LETTERS TO THE EDITOR

MEAN SQUARE AMPLITUDES FOR THE IN-PLANE VIBRATIONS IN ACETANILIDE AND DEUTERATED ACETANILIDE

THE authors in their earlier investigation have carried out the normal co-ordinate treatment of acetanilide and N-Deuterated acetanilide[1] using the general quadratic potential function as a force field. The calculation of potential energy distribution of each normal mode among various symmetry co-ordinates has enabled the authors to discuss the nature of the Amide I, Amide II and Amide III bands in acetanilide and N-Deuterated acetanilide. These results have indicated that the Amide I band is due to (C=O) stretch and the Amide II and Amide III bands are due to the combined contributions of δ (N–H) and ν (C–N) modes of vibrations as in the case of N-Methyl acetamide[2].

In the present note, we report the mean square amplitudes and the mean amplitudes of vibration of the various linkages of the acetanilide and N-Deuterated acetanilide using the 'L' matrix method. The mean square amplitudes of vibration is given by $L \Delta \tilde{L}$, where $\tilde{L}$ is the transpose of the L matrix and Δ is the diagonal matrix with elements

$$\Delta_k = \langle Q_k^2 \rangle = \frac{h}{8\pi^2 \nu_k} \coth\left(\frac{h\nu_k}{2kT}\right)$$

Where $\langle Q_k^2 \rangle$ is the mean square of the kth normal co-ordinate. The mean square amplitudes and the mean amplitudes at temperatures 0° K and 300° K are given in Table I.

TABLE I

Mean square amplitudes and mean amplitudes of various linkages in acetanilide and N-Deuterated acetanilide

Bond and mode of vibration	Molecule	Mean square amplitudes (in Å²) at		Mean amplitudes (in Å) at	
		T = 0° K	T = 300° K	T = 0° K	T = 300° K
ν (C–N)	Acetanilide	0·001872	0·001914	0·0433	0·0438
	Deuterated Acetanilide	0·001853	0·001876	0·0430	0·0433
ν (C=O)	Acetanilide	0·001636	0·001650	0·0404	0·0406
	Deuterated Acetanilide	0·001639	0·001652	0·0405	0·0410
ν (C–CH_3)	Acetanilide	0·002522	0·002635	0·0502	0·0513
	Deuterated Acetanilide	0·002525	0·002622	0·0504	0·0512
ν (N–C_6H_5)	Acetanilide	0·001626	0·001773	0·0403	0·0421
	Deuterated Acetanilide	0·001613	0·001734	0·0401	0·0416

The mean amplitudes of vibration of ν (C=O) and ν (C–N) in acetanilide and N-Deuterated acetanilide are lower than that of the same linkages in N-Methyl acetamide[2]. The variation of the mean amplitude of vibration with temperature is observed to be small in all these linkages.

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1. Venkata Chalapathi, V. and Venkata Ramiah, K., *Proc. Indian Acad. Sci.*, 1968, **67**, 184.
2. — and —, *Ibid.*, 1966, **64**, 148.