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Chemistry of Laser-Coolable Polyatomic Molecules[1] JACEK KLOS, Temple University, University of Maryland, MING LI, ALEXANDER PETROV, SVETLANA KOTOCHIGOVA, Temple University — Gasses of cooled molecules containing heavy atoms might have practical benefits for precision measurements and controlled chemical reactions. Cold and thus slow molecules lead to longer interrogation times, while novel quantum reaction pathways might be explored to control product molecules. Recently, J. Doyle's group at Harvard University successfully demonstrated [2] laser cooling of polyatomic SrOH molecules, in which the Sr atom acts as a photon cycling site. Here, we report on a quantum mechanical study of the electronic structure of the SrOH molecule using a combination of the ab-initio coupled-cluster method with single, double, and perturbative triple excitations (CCSD(T)) and the configuration-interaction (MRCI) method. These calculations reveal the presence of multiple Conical Intersections (CIs) between potential surfaces and the richness of the SrOH electronic structure. We have located the CIs and determined their non-adiabatic couplings.

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[2]I. Kozyrev et al. Phys. Rev. Lett. **118**, 173201 (2017)

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