THE ROTATIONAL SPECTRA AND STRUCTURES OF TWO ISOMERS OF THE HCCH-OCS DIMER

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Two isomers of the HCCH-OCS dimer have been characterized by pulsed supersonic nozzle, Fourier-transform microwave spectroscopy. The more stable isomer has the acetylene and OCS molecules aligned almost parallel, while the higher energy form is T-shaped, with the S atom of the OCS interacting with the triple bond of the acetylene. The experimentally determined structures will be compared to results obtained from a semi-empirical modeling program and *ab initio* calculations.