OBSERVATION OF THE $\widetilde{A}$ - $\widetilde{X}$ ELECTRONIC TRANSITION OF β-HYDROXYETHYL PEROXY VIA CAVITY RING DOWN SPECTROSCOPY

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Peroxy radicals, formed by the addition of oxygen to organic radicals, are key intermediates in combustion and atmospheric chemistry. β-hydroxyethyl peroxy (HOC_2H_4OO/ β-HEP) in particular is a key intermediate in the OH radical mediated oxidation of ethene in the atmosphere and the combustion of ethanol. Historically, $\widetilde{B}$-$\widetilde{X}$ transitions of peroxy radicals have been monitored in kinetic studies. However, this system cannot be used to extract detailed structural information due to predissociation in the $\widetilde{B}$ state. Recently, the $\widetilde{A}$-$\widetilde{X}$ transitions, which are weak but structured and specific to conformers and isomers, have been studied for a number of aliphatic and aromatic peroxy radicals using the sensitive cavity ring down spectroscopy (CRDS) technique. In this work we present for the first time the observation and analysis of the $\widetilde{A}$-$\widetilde{X}$ transition of the β-HEP using CRDS. Aided by *ab inito* and DFT calculations, we tentatively assign our spectrum to low energy conformers involving different G($\pm$120°) and T(O°) orientations of the three dihedral angles between the OOC and OCC, the OCC and CCO, and the CCO and COH planes.