

## NOTE

**Fourier transform infrared and laser Raman spectral analysis of 5-fluorouracil**V KRISHNAKUMAR, N SUNDARESAN\* and A NATARAJAN<sup>†</sup>*Department of Physics, Nehru Memorial College  
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The FTIR of 5-fluorouracil was recorded in the region 400–4000  $\text{cm}^{-1}$  and its Raman spectrum in the region 200–4000  $\text{cm}^{-1}$ . The spectra have been analysed by assuming that the molecule belongs to  $C_s$  point group symmetry. The assignments of the infrared and Raman bands are made on the basis of magnitude and relative intensity of the observed bands.

Recent spectroscopic studies of uracil and its derivatives<sup>1,2</sup> have been motivated by their biological importance. Detailed band assignments are not possible for such type of molecules because of their high complexity and low symmetry. In the present note we report the vibrational spectra of 5-fluorouracil.

5-fluorouracil is a fluorinated pyrimidine derivative obtained from M/s Sigma Chemical Co, USA. The FTIR spectra was recorded in KBr disc on perkin-Elmer FTIR Spectrometer in the region 400–4000  $\text{cm}^{-1}$ . The laser Raman spectrum was recorded in the standard 90° configuration in the region 200–4000  $\text{cm}^{-1}$  on Dilor Z-24 Raman Spectrometer. Argon-ion laser operating at 200 mW power continuously on the 488.0 nm line was used as the laser source.

From the structural point of view, the molecule has been assumed to belong to  $C_s$  point group. The 30 fundamental modes of vibration of the molecule may be classified as 21 in-plane and 9 out-of-plane vibrations. The observed frequencies together with their relative intensities and probable assignments are presented in Table 1. As the Table 1 is self explanatory, therefore, we shall discuss here only some important modes.

**N–H Stretching Vibrations :** According to Bellamy<sup>4</sup> the N–H stretching vibrations of aromatic compounds occur in the region 3300–3500  $\text{cm}^{-1}$ . Accordingly, the bands at 3349  $\text{cm}^{-1}$  and 3290  $\text{cm}^{-1}$  are designated to represent N–H stretching modes.

**C–H Stretching Vibrations :** Heterocyclic aromatic compounds like uracil and its derivatives are structurally very close to benzene. The C–H stretching

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frequency of such compounds<sup>4</sup> fall nearly in the region  $3020\text{ cm}^{-1}$ . Hence the strong bands observed at  $3194\text{ cm}^{-1}$  and  $2943\text{ cm}^{-1}$  are assigned to  $\nu(\text{C-H})$  modes.

Table 1. Assignments of the vibrational frequencies of 5-fluorouracil

IR	Raman	Assignments	IR	Raman	Assignments
3349 vs	—	$a'$ $\nu$ (N-H)	1039 s	1090 w	$a'$ $\beta$ -ring
3290 s	—	$a'$ $\nu$ (N-H)	1022 w	1014 s	$a''$ $\gamma$ (C-H)
3194 s	2923 s	$a'$ $\nu$ (C-H)	980 w	—	$a'$ C-H bending
2943 s	2811 vs	$a'$ $\nu$ (C-H)	914 w	—	$a''$ $\gamma$ (N-H)
1686 s	—	$a'$ $\nu$ (C=O)	893 w	—	$a''$ $\gamma$ (C-H)
1649 m	—	$a'$ $\nu$ (C=O)	851 m	—	$a''$ $\gamma$ (N-H)
1588 m	—	$a'$ $\nu$ (C=C)	820 m	—	$a''$ $\gamma$ (C-H)
1539 m	—	$a'$ $\beta$ (N-H)	800 m	—	$a''$ $\beta$ (C-N-C)
1463 m	1434 m	$a'$ $\nu$ -ring	776 w	—	$a'$ $\gamma$ (C-N)
1400 m	—	$a'$ $\beta$ (C-H)	714 w	—	$a''$ $\phi$ (N-H)
1341 m	—	$a'$ $\nu$ (C=C-F)	630 w	—	$a'$ $\nu$ (C-F)
1306 w	—	$a'$ $\nu$ (C=C-F)	586 w	—	$a'$ $\beta$ (C-F)
1282 s	—	$a'$ $\nu$ (C-N)	527 m	—	$a''$ $\gamma$ (C-F)
1217 m	—	$a'$ $\beta$ (N-H)	470 w	—	$a''$ $\gamma$ (C-F)
1157 w	—	$a'$ $\beta$ (C-H)	450 w	451 w	$a''$ $\gamma$ (C=O)

vs—very strong, s—strong, m—medium, w—weak,  $\nu$ —stretching,  $\beta$ —in-plane bending,  $\gamma$ —out-of-plane bending,  $\phi$ —wagging.

**C=O Vibrations** : Although the two C=O groups of the uracil derivatives are in chemically different environments, they seem to be interacting with each other within the uracil molecule<sup>5</sup>. The interaction of carbonyl groups with a hydrogen donor group does not produce drastic characteristic changes in the frequency of C=O. In the earlier work on pyridine derivatives<sup>2</sup> the band at  $1680\text{ cm}^{-1}$  was assigned to  $\nu(\text{C=O})$ . Consideration of these factors lead to assign the bands observed at  $1686\text{ cm}^{-1}$  and  $1649\text{ cm}^{-1}$  to  $\nu(\text{C=O})$  vibrations. The lower frequencies observed at  $450\text{ cm}^{-1}$  in IR and at  $451\text{ cm}^{-1}$  in Raman are assigned to  $\gamma(\text{C=O})$  modes.

**C=C Stretching Vibrations** : In the present work, the band observed at  $1588\text{ cm}^{-1}$  is assigned to C=C stretching. This assignment is in good agreement with the literature values available for aromatic compounds<sup>6</sup>.

**In-Plane Vibrations** : The bands observed in the region  $1539\text{--}1217\text{ cm}^{-1}$  are assigned to N-H in-plane bending modes. These assignments are also supported by the literature values<sup>5</sup>. The weak band at  $1157\text{ cm}^{-1}$  is designated as C-H in-plane bending vibration.

**Ring Vibrations** : Fairly medium bands observed in the region  $1465\text{--}1430\text{ cm}^{-1}$  were assigned to ring vibrations for aromatic compounds by the earlier workers<sup>2</sup>. Accordingly, the medium bands observed at  $1463\text{ cm}^{-1}$  in I.R. and  $1434\text{ cm}^{-1}$  in Raman spectra in the present study are assigned to ring stretching

vibrations.

**Out-of-Plane Bending Vibrations :** The vibrational frequencies observed in the region  $893\text{--}851\text{ cm}^{-1}$  are assigned to C–H and N–H out-of-plane bending vibrations respectively. These assignments are in good agreement with the earlier work<sup>7</sup>. The larger frequency shifts of  $\nu(\text{N–H})$  and  $\gamma(\text{N–H})$  suggest that the interaction is stronger<sup>8</sup>.

**C–F Stretching Vibrations :** The frequencies observed in the region  $1400\text{--}1306\text{ cm}^{-1}$  are assigned to C=C–F stretching modes. The literature values available for these modes of vibrations and the observed values are quite comparable<sup>9</sup>. The band in the region  $586\text{ cm}^{-1}$  is assigned to  $\beta$  (C–F) vibration. The bands at  $527\text{ cm}^{-1}$  in IR and at  $470\text{ cm}^{-1}$  in Raman are assigned to  $\gamma$  (C–F).

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