MICROWAVE AND AB INITIO STUDY OF $(CH_3)_3CCN\text{-}SO_3$

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The microwave spectrum of the partially bound complex $(CH_3)_3CCN\text{-}SO_3$ has been recorded. The nitrogen-sulfur bond length is 2.34 $\mathring{A}$, which is almost exactly half way between that in weakly bound $N_2\text{-}SO_3$ and the more strongly bonded $(CH_3)_3N\text{-}SO_3$. A simple Townes and Dailey analysis of the ^{14}N nuclear quadrupole coupling constant gives a value of about 0.19 e^- transferred away from the $(CH_3)_3CCN$ upon complexation. Ab initio calculations at the MP2/aug-cc-pvtz level yield a binding energy relative to free $(CH_3)_3CCN$ and SO_3 of 11.0 kcal/mol, which is only about a fourth of that of $(CH_3)_3N\text{-}SO_3$. As noted previously for the complex $HCCCN\text{-}SO_3$,[a] comparison of the N-S bond length with those of a series of SO_3 adducts indicates that the proton affinity Lewis base is a good predictor of the properties of the complex. Indeed, spectra of this adduct were readily located on the basis of the proton affinity value for $(CH_3)_3CCN$.

[a] S. W. Hunt, D. L. Fiacco, and K. R. Leopold, *J. Mol. Spectrosc.* **212**, 213 (2002).