

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 M06-2X/6-311++G(3df,3pd) level. The good agreement, together with the small observed ^{14}N quadrupole coupling constants, indicate essentially complete proton transfer from the triflic acid to the trimethylamine. Ion pair formation in un-solvated acid – base complexes, while not unprecedented, is unusual and likely related to the superacidity of triflic acid.