JET-COOLED \tilde{A} - \tilde{X} SPECTRA OF THE β -HYDROXYETHYLPEROXY and β -HYDROXYETHYLPEROXY-OD RADICALS

MING-WEI CHEN, GABRIEL M. P. JUST^a, TERRANCE CODD, and TERRY A. MILLER, Laser Spectroscopy Facility, Department of Chemistry, The Ohio State University, 120 W. 18th Avenue, Columbus, Ohio 43210.

The β -hydroxyethylperoxy (HOCH₂CH₂OO, β -HEP) radical in the atmosphere arises from the reaction of ethene (CH₂CH₂) and hydroxyl radical (OH), followed by the reaction with oxygen (O₂). It is also an important intermediate in the oxidation of ethanol, a component of automotive fuel. High-resolution, jet-cooled cavity ring-down spectroscopy (resolution of $\Delta\nu\approx$ 250MHz, considering the instrumental linewidth and the residual Doppler broadening) has been applied to observe the \tilde{A} - \tilde{X} origin band of the most stable conformer of both β -HEP and mono-deuterated β -HEP (DOCH₂CH₂OO, β -HEP-OD). Broadened rotational contours are observed for both isotopologues, but more resolved structure is shown in the β -HEP-OD spectrum. The evolutionary algorithm approach is applied to analyze the spectra, which gives fitted rotational constants and the homogeneous linewidths for both isotopologues using an asymmetric-top model for the rotational Hamiltonian. Evidence corresponding to a narrower homogeneous linewidth in the β -HEP-OD spectra implies that the broad rotational contour of β -HEP likely involves the motion of the hydrogen of the OH group.

^apresent address: Lawrence Berkeley National Laboratory, Lawrence Berkeley National Laboratory