MICROWAVE INVESTIGATION OF C-H HYDROGEN BONDING INTERACTIONS IN THE DIMETHYL ETHER - OCS DIMER

JOSH J. NEWBY, REBECCA A. PEEBLES, and SEAN A. PEEBLES, *Department of Chemistry, Eastern Illinois University, 600 Lincoln Ave., Charleston, IL 61920 USA*.

The rotational spectrum of a weakly bound dimer formed between dimethyl ether and OCS has been observed by Fourier-transform microwave spectroscopy. The rotational constants of the normal isotopic species are found to be $A = 4069.4106(23)$ MHz, $B = 1431.7413(7)$ MHz and $C = 1074.2925(5)$ MHz and the dipole moment components are $\mu_a = 1.3046(25)$ D and $\mu_b = 0.8159(35)$ D. The rotational constants and dipole moment components are consistent with a heavy atom planar structure in which the OCS lies across the C_2 axis of the dimethyl ether (the O=C...O angle is estimated to be about 83° by *ab initio* calculation); the oxygen atom of OCS appears to interact with one of the methyl group hydrogen atoms. Isotopic shifts in the spectra of the DME-O^{13}CS and DME-OC^{34}S isotopomers have been found to be consistent with this structure. *Ab initio* optimizations at the MP2/6-311++G(2d,2p) level will be presented and shown to give very good agreement with the rotational constants obtained from experiment.