H Vibrations⁸ in the region 3100–3000 cm^{-1} . In this region bands are not much affected due to the nature of the substituents. Hence, in the present work, the bands identified at 3210 cm^{-1} and 3160 cm^{-1} have been designated to C—H stretching modes of vibrations. These assignments are in good agreement with an earlier work on 2-pyridyl formamide.⁴

C=O vibrations: The strong band observed at 1685 cm^{-1} in 6-methyl 2-pyridyl formamide has been designated to C=O stretching modes of vibrations, which is in good agreement with our earlier assignments, and it is found that there is no much frequency shift in C=O stretching vibrations between 2-pyridyl formamide and 6-methyl 2-pyridyl formamide.

C—C vibrations: Bands between 1650 cm^{-1} and 1400 cm^{-1} in benzene derivatives are assigned to these modes of vibrations.⁹ In the present investigation the bands at 1570 cm^{-1} , 1560 cm^{-1} and 1460 cm^{-1} have been designated to C—C stretching vibrations.

C—CH₃ vibrations: The bands identified at 1445 cm^{-1} and 1435 cm^{-1} have been designated to C—CH₃ asymmetric and symmetric modes of vibrations respectively. These conclusions agree favourably with earlier workers.¹⁰ In 2-pyridyl formamide, these modes are absent.

C—N vibrations: The strong bands at 1330 cm^{-1} and 1310 cm^{-1} have been assigned to C—N stretching modes of vibrations, which is in good agreement with the assignments made by Horak *et al.*¹¹ for aromatic compounds.

TABLE-I
OBSERVED INFRARED FUNDAMENTALS OF 6-METHYL 2-PYRIDYL FORMAMIDE
AND ASSIGNMENTS

IR frequencies (cm ⁻¹)	Intensity	Assignments
3315	m	N—H Stretching
3210	w	C—H stretching
3160	s	C—H stretching
1685	s	C=O stretching
1595	s	N—H in-plane bending
1570	sh	C—C ring stretching
1560	sh	C—C ring stretching
1460	s	C—C ring stretching
1445	sh	C—CH ₃ asymmetric stretching
1435	sh	C—CH ₃ symmetric stretching
1415	m	C—CH ₃ stretching
1370	s	C—C stretching
1330	s	C—N stretching
1310	s	C—N stretching
1250	sh	Pyridine —CH ₃ stretching
1230	sh	N—H in-plane bending
1220	sh	C—H in-plane bending
1205	s	C—H in-plane bending
995	s	Ring breathing mode
950	w	Ring breathing mode
825	s	C—H out-of-plane bending
795	sh	C—H out-of-plane bending
560	s	Ring deformation
525	s	C—C deformation
360	m	Ring deformation

s = strong, m = medium, w = weak, sh = shoulder

In-plane vibrations: The strong bands identified at 1595 cm⁻¹ and 1230 cm⁻¹ have been designated to N—H in-plane bending modes of vibrations. The bands at 1220 cm⁻¹ and 1205 cm⁻¹ have been assigned to C—H in-plane bending vibrations. These assignments are made in analogy with the assignments proposed by Ohsaku *et al.*¹² and Hendra *et al.*¹³

Out-of-plane vibrations: The bands observed at 825 cm⁻¹ and 795 cm⁻¹ are due to C—H out-of-plane bending vibrations, which fairly agree with the assignments of Ohsaku *et al.*¹⁴

ACKNOWLEDGEMENT

Thanks in due to Professor C.R. Gopinath to provide 6-methyl 2-pyridyl formamide as gift sample for this study.

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(Received: 8 November 1994; Accepted: 9 March, 1995).

AJC-951