University of Louisville
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Research Seminar

When: February 22, 2024
Time: 12:00 p.m.
Location: CBLL-16

Spectroscopic Studies of Asymmetric-Top Ca-1-Propoxide Free Radicals by Laser Induced Fluorescence (LIF) and Dispersed Fluorescence (DF) Techniques

Abstract:

Metal-containing molecules are gaining attention in astrochemistry due to their presence in the interstellar medium and in synthetic chemistry because metal-containing free radicals are important reaction intermediates. [1] Many radicals containing alkaline-earth metals are also promising candidates for direct laser cooling.[2] Ultracold molecules can be used for precision measurements, quantum information storage, and quantum computing. Laser cooling has proven to be an effective tool to produce cold molecules. In recent years, our group has conducted computational calculations and spectroscopic studies on calcium alkoxide radicals, including $CaOCH_3$, $CaOC_2H_5$, and $CaOCH(CH_3)_2$ under jet-cooled conditions.[3] In the laser-induced fluorescence (LIF) and dispersed fluorescence (DF) spectroscopic measurements, we observed electronic transitions with largely diagonal Franck-Condon (FC) matrices and high vibrational branching ratios for the origin (v=0-0) bands, making these radicals potential candidates for laser cooling.

In the present project, we study the electronic and vibrational structure of Ca-1-propoxide radicals with a particular focus on the influence of its different conformations on the vibrational branching ratios furthermore and the role of C-H stretching modes in vibronic transitions. The Ca-1-propoxide radical has two conformers with gauche (G) and trans (T) OCCC dihedral angles, which are distinguishable by their unique spectroscopic signatures. Initially, we identified two pairs of origin bands, corresponding to the $\widetilde{A_2}/\widetilde{A_1} - \tilde{X}$ electronic transition of the G and T conformers, each separated by the spin-orbit (SO) interaction. Experimentally obtained LIF and DF spectra of the Ca-1-propoxide radical provide valuable insights into its ground- and excited-state energy level structure and conformational behaviors, leading to the construction of the FC matrix of each conformer. Transitions to the CH-stretch levels were also observed in the LIF/DF spectra of the two conformers, which are absent in the three calcium monoalkoxide radicals previously studied by our groups. The potential of Ca-1-propoxide radical as a laser-cooling candidate has been explored through experimental spectroscopic measurements and quantum chemistry calculations using the density functional theory (DFT) and time-dependent (TD-)DFT methods.

Our future endeavors will utilize narrow-linewidth continuous-wave (CW) ring lasers for high-resolution spectroscopy measurements to elucidate the rational and fine structure of the Ca-1-propoxide radical. Moreover, the cavity ring-down (CRD) spectroscopy apparatus in our lab can be used to obtain more precise values of vibrational and even rotational branching ratios.

References:

1. Sandford, S.A., et al., *Prebiotic astrochemistry and the formation of molecules of astrobiological interest in interstellar clouds and protostellar disks.* Chemical reviews, 2020. **120**(11): p. 4616-4659.
2. Mitra, D., et al., *Direct laser cooling of a symmetric top molecule.* Science, 2020. **369**(6509): p. 1366-1369.
3. Telfah, H., et al., *A combined experimental and computational study on the transition of the calcium isopropoxide radical as a candidate for direct laser cooling.* Physical Chemistry Chemical Physics: PCCP, 2022.
4. Ulenikov, O.N., et al., *High resolution spectroscopy of asymmetric top molecules in nonsinglet electronic states: the ν 3 fundamental of chlorine dioxide (16 O 35 Cl 16 O) free radical in the X 2 B 1 electronic ground state.* Physical Chemistry Chemical Physics, 2023. **25**(8): p. 6270-6287.