STRUCTURAL INVESTIGATION AND ANALYSIS OF INTERNAL MOTIONS IN THE DIMETHYL ETHER–CS_2 DIMER

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The microwave spectrum of the weakly bound dimer between dimethyl ether (DME) and carbon disulfide was first presented at the 60th International Symposium on Molecular Spectroscopy (talk RH13) and published in Chemical Physics Letters.[a] Experimental and ab initio rotational constants for the normal isotopomer were consistent with a structure in which the sulfur atom of CS_2 interacts with the lone pair on the oxygen atom of the DME. Recent assignment of the spectra of two additional isotopomers of DME–CS_2 allowed an inertial fit of the structural parameters to the observed moments of inertia as well as a Kraitchman analysis of the principal axis coordinates of the substituted atoms. These analyses lead to a structure in which the CS_2 axis is aligned roughly perpendicular to the heavy atom plane of DME. The structure has an R(O-C) distance of $4.570(8)$ Å and a DME center of mass–O–C angle of $115.7(9)^\circ$. In light of the additional structural data, the tunneling pathway of the CS_2 from one side of the DME to the other and the potential energy barrier to this inversion motion have been reexamined.

[a] S. A. Peebles, R. A. Peebles, J. J. Newby and M. M. Serafin, *Chem. Phys. Lett*, **410** (2005) 77.