

## MICROWAVE CHARACTERIZATION OF PROPIOLIC SULFURIC ANHYDRIDE AND TWO CONFORMERS OF ACRYLIC SULFURIC ANHYDRIDE

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Sulfur trioxide reacts with propiolic acid and acrylic acid to form propiolic sulfuric anhydride ( $\text{HC}\equiv\text{C-COOSO}_2\text{OH}$ ) and acrylic sulfuric anhydride ( $\text{H}_2\text{C}=\text{CH-COOSO}_2\text{OH}$ ), respectively. Both species have been observed by chirped-pulse and conventional cavity microwave spectroscopy. In the case of acrylic acid, two conformers derived from the cis and trans form of the acid have been observed. The reaction mechanism and energetics are investigated by density functional theory and CCSD calculations. These results add to a growing body of evidence that establishes carboxylic sulfuric anhydrides,  $\text{RCOOSO}_2\text{OH}$ , as a class of molecules formed readily from  $\text{SO}_3 + \text{RCOOH}$  in the gas phase and which, therefore, may be of significance in the nucleation and growth of atmospheric aerosol particles.