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FTIR Spectroscopic Study of 2-Hydroxy-4-methyl Pyrimidine Hydrochloride

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The FTIR absorption spectrum of 2-hydroxy-4-methyl pyrimidine hydrochloride has been recorded on Perkin Elmer spectrophotometer and analyzed in the region 4000-400 cm^{-1} using Nujol mull technique. The modes of vibration for the different fundamentals have been proposed. The group sensitive fundamentals are compared with those of similar molecules.

Key Words: FTIR, 2-Hydroxy-4-methylpyrimidine hydrochloride.

INTRODUCTION

Inspite of great biological importance of N-heterocyclic molecules like pyrimidine, cytosine uracil and their derivatives, lesser spectroscopic work has been carried out on pyrimidine compounds[1,2]. Although the vibrational spectra of some disubstituted pyrimidines have been studied by some workers[3]; but very little work appears on the FTIR spectra of disubstituted pyrimidines. N-Heterocyclic molecules like pyrimidine, uracil and cytosine also show a great importance as they play a central role in the structure and properties of nucleic acids[4-6]. Hence the present investigation has been undertaken to study the infrared spectrum of 2-hydroxy-4-methyl pyrimidine hydrochloride and to identify the frequencies of different modes of vibration in the molecule.

EXPERIMENTAL

The spec-pure grade sample of 2-hydroxy-4-methyl pyrimidine hydrochloride (2,4-HMP-HCl) (Fig. 1) was obtained from M/s Aldrich Chemie, Germany and used as such. The purity of the compound was also confirmed by elemental analysis and melting point determination. The FTIR absorption spectrum of 2,4-HMP-HCl was recorded on Perkin Elmer spectrophotometer in the region 4000-400 cm^{-1} using Nujol mull technique.

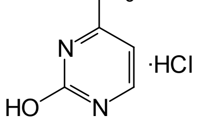

Fig. 1. Structure of 2-hydroxy-4-methyl pyrimidine hydrochloride

RESULTS AND DISCUSSION

The observed fundamental frequencies and their proposed assignments are given in Table-1.

TABLE-1
ASSIGNMENTS OF FREQUENCIES OF 2,4-HMP-HCl
(All values are in cm^{-1})

FTIR frequencies	Intensity	Assign.	FTIR frequencies	Intensity	Assign.
432	ms	(O–H) torsion, (H–Cl) wagging	1377	ms	CH_3 sym. def.
512	s	γ(C–N)	1403	s	CH_3 asym. def.
530	s	β(C–CH_3)	1426	s	ν ring
588	s	β(C–OH)	1523	ms	ν ring
611	w	γ(C–C), γ(N–H)	1556	ms	ν(C–C)
761	s	Ring breathing, C–N–C trigonal bending	1581	s	ν(C–C)
837	s	γ(C–H)	1627	s	ν(C–N)
919	ms	β(C–C)	1650	ms	ν(C–N), ν(N–H)
925	s	β(C–N), C–C–C trigonal bending	2900	ms	ν sym. CH_3
1026	ms	β(C–N)	2949	w	ν asym. CH_3
1035	ms	CH_3 rocking	2981	s	ν asym. CH_3
1158	s	β(C–H)	3010	vw	ν(C–H)
1190	ms	ν(C–CH_3)	3038	vw	ν(C–H)
1230	s	β(O–H)	3154	s	ν(N–H)
1250	s	ν(C–OH)	3460	w	ν(O–H)

Ring vibration

The molecule 2,4-HMP-HCl is a disubstituted pyrimidine, so two C-H valence oscillations are expected in the region 3100-3000. Thus, two bands at 3038 and 3010 cm^{-1} have been assigned to C–H stretching mode in the study of present molecule. These assignments are in good agreement with the literature values[6,7].

