MICROWAVE AND AB INITIO INVESTIGATIONS OF $CHCl_2F$–OCS AND RELATED HYDROCHLOROFLUOROCARBON COMPLEXES

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The microwave spectrum of the weakly bound dimer of Freon-21 ($CHCl_2F$) with OCS has been investigated by Fourier-transform microwave spectroscopy and ab initio calculations. The two equivalent chlorine atoms in $CHCl_2F$ lead to extensive hyperfine splittings in the spectra, and since they do not lie in any of the planes defined by the principal axes of the complex, all three off-diagonal elements of the quadrupole coupling tensor are expected to be nonzero. Initial analysis of the extensive hyperfine splitting from the two chlorine atoms leads to fitted rotational constants that are in excellent agreement with MP2/6-311++G(2d,2p) predictions for a structure with a 2.49 Å C-H...O interaction between the $CHCl_2F$ and OCS and a secondary interaction between the chlorine atoms from the $CHCl_2F$ and the carbon atom of the OCS (C...C $= 3.60$ Å; C...Cl $= 3.57$ Å). Ab initio structures for the $CHCl_2F$–CO_2, $CHClF_2$–OCS and $CHClF_2$–CO_2 complexes will also be examined and comparisons will be made to the analogous series of CH_nF_{4-n} ($n = 1 - 3$) complexes with OCS and CO_2.