INVERSION MOTIONS IN THE DIMETHYL ETHER–CARBON DISULFIDE DIMER

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The rotational spectrum of the 1:1 dimer formed between dimethyl ether (DME) and CS_2 has been assigned using Fourier transform microwave spectroscopy. The spectrum shows tunneling splittings of approximately 180 MHz in the c-type transitions and smaller splittings of a few hundred kilohertz in the a-type transitions. The splittings are attributed to a motion of the CS_2 between the lone pairs of the DME, causing an inversion of the c-component of the dipole moment. The $\Delta E(0^- - 0^+)$ splitting between the two tunneling states is $90.3411(14)$ MHz. The B and C rotational constants for the two states were fit separately, along with an average A rotational constant, giving values of $A = 8099.5906(12)$ MHz, $B_0 = 604.67510(18)$ MHz, $B_1 = 604.65215(18)$ MHz, $C_0 = 582.50781(23)$ MHz, and $C_1 = 582.55142(23)$ MHz. A barrier to the tunneling motion has been estimated using both ab initio techniques and the one dimensional model of Meyer.[a] Dipole moment components of $\mu_a = 0.961(1)$ MHz, $\mu_c = 1.104(1)$ MHz, and $\mu_{total} = 1.464(1)$ MHz have been measured and are also consistent with the CS_2 interacting with a DME lone pair.

[a] R. Meyer, *J. Mol. Spectrosc.*, **76** (1979) 266.