

CHARACTERIZATION OF OCS-HCCCCCH AND N₂O-HCCCCCH DIMERS: THEORY AND EXPERIMENT

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The infrared spectra of the weakly-bound dimers OCS-HCCCCCH, in the region of the ν_1 fundamental band of OCS (2050 cm^{-1}), and N₂O-HCCCCCH, in the region of the ν_1 fundamental band of N₂O (2200 cm^{-1}), are observed in a pulsed supersonic slit jet expansion probed with tunable diode/QCL lasers. Both OCS-HCCCCCH and N₂O-HCCCCCH were found to have planar structure with side-by-side monomer units having nearly parallel axes. These bands have hybrid rotational structure which allow for estimates of the orientation of OCS and N₂O in the plane of their respective dimers. Analogous bands for OCS-DCCCCD and N₂O-DCCCCD were also observed and found to be consistent with the normal isotopologues. Various levels of ab initio calculations were performed to find stationary points on the potential energy surface, optimized structures and interaction energies. Three stable geometries were found for OCS-HCCCCCH and two for N₂O-HCCCCCH. The rotational parameters at CCSD(T*)-F12c level of theory give results in very good agreement with those obtained from the observed spectra. In both dimers, the experimental structure corresponds to the lowest energy isomer.