MOLECULAR-SPECTROSCOPIC CONSIDERATIONS IN LASER-COOLING ASYMMETRIC-TOPS: ENERGY LEVEL STRUCTURE, ROTATIONAL BRANCHING, PARITY, AND CHIRALITY.

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Molecules that have been laser-cooled in the lab are still limited to diatomic and linear triatomic species. Extension of laser cooling to include symmetric as well as asymmetric tops could significantly broaden the applications of cold (and ultra-cold) molecules. Recently, a practical roadmap to achieve optical cycling and laser cooling of asymmetric-top molecules has been proposed by Kozyryev et al.[a] Successful optical cycling and laser cooling require a detailed understanding of ro-vibronic structure and transition probabilities between ro-vibronic levels. Most candidate molecules for laser cooling are open-shell molecules (free radicals), and degenerate or quasi-degenerate electronic states are involved. Therefore, vibronic interactions (e.g., Renner-Teller, Jahn-Teller, or pseudo-Jahn-Teller interactions) and related effects (e.g., spin-orbit and Coriolis couplings) need to be taken into account. In this talk, we will discuss (i) the rotational and fine structure of asymmetric tops in quasi-degenerate electronic and vibronic states that are subject to vibronic, spin-orbit, and Coriolis couplings; (ii) symmetry properties of the rotational energy levels and their implications on the search for the permanent electric dipole moment of the electron (eEDM) and parity-violating interactions in molecules; (iii) transition intensities between vibronic levels and the rotational branching, which determine the practicality of optical cycling and laser cooling.

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[a] B. L. Augenbraun, J. M. Doyle, T. Zelevinsky, and I. Kozyryev, arXiv:2001.11020 [physics.atom-ph] (2020).