INFRARED SPECTRA OF CARBONYL SULFIDE-ACETYLENE TRIMERS: OCS- $(C_2H_2)_2$ AND TWO ISOMERS OF $(OCS)_2$ - C_2H_2

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Spectra of acetylene-carbonyl sulphide trimers in the region of the OCS ν_1 fundamental (~2062 cm⁻¹) are observed using a tunable diode laser to probe a pulsed supersonic slit jet expansion. A previous microwave study of (OCS)₂- C₂H₂ by Peebles and Kuczkowski^a gave a nonplanar triangular twisted structure, which could be thought of as a polar OCS dimer plus a C₂H₂ monomer lying above the dimer plane. In the present work, three infrared bands are analyzed. The first band clearly belongs to this previously known (OCS)₂-C₂H₂ complex. The second band can be assigned as an isomer of (OCS)₂-C₂H₂ having a similar structure, but with a nonpolar OCS dimer plus a C₂H₂ monomer above the dimer plane. The third band is assigned to OCS-(C₂H₂)₂. The rotational constants and dipole moment components of all three bands are consistent with barrel shape structures having C₁, C₂ and C_s symmetries, respectively.

^aS.A. Peebles and R.L. Kuczkowski, J. Chem. Phys. 111, 10511 (1999).