INVESTIGATION OF ETHYL PEROXY RADICAL CONFORMERS VIA CAVITY RINGDOWN SPECTROSCOPY OF THE $\tilde{A} - \tilde{X}$ ELECTRONIC TRANSITION

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Alkyl peroxy radicals ($C_nH_{2n+1}O_2$) are notoriously important reactive intermediates in the low temperature (T<700 K) combustion of hydrocarbons and in the chemistry of the atmosphere. Previous spectroscopic studies of the alkyl peroxy radicals, such as propyl peroxy[a], using cavity ringdown spectroscopy (CRDS) of the $\tilde{A} - \tilde{X}$ electronic transition have shown that this technique can distinguish between different alkyl peroxy radicals, as well as between different isomers and conformers of the same alkyl peroxy radical.
An earlier CRDS study[b] of ethyl peroxy radical (n=2) assigned a single band in the origin region of the $\tilde{A} - \tilde{X}$ electronic spectrum. However, calculations[c] predict two stable conformers of ethyl peroxy, namely trans (T) and gauche (G), that should be populated at room temperature and give distinct origin bands. In this talk, we present the results from our CRDS re-investigation of ethyl peroxy radical, both normal ($C_2H_5O_2$) and deuterated ($C_2D_5O_2$), via the $\tilde{A} - \tilde{X}$ electronic transition. With the help of equation of motion (EOMIP) quantum chemical calculations, we have assigned the 0_0^0 band for both the T and G conformers, as well as several vibrational hot bands, for $C_2H_5O_2$ and $C_2D_5O_2$. In addition for $C_2H_5O_2$, we have also assigned $\tilde{A}$ state COO bend and OO stretch vibrations.

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[b] M. B. Pushkarsky, S. J. Zalyubovsky and T. A. Miller, *J. Chem. Phys.* **112**, 10695 (2000).
[c] J. C. Rienstra-Kiracofe, W. D. Allen and H. F. Schaefer III, *J. Phys. Chem. A* **104**, 9823 (2000).