C–H HYDROGEN BONDING INTERACTIONS IN THE CARBONYL SULFIDE–FLUOROFORM DIMER

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The rotational spectrum of the weakly bound dimer of carbonyl sulfide (OCS) and fluoroform (HCF_3) has been assigned using Fourier-transform microwave spectroscopy. The rotational constants for the normal isotopomer are $A = 4745.7157(25)$ MHz, $B = 813.9222(27)$ MHz, and $C = 790.9238(27)$ MHz, and dipole moment components are $\mu_a = 0.828(4)$ D and $\mu_b = 0.858(7)$ D. The experimental rotational constants are found to be in very good agreement with ab initio optimizations at the MP2/6-311++G(2d,2p) level of calculation. This C_s symmetry structure has the OCS and HCF_3 aligned such that there is a C–H...O and C–F...C interaction, with an approximate C...C intermolecular distance of 3.60 Å.