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Cooling polyatomic molecules with single and double optical cycling centers[1] JACEK KLOS, SVETLANA KOTOCHIGOVA, Physics Department, Temple University — Cooling polyatomic molecules is challenging in comparison to atoms. Nevertheless, laser cooling to μK temperature of SrOH molecule by Dr. Doyle's group [1] was possible due to the existence of diagonal Frank-Condon factors (FCFs) between the vibrational modes of optical transitions. To elucidate the role of molecular complexity on the diagonal nature of electronic transitions, we study optical transitions in the family of molecules M-O-$(CH_2)_n$-CH_3, where $n = 1 - 3$ and optical cycling center (OCC) M=Sr or Ca. We have performed geometry optimization of ground X and excited A and B states using time-dependent density functional theory and simulated excitation spectra from the X (0,0,0) state to vibrational states of the A and B potentials. This has shown that FCFs are close to one for all systems but decrease with complexity indicating that longer chains of ligands do change the coupling between M and O and make cooling less efficient. The B state is more favorable for cooling. It can be advantageous to attach two OCCs, thereby possibly doubling the photon scattering rate. We show that cycling rates can indeed be significantly increased for MO-$(CH_2)_n$-CH_3-OM with two optical centers. [1] I. Kozyrev et al., Phys. Rev. Lett. 118, 173201 (2017).

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Svetlana Kotochigova
Physics Department, Temple University

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