THE CRIEGEE INTERMEDIATE-ACETIC ACID REACTION EXPLORED BY FOURIER TRANSFORM MICROWAVE SPECTROSCOPY

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Rapid reactions of organic acids with Criegee intermediates provide efficient gas phase removal process and are proposed to trigger the formation of atmospheric aerosols. The gas phase reaction between the simplest Criegee intermediate, CH_2OO, and acetic acid has been investigated by pulsed discharge nozzle Fourier transform microwave spectroscopy (PDN-FTMW). Two low lying conformers of hydroperoxymethyl acetate ($HOOCH_2OCOCH_3$, HPMA),which serves as the dominate nascent product from this reaction, was observed in the discharged plasma of a CH_2I_2/O_2/acetic acid gas mixture. Due to the three-fold methyl internal rotation and the low barrier height of the hindered methyl rotation, most of the observed pure rotational transitions in 13-21 GHz show large splitting corresponding to the A/E components. The relative abundance of the two observed hydroperoxymethyl acetate isomers is in agreement with the calculated relative energy. Also, the dehydrated product of HPMA, formic acid anhydride ($OHCOCOCH_3$), was observed in this work.