# ACCURATE PREDICTION OF VIBRONIC LEVELS AND BRANCHING RATIOS FOR LASER-COOLABLE LINEAR POLYATOMIC MOLECULES: THE CONSTRUCTION OF THE QUASIDIABATIC HAMILTONIAN

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The vibronic structures of the low-lying electronic states in linear polyatomic molecules, which are utilized to construct closed optical cycling, play crucial roles in the laser-cooling processes. The construction of a multi-state Köeppel-Domcke-Cederbaum (KDC) quasidiabatic Hamiltonian with spin-orbit coupling, linear vibronic coupling, and Renner-Teller effects taken into account is reported aiming to obtain accurate vibronic levels and wave functions for laser-coolable triatomic molecules. The parameters for this KDC Hamiltonian were obtained from relativistic equation-of-motion coupled-cluster singles and doubles (EOM-CCSD) calculations. Discrete variable representation (DVR) calculations were then carried out to obtain the vibronic levels and wave functions. The accuracy of the present parametrization for the KDC Hamiltonian is demonstrated with calculations for vibronic levels of the $X^2\Sigma$ and $A^2\Pi$ states of the SrOH molecule.