THE ROTATIONAL SPECTRA AND STRUCTURES OF THE HCCH-$(OCS)_2$ and OCS-$(HCCH)_2$ TRIMERS

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The two mixed trimers HCCH-$(OCS)_2$ and OCS-$(HCCH)_2$ have been identified and assigned by FTMW spectroscopy. Rotational constants and dipole moment components for both species are consistent with triangular, barrel-shaped configurations of the monomers.

The assignment of the rotational spectra of eight isotopomers for HCCH-$(OCS)_2$ enabled an unambiguous structure determination and the discovery that this trimer contains a polar OCS dimer fragment. The two OCS molecules are found to be aligned in an unusual parallel arrangement with their dipole moments reinforcing one another.

Four isotopomers of the OCS-$(HCCH)_2$ trimer were assigned. Due to a lack of isotopic data, a full structure determination was not possible. Semi-empirical calculations did, however, give a structure that aligned the acetylene monomers in a geometry intermediate between T-shaped and parallel that was consistent with the experimental data.