THE INFLUENCE OF FLUORINATION ON STRUCTURE OF THE TRIFLUOROACETONITRILE WATER COMPLEX

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Acetonitrile, CH_3CN, and trifluoroacetonitrile, CF_3CN, 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[a], with the external hydrogen freely rotating about the $O-H$ bond aligned towards the nitrogen of the cyanide of CH_3CN. Unlike the CH_3CN-H_2O complex, the CH_3CN-Ar and CF_3CN-Ar complexes were observed to be asymmetric tops. Having a series of symmetric and asymmetric top complexes of acetonitrile and trifluoracetonitrile 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 CF_3CN-H_2O will be revealed.

SPOILER ALERT: It's an asymmetric top.

[a]Lovas, F.J.; Sobhanadri, J. Microwave rotational spectral study of CH_3CN-H_2O and $Ar-CH_3CN$. *J. Mol. Spetrosc.* **2015**, *307*, 59-64.