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Mid-IR spectra of the bio-related molecules in the gas phase

YONGJUN HU, ELLIOT R. BENSTEIN, Department of Chemistry, Colorado State Univ. — Mid-IR spectra of gas phase bio-related molecules R-OH, R-COOH and simple non-aromatic amino acids, such as glycine and valine, detected by vacuum ultraviolet (VUV), 10.5 eV single photon ionization of supersonically expanded and cooled samples, are presented and discussed. Molecules and their fragment species, generated by a proton transfer reaction following ionization, are identified by time of flight mass spectroscopy. The fundamentals and overtones of the CH and OH stretches and some combination bands are identified in the spectra. Rotational resolution for the OH mode and its first overtone yield an estimate of ~ 50 K for the methanol monomer in the supersonic beam. Two neutral C_2H_5OH conformers can be identified by high sensitivity IR plus VUV nonresonant ionization and fragmentation detected (NRIFD-IR) vibrational spectroscopy. Free OH and NH stretches are missing in the spectrum of glycine and valine, indicating that the strong intramolecular hydrogen bonds are formed in these gas phase species.

Yongjun Hu
Department of Chemistry, Colorado State Univ.

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