INFRARED SPECTROSCOPY OF TWO ISOMERS OF THE OCS-CS_2 COMPLEX

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A second isomer of OCS-CS_2 complex, with a nonplanar cross-shaped structure, has been studied for the first time by analysing an infrared band in the region of the OCS stretching vibration (2062 cm^{-1}). This isomer has C_s symmetry and the observed band consists of purely c-type rotational transitions. The ground state rotational parameters are found to be A=0.07306 cm^{-1}, B=0.03325 cm^{-1} and C=0.02879 cm^{-1}, in good agreement with a previous semi-empirical calculation.[a] In addition, a hybrid band with a- and b-type rotational transitions has been assigned to be due to the known planar form of OCS-CS_2, as previously studied by microwave spectroscopy.[a] The spectra were recorded using a rapid-scan tunable diode laser spectrometer to probe a pulsed supersonic jet expansion. Calculations indicate that the planar isomer of OCS-CS_2 is the lowest in energy, in contrast to CO_2-CS_2 where the crossed form is believed to be the lowest.[b]

[a] J. J. Newby, M. M. Serafin, R. A. Peebles and S. A. Peebles, *Phys. Chem. Chem. Phys.* **7**, 487 (2005).
[b] C. C. Dutton, D. A. Dows, R. Eikey, S. Evans and R. A. Beaudet, *J. Phys. Chem. A* **102**, 6904 (1998).