VIBRONIC ANALYSIS FOR $\widetilde{B}$ - $\widetilde{X}$ TRANSITION OF ISOPROPOXY RADICAL

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Alkoxy radicals are important intermediates in combustion and atmospheric chemistry. Alkoxy radicals are also of significant spectroscopic interest for the study of Jahn Teller and pseudo Jahn Teller effects, involving the $\widetilde{X}$ and $\widetilde{A}$ states. The Jahn Teller effect has been studied in methoxy. Substitution of one or two hydrogens by methyl groups transforms the interaction to a pseudo Jahn Teller effect in ethoxy and isopropoxy. Previously, moderate resolution scans have been obtained for $\widetilde{B}$ - $\widetilde{X}$ and $\widetilde{B}$ - $\widetilde{A}$ transition systems, the latter observable at higher temperature. These measurements have shown that the $\widetilde{X}$ and $\widetilde{A}$ states of isopropoxy are separated by only 60.7(7) cm^{-1} which indicates a strong pseudo Jahn Teller effect in the $\widetilde{X}$ state. Such pseduo Jahn Teller coupling should also introduce additional bands into the $\widetilde{B}$ - $\widetilde{X}$ spectrum and a number of weaker transitions have been observed which may be caused by such effects. In this talk we present a vibronic analysis for the $\widetilde{B}$ - $\widetilde{X}$ transition based on the experimental results and also the results from recent quantum chemistry calculations.