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Observation of the $\tilde{A} - \tilde{X}$ Electronic Transitions of Cyclopentyl and Cyclohexyl Peroxy Radicals Via Cavity Ringdown Spectroscopy

RABI CHHANTYAL PUN, PHILLIP THOMAS, TERRY MILLER, Ohio State University — Organic peroxy radicals are important intermediates in combustion chemistry. These molecules, formed from the addition of oxygen to alkyl radicals, are pivotal species in many atmospheric processes. We have previously targeted the $\tilde{A}$-$\tilde{X}$ transitions of straight and branched aliphatic peroxy radicals. This research has now been extended towards cyclic systems starting with cyclopentyl peroxy ($C_5H_9O_2$) and cyclohexyl peroxy ($C_6H_{11}O_2$), which are predicted by *abinitio* and DFT calculations to have four and two low-lying conformers respectively. Both have conformers which differ on the orientation of the O-O bond with respect to the cyclic carbon skeleton namely, *cis*- and *gauche*-, with $C_6H_{11}O_2$ also having conformers with axial and equatorial placement on the ring. We observe strong bands for both peroxies in the near-IR which are favorably assigned as the origin and the O-O stretch in agreement with the calculations. We have also obtained the spectrum of $C_6D_{11}O_2$ which facilitates the assignments of the weaker vibrational structure in $C_6H_{11}O_2$.

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