ANALYSIS OF PSEUDO-JAHN-TELLER EFFECT IN METAL ALKOXIDES

KETAN SHARMA, TERRY A. MILLER, Department of Chemistry and Biochemistry, The Ohio State University, Columbus, OH, USA; ANAM C. PAUL, JINJUN LIU, Department of Chemistry, University of Louisville, Louisville, KY, USA.

The proposed possibility of laser cooling of alkaline earth monoalkyl (MR) and monoalkoxide (MOR) free radicals, e.g. $CaCH_3$ and $CaOCH_3$, has generated significant experimental interest in the spectroscopic analysis of these openshell molecules with orbitally degenerate or nearly degenerate low-lying electronic states. The analysis of laser induced fluorescence (LIF) and dispersed fluorescence (DF) spectra of such molecules requires an in-depth analysis of couplings between close lying electronic states. The Jahn-Teller and psuedo-Jahn-Teller effect plays an important role in the spectra of these molecules. The molecular interaction picture is even more complex due to the presence of spin-orbit couplings between electronic states. In this talk we present our methodology for treating psuedo Jahn-Teller couplings for calcium methoxide ($CaOCH_3$), calcium ethoxide ($CaOC_2H_5$) and calcium iso-propoxide (iso- $CaOC_3H_7$). A combination of EOM-CCSD and multi-mode Spin-Vibronic calculations have been employed to calculate transition frequencies and intensities for the excitation and emission spectra of these molecules. These calculations are used to understand the LIF and DF spectra, and to predict the feasibility of laser cooling of these molecules.