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Probing Binding-Site Preferences in Propiolic Acid Complexes with Water and H2S inside Helium Nanodroplets

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Binary molecular complexes serve as model systems for probing hydrogen bond (HB) interactions and are studied using molecular beam and matrix isolation techniques, which favor the isolation of thermodynamically stable structures. In contrast, the helium nanodroplet (HND) technique, owing to its ultracold environment (0.4 K) and efficient energy dissipation, enables the kinetic trapping of higher-energy isomers, revealing a wider variety of hydrogen bonded motifs that are otherwise inaccessible.

Interaction of organic acids with small molecules are crucial in biology and atmospheric chemistry. So, we investigated the HB site preferences in 1:1 complexes of propiolic acid (HC≡C–COOH, PA) with D2O and H2S inside HNDs. Mass-selective vibrational spectra recorded in the C=O and C≡C stretching regions, complemented by MP2-computed harmonic IR spectra, confirmed the isolation of the cis-PA. Complexation with D_2O resulted in the formation of three isomers of the cis-PA···D2O. The dominant spectral features correspond to a kinetically trapped structure stabilized via a ≡C–H···OD_2 HB. Contrarily, PA···H_2S forms exclusively the global minimum structure, aggregated by two hydrogen bonds with the COOH moiety.

These findings demonstrate the balance of the dipole–dipole and higher order interactions in steering aggregation dynamics at 0.4 K. The polar D2O (1.85 D) and PA (1.59 D) promotes directional association, whereas the weaker dipole of H2S (0.97 D) favors the global minimum structure.

Keywords

Hydrogen bond, helium droplet, dipole steering, kinetic trapping

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