THE MOST STABLE ISOMER OF C_4H_2-$(OCS)_2$ VAN DER WAALS COMPLEX: THEORY AND EXPERIMENT CONFIRM A STRUCTURE WITH C_2 SYMMETRY

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We report the infrared spectrum of C_4H_2-$(OCS)_2$ trimer in the region of the ν_1 fundamental vibration of the OCS monomer. The van der Waals complexes are generated in a supersonic slit-jet apparatus and probed using a rapid-scan tunable diode laser. Both C_4H_2-$(OCS)_2$ and C_4D_2-$(OCS)_2$ are studied. Analysis of their spectra establishes that the trimer has C_2 symmetry. Theoretical calculations performed to find stationary points on the potential energy surface confirm that the experimental structure is the most stable form of the trimer. The rotational parameters computed using double hybrid functionals are in very good agreement with those obtained from the observed spectra.