

## THE TWO MISSING CONFORMERS OF GAS-PHASE ALANINE: A JET-COOLED RAMAN SPECTROSCOPY STUDY

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The jet-cooled spontaneous Raman spectrum of an amino acid – alanine (Ala, 2-aminopropanoic acid;  $\text{H}_2\text{NCH}(\text{CH}_3)\text{COOH}$ ) – is reported. The low-frequency vibrational spectrum (below  $500\text{ cm}^{-1}$ ) was recorded and assigned using quantum chemical data: *ab initio* (MP2) and density functional theory (DFT; BLYP, B3LYP, and PBE0/PBE1PBE). Band polarization measurements were used to confirm the vibrational assignments. The acquired medium resolution spectra (HWHM of approximately  $4\text{ cm}^{-1}$ ) allow the different alanine conformations to be distinguished. Four alanine conformers were observed and identified: two previously reported by microwave (MW) spectroscopy studies and two that were previously unreported. A set of reasons for why these conformers eluded previous studies are discussed. Selective collisional relaxation processes in the jet (associated with low interconversion barriers between different alanine conformations) that depopulate the high-energy conformers were experimentally demonstrated. Conclusions about conformational equilibrium in peptide/protein building block are made.