

## FT MICROWAVE SPECTROSCOPIC STUDY OF $(\text{CH}_3)_3\text{N}\cdots\text{HCN}\cdots\text{HCN}$

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Rotational spectra of the hydrogen-bonded trimer  $(\text{CH}_3)_3\text{N}\cdots\text{HCN}\cdots\text{HCN}$  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  $\text{N}\cdots\text{H}$  hydrogen bond contraction of approximately  $0.08 \text{ \AA}$  relative to the dimer  $(\text{CH}_3)_3\text{N}\cdots\text{HCN}$ . Changes in the secondary hydrogen bond between the two HCN subunits lie within the experimental uncertainty for the  $\text{N}\cdots\text{H}$  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  $\text{H}_3\text{N}\cdots\text{HCN}\cdots\text{HCN}$ <sup>a</sup>.

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