In disubstituted pyrimidine derivatives, two modes of vibration remain almost unchanged and are called C–H in-plane bending and out-of-plane bending vibrations. The C–H in-plane and C-H out-of-plane bending modes lie in the region 1500-1000 and 1000-750 cm^{-1}, respectively[8,9], in view of this the bands at 837 and 1158 cm^{-1} represent the C–H in-plane and C–H out-of-plane bending modes.

In the present study the two C–C stretching vibrations have been assigned at 1581 and 1556 cm^{-1}, while the C–C in-plane bending mode has been observed at 919 cm^{-1} and the C–C out-of-plane bending vibration is identified at 611 cm^{-1}. In the present molecule 2,4-HMP-HCl a C–C–C trigonal bending vibration is also observed at 925 cm^{-1}. These assignments are satisfied with the work of earlier workers[8,10].

Singh *et al.*[3] assigned the C–N stretching mode in the region 1650-1400 cm^{-1}, while Yadav *et al.*[13] assigned this mode at 1560 cm^{-1} in disubstituted pyrimidine. In view of this the bands at 1650 and 1627 cm^{-1} have been assigned as C–N stretching mode. The two C–N in-plane bending and a single out-of-plane bending modes are observed at 925, 919 and 512 cm^{-1}, respectively in the present investigation, while a C–N–C trigonal bending is detected at 761 cm^{-1} in the molecule 2,4-HMP-HCl, which finds support with the work of earlier researchers[11,12].

In the present molecule N–H stretching, in-plane bending and out-of-plane bending modes of vibration are possible due to the migration of H^+ atom of HCl to the N atom of the ring[15]. So the band observed at 3154, 1650 and 611 cm^{-1} have been assigned as N-H stretching, in-plane bending and out-of-plane bending vibrations in the present study which is in good agreement with the earlier literature[13,14].

With the support of earlier literature[10,11] the few bands have been assigned at 1523, 1426 and 761 cm^{-1} as ring stretching and ring breathing modes.

C-X Vibration

Singh *et al.*[9] have assigned C–OH stretching mode at 1301 and 1260 cm^{-1} in dihydroxy pyrimidine. In the present study the band observed at 1250 cm^{-1} has been assigned as C–O–H stretching mode while a band at 588 cm^{-1} is observed as C–OH in-plane bending vibration in the present molecule.

Mohan *et al.*[17] have assigned to C–CH_3 stretching vibration at 1200 cm^{-1} in 2,4,6-D MHP. In the present investigation the band observed at 1190 cm^{-1} in 2,4-HMP-HCl has been taken to represent C–CH_3 stretching mode. Yadav *et al.*[10] have observed the C–CH_3 in-plane bending mode at 570 cm^{-1}, while in the molecule 2,4-HMP-HCl the band identified at 530 cm^{-1} as C–CH_3 in-plane bending vibration.

Group vibration

–OH Group: The –OH group gives rise to three characteristic vibrations *i.e.* stretching, in-plane bending and out-of-plane bending. Molecules containing –OH group, the O–H valance oscillation appears in the region 3700-3450 cm^{-1}. Patel and Simoes[15] have assigned this mode at 3500 cm^{-1}. In view of this a band observed at 3460 cm^{-1} have been assigned as O–H stretching mode, while the bands observed at 1230 and 432 cm^{-1} are identified as O–H in-plane bending and O-H torsion modes, respectively in the present investigation, which is in good agreement with the literature values[16].

–CH_3 Group: The C–H stretching and C–H deformation due to methyl group have been assigned in their respective region in Table-1. The CH_3 rocking mode has been identified at 1035 cm^{-1}. In the methyl group there are three C–H stretching vibrations are possible, one being symmetric and the other two asymmetric[17]. The frequencies of asymmetric vibration are higher than that of symmetric. In the present case the frequencies 2981 and 2949 cm^{-1} have been assigned to asymmetric stretching while the frequency 2900 cm^{-1} has been assigned to symmetric stretching. In the present investigation two CH_3 symmetric deformation modes have also been identified at 1403 and 1377 cm^{-1}. These are in good accordance with the values reported in the literature[17].

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