

CHARACTERIZATION OF HYDROPEROXYMETHYL FORMATE BY MICROWAVE SPECTROSCOPY: MOLECULAR INSIGHT INTO AEROSOL FORMATION

JESSIE P PORTERFIELD, KELVIN LEE, *Radio and Geoastronomy Division, Harvard-Smithsonian Center for Astrophysics, Cambridge, MA, USA*; VALENTINA DELL'ISOLA^a, BRANDON CARROLL, MICHAEL C McCARTHY, *Atomic and Molecular Physics, Harvard-Smithsonian Center for Astrophysics, Cambridge, MA, USA*.

Hydroperoxide esters are important products in the class of reactions between Criegee intermediates and carboxylic acids. Such reactions are believed to play key roles in the formation of secondary organic aerosols by producing semivolatile and low-volatility organic compounds. We provide the first definitive evidence for the most fundamental reaction in this class, that between carbonyl oxide CH_2OO and formic acid HCOOH to form hydroperoxymethyl formate (HPMF), $\text{HOOCH}_2\text{OCHO}$. Using a modified continuous flow pulsed reactor, HPMF is characterized in the ozonolysis of ethylene by high resolution Fourier transform microwave spectroscopy. Evidence for the most stable conformer - a seven membered, hydrogen bond stabilized ring - is supported with high level calculations and observation of ^{13}C isotopologues in natural abundance.

^aCo-affiliation University of Bologna