ROTATIONAL SPECTRA AND STRUCTURES OF $(OCS)_2CO_2$ and $(OCS)_3$

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The structures of $(OCS)_2CO_2$ and $(OCS)_3$ have been determined from rotational spectra obtained using a pulsed nozzle Fourier transform spectrometer. The two trimers have a barrel like monomer arrangement commonly seen in similar complexes. In $(OCS)_2CO_2$, the two OCS units have an anti-parallel arrangement, like the OCS dimer, but twisted from planarity by 34°. The CO_2 straddles both of them in an approximately parallel orientation. In $(OCS)_3$, two of the OCS molecules are again nearly anti-parallel with the third OCS straddling them. Seven isotopic species were assigned for $(OCS)_2CO_2$. Two isotopic species were assigned for $(OCS)_3$, to supplement the normal species data previously reported.[a] The dipole moments of the trimers are consistent with the derived structures. Comparisons of the structures with results from a semi-empirical model including electrostatic, dispersion and repulsive terms will be presented.

[a] J.P. Connelly, A. Bauder, A. Chisholm and B. J. Howard, Mol. Phys. **88** (1996) 915