RAMAN STUDY OF 6-AZACYTIDINE AND RELATED COMPOUNDS

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Summary

Raman spectra of 6-azacytidine (6-azaC) in the microcrystalline state and in various solutions (H_2O) , D_2O , and DMSO) are measured for the first time. On the basis of the comparison with the measured Raman spectra of related compounds such as microcrystals of cytidine, cytosine, 5-azacytidine, and 6-azacytosine and solutions of cytidine, the main spectroscopic feature of the substitution of a CH group in the 6^{th} position of a pyrimidine base ring for an N atom is revealed as the absence of the low-frequency component of a characteristic doublet of cytidine in the region 1200–1300 $\rm cm^{-1}$. Blue shifts of some Raman peaks in $\rm D_2O$ solutions of 6-azaC and cytidine are observed. Apparently, they may be connected with the transformation of intramolecular H-bonds into D-bonds. In addition, improved X-ray data for 6-azaC single crystals are obtained.