

PROBING THE CONFORMATIONAL BEHAVIOR OF THE C₃ ALKYL-SUBSTITUTED CRIEGEE INTERMEDIATES BY FTMW SPECTROSCOPY

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Carbonyl oxides (R₁R₂COO), often called Criegee intermediates (CIs), have been assumed as intermediates generated by the ozonolysis reaction of alkenes, and are thought to play important roles in atmospheric chemistry. After the first laboratory observation of the simplest CI, CH₂OO, their experimental characterization has been drastically progressing. Especially alkyl-substituted CIs have attracted much attention. Here we report rotational spectra of alkyl-substituted CIs with three carbon atoms in the substituent groups, named C₃ alkyl-substituted CIs. This group includes methyl-ethyl-ketone oxide or 2-butanone oxide (C₂H₅CCH₃OO) and its structural isomers n-butyraldehyde oxide (C₃H₇CHOO) and isobutyraldehyde oxide ((CH₃)₂CHCHOO). These molecules have been produced in the discharge plasma of diiodo-alkyl-derivative/O₂ gas mixtures, and characterized by Fourier-transform microwave spectroscopy. For the first of them, C₂H₅CCH₃OO, four different conformers were observed coexisting in the supersonic expansion. Spectra of the four species show small splittings due to the threefold methyl internal rotation which made possible to determine their respective barrier heights of the hindered methyl rotation. Preliminary results of the ongoing investigation of C₃H₇CHOO and (CH₃)₂CHCHOO molecules are also presented.