VIBRATIONAL TRANSITION MOMENT ANGLE STUDY OF URACIL AND THYMINE IN HELIUM NANODROPLETS

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Infrared spectroscopy has been used to characterize the vibrational bands in the NH stretching region for uracil(U) and thymine(T) monomers in helium nanodroplets. Each monomer shows only a single isomer, the global minimum, in agreement with previous experimental and theoretical studies. The assignment of the infrared vibrational bands in the spectra is aided by the measurement of the corresponding vibrational transition moment angles (VTMAs) and ab initio frequency calculations. The ambiguity in the VTMA assignment of the N3H band for the urail monomer is explained by the presence of dimer bands, which are overlapped with the monomer band.

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