PARTIAL PROTON TRANSFER IN THE TRIFLUOROACETIC ACID - TRIMETHYLAMINE COMPLEX

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Chirped-pulse and cavity microwave spectra are presented for the complex formed from trifluoroacetic acid (TFA) and trimethylamine (TMA). Both the parent complex and that formed from deuterated TFA have been observed. Based on measured ^{14}N nuclear quadrupole coupling constants and supplemental computations at the MP2/6-311++G(df,pd) level of theory, the complex is shown to involve partial transfer of the TFA proton to the amine. Structural indicators of the degree of proton transfer are used to support this conclusion and comparisons with other related hydrogen bonded systems are presented. The relatively strong acidity of TFA as compared with other carboxylic acids, together with the relatively strong Brønsted basicity of TMA, likely underlie the ability of this system to undergo partial proton transfer in the gas phase without the aid of microsolvation.