FACILE FORMATION OF ACETIC SULFURIC ANHYDRIDE IN A SUPERSONIC JET: CHARACTERIZATION BY MICROWAVE SPECTROSCOPY AND COMPUTATIONAL CHEMISTRY

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Sulfur trioxide and acetic acid are shown to react under supersonic jet conditions to form acetic sulfuric anhydride, CH_3COOSO_2OH. Rotational spectra of the parent, ^{34}S, methyl ^{13}C, and fully deuterated isotopologues have been observed by chirped-pulse and conventional cavity microwave spectroscopy. A and E internal rotation states have been observed for each isotopologue studied and the methyl group internal rotation barriers have been determined (241.043(65) $\mathrm{cm}^{-1}$for the parent species). The reaction is analogous to that of our previous report on the reaction of sulfur trioxide and formic acid. DFT and CCSD calculations are also presented which indicate that the reaction proceeds via a π_2 + π_2 + σ_2 cycloaddition reaction. These results support our previous conjecture that the reaction of SO_3 with carboxylic acids is both facile and general. Possible implications for atmospheric aerosol formation are discussed.