MICROWAVE AND *AB INITIO* INVESTIGATION OF $(CH_3)_3N\cdots HF\cdots HF$

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Rotational spectroscopy and *ab initio* calculations have been used to examine the effect of a single HF solvent molecule on the gas phase proton transfer in the hydrogen bonded complex $(CH_3)_3N\cdots HF$. The rotational spectra of $(CH_3)_3N\cdots HF\cdots HF$ and five of its isotopically substituted derivatives have been observed by Fourier transform microwave spectroscopy. This follows a previous study by our group on $H_3N\cdots HF\cdots HF$, in which the addition of the second HF decreased the $N\cdots H$ hydrogen bond distance in $H_3N\cdots HF$ by 0.21(6) Å. The present study investigates the effect of the increased basicity of the amine on the $N\cdots H$ hydrogen bond. We observe a simple asymmetric rotor spectrum with strong a- and b- type transitions, consistent with a ring structure for the $N\cdots HF\cdots HF$ frame. No evidence of internal rotation is observed. Structural analysis is underway and will be discussed, but preliminary analysis indicates an $N\cdots H$ hydrogen bond distance of about 1.4 Å, approximately halfway between the hydrogen bond distance in $H_3N\cdots HF$ of 1.7 Å and the N-H covalent length of 1.1 Å. *Ab initio* calculations concur with experiment, indicating that, as with $H_3N\cdots HF\cdots HF$, the trimethylamine complex forms a ring in which both the $N\cdots H$ hydrogen bond and the HFH angle are significantly perturbed. In addition, two of the methyl groups of the trimethylamine assume an eclipsed conformation, apparently participating in a bifurcated interaction with the fluorine atom of the second HF. This complex provides the first step in microsolvation of $(CH_3)_3N\cdots HF$ and is useful in understanding the role of local environment in promoting proton transfer.