FT MICROWAVE SPECTROSCOPIC STUDY OF $(CH_3)_3N\cdots HCN\cdots HCN$

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Rotational spectra of the hydrogen-bonded trimer $(CH_3)_3N\cdots HCN\cdots HCN$ and10 isotopically substituted derivatives have been observed using Fourier transform microwave spectroscopy. The complex is a symmetric top with the atomic arrangements indicated above. A central focus of this work is to test the effect of microsolvation in promoting proton transfer across a strong hydrogen bond. Analysis of the rotational and quadrupole coupling constants will be presented, along with *ab initio* binding energy and geometry optimization results. Preliminary structural analysis indicates an $N\cdots H$ hydrogen bond contraction of approximately 0.08 $\AA$ relative to the dimer $(CH_3)_3N\cdots HCN$. Changes in the secondary hydrogen bond between the two HCN subunits lie within the experimental uncertainty for the $N\cdots H$ distance in HCN dimer. The effect of increasing the basicity of the amine in amine-HCN systems will be discussed in the context of previous work on the closely related system $H_3N\cdots HCN\cdots HCN$[a].

[a]R. S. Ruoff, T. Emilsson, C. Chuang,T. D. Klots,H. S. Gutowsky *J. Chem. Phys.* **93**(9), 6363, (1990).