

## THE INFLUENCE OF FLUORINATION ON STRUCTURE OF THE TRIFLUOROACETONITRILE WATER COMPLEX

WEI LIN, *Department of Chemistry, University of Texas, Brownsville, TX, USA*; ANAN WU, XIN LU, *Department of Chemistry, Xiamen University, Xiamen, China*; DANIEL A. OBENCHAIN, STEWART E. NOVICK, *Department of Chemistry, Wesleyan University, Middletown, CT, USA*.

Acetonitrile,  $\text{CH}_3\text{CN}$ , and trifluoroacetonitrile,  $\text{CF}_3\text{CN}$ , are symmetric tops. In a recent study of the rotational spectrum of the acetonitrile and water complex, it was observed that the structure was also an effective symmetric top<sup>a</sup>, with the external hydrogen freely rotating about the O – H bond aligned towards the nitrogen of the cyanide of  $\text{CH}_3\text{CN}$ . Unlike the  $\text{CH}_3\text{CN} - \text{H}_2\text{O}$  complex, the  $\text{CH}_3\text{CN} - \text{Ar}$  and  $\text{CF}_3\text{CN} - \text{Ar}$  complexes were observed to be asymmetric tops. Having a series of symmetric and asymmetric top complexes of acetonitrile and trifluoroacetonitrile for comparison, we report the rotational spectrum of the weakly bound complex between trifluoroacetonitrile and water. Rotational constants and quadrupole coupling constants will be presented, and the structure of  $\text{CF}_3\text{CN} - \text{H}_2\text{O}$  will be revealed.

SPOILER ALERT: It's an asymmetric top.

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<sup>a</sup>Lovas, F.J.; Sobhanadri, J. Microwave rotational spectral study of  $\text{CH}_3\text{CN} - \text{H}_2\text{O}$  and  $\text{Ar} - \text{CH}_3\text{CN}$ . *J. Mol. Spectrosc.* **2015**, *307*, 59-64.