

EVIDENCE FOR SPONTANEOUS PROTON TRANSFER IN THE COMPLEX FORMED FROM TRIFLIC ACID AND TRIMETHYLAMINE: MICROWAVE SPECTRUM AND COMPUTATIONAL ANALYSIS OF THE TRIMETHYLAMMONIUM TRIFLATE ION PAIR

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Gas phase trimethylammonium triflate, $(\text{CH}_3)_3\text{NH}^+ - ^-\text{OSO}_2\text{CF}_3$, has been observed by microwave spectroscopy. The ion pair was produced by on-the-fly mixing of trimethylamine and the superacid triflic acid in a supersonic jet. An initial fit with unresolved ^{14}N hyperfine structure was obtained within several minutes from the chirped-pulse spectrum using a new fitting program for dense spectral, DAPPERS, and the nitrogen hyperfine structure was then measured by cavity FTMW spectroscopy. Rotational constants are in good agreement with those calculated at the MP2/6-311++G(df,pd) level, which indicate a covalent N-H bond distance. Moreover, the measured ^{14}N nuclear quadrupole coupling constants, together with those calculated at a series of N-H distances, provide definitive evidence of the transfer of a proton in this cold, 1:1 complex.