THE SIMPLEST CRIEGEE INTERMEDIATE ($H_2C = O$–O): EQUILIBRIUM STRUCTURE AND POSSIBLE FORMATION FROM ATMOSPHERIC LIGHTNING

MICHAEL C McCARTHY, *Atomic and Molecular Physics, Harvard-Smithsonian Center for Astrophysics, Cambridge, MA, USA*; LAN CHENG, *Department of Chemistry, The University of Texas, Austin, TX, USA*; KYLE N CRABTREE, OSCAR MARTINEZ JR., *Atomic and Molecular Physics, Harvard-Smithsonian Center for Astrophysics, Cambridge, MA, USA*; THANH LAM NGUYEN, *Department of Chemistry, The University of Texas, Austin, TX, USA*; CARRIE WOMACK, *Department of Chemistry, MIT, Cambridge, MA, USA*; JOHN F. STANTON, *Department of Chemistry, The University of Texas, Austin, TX, USA*.

Fourier transform microwave spectroscopy in combination with double-resonance techniques has been used to detect the rotational spectra of all five singly-substituted isotopic species of $H_2C = O$–O, the simplest Criegee intermediate. By correcting the rotational constants of these species and those of four others previously reported by Nakajima and Endo (*J. Chem. Phys.* **39**, 101103, 2013) for zero-point vibrational motion calculated theoretically, a highly precise equilibrium structure is reported for this important atmospheric intermediate. In contrast to the production method employed by most other groups, which has emphasized the use of halogenated percursors, we find that $H_2C = O$–O is produced in good yield and fairly selectively by passing a mixture of methane and excess molecular oxygen through an electrical discharge. For this reason $H_2C = O$–O may be produced in the direct vicinity of atmospheric lightning.