Guanine – A combined study using vibrational spectroscopy and theoretical methods

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Abstract

The present work reports a conformational study of solid-state anhydrous guanine, using vibrational spectroscopy techniques – infrared, Raman and inelastic neutron scattering – coupled to quantum mechanical methods at the DFT level, both for the isolated molecule and the condensed state. In both cases, the 7H-keto-amino tautomer was found to be the prevalent form, contrary to aqueous solutions and hydrated polycrystalline guanine, where the 9H-keto-amino tautomer is the most favoured species. This study is a significant contribution for the existing spectroscopic characterisation of this purine base, by unambiguously assigning its vibrational spectra.