CALCULATION OF THE TRANSITION DIPOLE MOMENT OF THE $\tilde{A} \leftarrow \tilde{X}$ ELECTRONIC TRANSITION OF THE $C_2H_5O_2$ FROM THE PEAK ABSORPTION CROSS-SECTION

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With the advent of sensitive spectroscopic techniques such as cavity ring-down spectroscopy (CRDS), the $\tilde{A} \leftarrow \tilde{X}$ electronic transition of the organic peroxy radicals becomes an attractive analytical tool to study such species which play crucial roles in atmospheric and combustion chemistry. Since both the $\tilde{X}$ and $\tilde{A}$ states are bound, the electronic transition between them bears structural information on the both states and therefore the $\tilde{A} \leftarrow \tilde{X}$ absorption is highly species-selective. To utilize this selectivity in quantitative studies, the accurate knowledge of the absorption properties must be known. The electronic transition moment, $|\mu_e|^2$, is the key piece of information that allows one to calculate absorption spectra of the radicals over wide range of the experimental conditions.

Additionally, the experimentally obtained values of the $|\mu_e|^2$ for $\tilde{A} \leftarrow \tilde{X}$ transition in organic peroxy radicals prowide a benchmark for quantum chemical calculations of the electronic structure of these species.

In this work we obtain the value for $|\mu_e|^2$ for the G-conformer of ethyl peroxy radicals using their experimentally measured peak absorption cross-section in the room-temperature spectra and the results of quantum chemical calculations of the vibrational structure and the high resolution CRDS study of the rotational structure of these species. The results of this analysis will be compared to the calculated values, and the major sources of errors will be discussed.