

CONFORMATIONAL EQUILIBRIUM IN GLYCINE: EXPERIMENTAL JET-COOLED RAMAN SPECTRUM

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The first observation of a gas-phase spontaneous Raman spectrum of an amino acid – glycine (Gly, $\text{H}_2\text{NCH}_2\text{COOH}$) – is reported. A molecular beam source was combined with a high sensitivity Raman setup to record a low-frequency (below 500 cm^{-1}) vibrational spectrum. *Ab initio* (first principles; MP2) and density functional theory (DFT; BLYP, B3LYP, and PBE0/PBE1PBE) calculations with the aug-cc-pVTZ Dunning-type basis set were used to support vibrational assignments. Jet-cooling of glycine molecules was observed by varying the laser-nozzle distance. The acquired medium resolution spectra (4 cm^{-1}) allow the different glycine conformations to be distinguished. The structures of the two most stable glycine conformers, previously observed by electron diffraction and microwave spectroscopy, have been confirmed. Evidence is reported for a third conformation (*gauche-trans-trans*), which has not been previously experimentally reported. Band polarization measurements were used to confirm the vibrational assignments.