FT MICROWAVE SPECTROSCOPIC STUDY OF (CH₃)₃N⋯HCN⋯HCN

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Rotational spectra of the hydrogen-bonded trimer (CH₃)₃N⋯HCN⋯HCN and 10 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⋯H hydrogen bond contraction of approximately 0.08 Å relative to the dimer (CH₃)₃N⋯HCN. Changes in the secondary hydrogen bond between the two HCN subunits lie within the experimental uncertainty for the N⋯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 H₃N⋯HCN⋯HCN⁴.