HALOGEN BONDING VS HYDROGEN BONDING IN CHF_2I COMPLEXES WITH NH_3 AND $N(CH_3)_3$

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Ammonia and trimethylamine (TMA) were used to probe preference of hydrogen over halogen bonding in molecular complexes containing CHF_2I via chirped pulse Fourier transform microwave spectroscopy. The halogen bonded complex of TMA is $\approx$ 2 kJ/mol more energetically favourable (extrapolation to CCSD(T)/CBS level) than the hydrogen bonded complex. The reverse is true for the ammonia complex where the hydrogen bonded complex is $\approx$ 3kJ/mol more favourable. Although the spectra of both complexes were perturbed by large amplitude motions around the intermolecular bond effective fits of the lower rotational energy levels appear to confirm that TMA prefers to bind to the iodine whilst ammonia prefers the hydrogen.