ANALYSIS OF THE ROTATIONALLY-RESOLVED SPECTRA OF ISOPROPOXY RADICAL USING MULTIMODE VIBRONIC CALCULATIONS

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We have recorded the high resolution spectra of $\tilde{B} \leftarrow \tilde{X}$ of isopropoxy radical. The isopropoxy radical can be qualitatively viewed as a "chemically substituted" methoxy (with two methyl groups playing roles of "isotopes" of hydrogen), and the calculations[a] indicate the methyl substitution only moderately removes the degeneracy of the $\tilde{X}^2E$ state of methoxy. Therefore, isopropoxy is expected to exhibit the effects of the vibronic coupling within near-degenerate electronic state twofold. Such a coupling can affect the selection rules of vibronic transitions as well as the observed parameters of the effective rotational Hamiltonian. These effects can be understood if the details of the vibronic eigenstates are available. To obtain such information we used a simple semi-quantitative model which accounts for spin-orbit and vibronic coupling involving several vibrational modes. We have subsequently use these results to predict the effects of the vibronic coupling on the observed parameters of the molecule. The results of these calculations will be discussed.

[a] R. A. Young and D. R. Yarkony, *J. Chem. Phys.*, **125**, 234301 (2006)