VAPOR-PHASE RAMAN SIGNATURE BANDS AND AB INITIO CALCULATIONS OF 3-METHYLINDOLE

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3-Methylindole (3MI), which is a structural model for the tryptophan side chain in proteins, has been investigated using vapor-phase infrared and Raman spectroscopy. The vapor Raman spectrum identifies the signature of the indolyl moiety free of intermolecular interaction. We have also utilized ab initio calculations to refine and extend previous vibrational assignments. The present results provide an improved basis for assessing the dependence of the indolyl Raman signature on the local environment of the tryptophan side chain of proteins. The vapor Raman bands at 3506, 1585, 1409, 1349/1341 (Fermi doublet) and 881 cm^{-1} differ greatly from their counterparts in the spectrum of the liquid and thus serve as spectral markers of the intermolecular interactions of the indolyl ring environment. The maximum value of the Fermi doublet intensity ratio (3.0) is observed for 3MI vapor, while the minimum value (0.43) is observed for 3MI in $CHCl_3$ solution.