

University of Louisville  
Department of Chemistry  
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**Literature Seminar**

When: February 29, 2024

Time: 12:00 p.m.

Location: CBL-16

## **Spectroscopic Investigations of Nonlinear Molecules as Candidates for Laser Cooling**

### **Abstract:**

Laser cooling of molecules has drawn significant interest due to its broad applications in cold chemistry, fundamental physics, quantum information science (QIS), and other related fields.<sup>1</sup> Many radicals containing alkaline-earth metals are promising candidates for laser cooling. Until recently, people thought it was impossible to use laser cooling techniques on molecules because of the complex structure of molecular levels and the absence of closed cyclic transition between electron levels of molecules. But now, it has been discovered that laser cooling can actually work on a wide range of molecules. This includes not only the basic two-atom molecules but also those with many atoms. High-resolution laser-spectroscopic studies using techniques like laser-induced fluorescence (LIF), dispersed fluorescence (DF), and cavity ring-down (CRD) supported by quantum chemistry calculations play a crucial role in identifying and selecting suitable candidate molecules and energy levels for laser cooling.<sup>2</sup>

In particular, accurate measurement and prediction of vibrational and rotational branching ratios (VBRs and RBRs) are necessary to achieve optical cycling closure, a prerequisite for laser cooling.<sup>3</sup> In my literature seminar, I will review three papers that report spectroscopic studies of nonlinear candidate molecules for laser cooling, focusing on how to utilize highly diagonal Franck-Condon (FC) matrices and favorable Honl-London factors, two molecular parameters that govern the VBRs and RBRs, respectively. Despite the complex structure of nonlinear molecules, basic physical chemistry principles, including the perturbation theory, the ligand field theory, and the theory of electron transfer, can be used to guide the design and synthesis of candidate molecules for laser cooling.<sup>4</sup> Finally, I will provide a comparison and critique of these three papers and discuss the direction of spectroscopic and dynamics studies in this burgeoning new research field of laser-cooling molecules.

### **References:**

1. Michael R. Wasielewski *et al.* Exploiting chemistry and molecular systems for quantum information science. *Nat Rev Chem* **4**, 490-504 (2020).
2. Benjamin L. Augenbraun *et al.* Molecular asymmetry and Optical Cycling: Laser Cooling Asymmetric Top Molecules. *Physical Review X* **10**, 031022 (2020).
3. Guanming Lao *et al.* Laser Spectroscopy of Aromatic Molecules with Optical Cycling Centers: Strontium (I) Phenoxides. *J. Phys. Chem. Lett.* **13**, 11029-11035 (2022).
4. <https://arxiv.org/abs/2302.10161> [physics.atom-ph] [Submitted on 20 Feb 2023]