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 CS₂ has been assigned using Fourier transform microwave spectroscopy. The spectrum shows tunneling splittings of approximately 180 MHz in the e-type transitions and smaller splittings of a few hundred kilohertz in the α-type transitions. The splittings are attributed to a motion of the CS₂ between the lone pairs of the DME, causing an inversion of the c-component of the dipole moment. The ΔE(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, B₀ = 604.67510(18) MHz, B₁ = 604.65215(18) MHz, C₀ = 582.50781(23) MHz, and C₁ = 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. Dipole moment components of μₐ = 0.961(1) MHz, μₑ = 1.104(1) MHz, and μₐₑₐₜₒ₉ₑₑ = 1.464(1) MHz have been measured and are also consistent with the CS₂ interacting with a DME lone pair.