

SIMULATION OF THE ABSORPTION SPECTRUM OF CHLORINE PEROXIDE (ClOOCl)

MEGAN R BENTLEY, *Chemistry, University of Florida, Gainesville, FL, USA*; JOHN F. STANTON, *Quantum Theory Project, University of Florida, Gainesville, FL, USA*.

Chlorine oxides, namely chlorine monoxide (ClO) and its head-to-tail dimer (ClOOCl), are thought to be important participants in the catalytic destruction of ozone in the Antarctic polar vortex. Chlorine peroxide photolysis is the crucial step in the ozone-depleting mechanism, requiring accurate measurements of absorption cross sections to estimate the amount of ozone destroyed by this process in the polar stratosphere. However, there are large inconsistencies in previous experimental determinations of absorption cross sections in the longer wavelength tail region, where chlorine peroxide photolysis is atmospherically relevant. We have used a model based upon Condon's reflection principle to construct a simulated absorption spectrum for dissociative excited states, as is the case for chlorine peroxide. The simulated spectrum uses oscillator strengths and excitation energies generated from equation-of-motion coupled-cluster (EOM-CC) techniques that include effects of triple excitations and agrees well with experimental spectra. This method shows promise in elucidating semi-quantitative features of the absorption cross sections without encountering common experimental complications.