THEORETICAL INVESTIGATION OF SPIN-ORBIT VIBRONIC COUPLING EFFECTS IN THE ELECTRONIC GROUND STATE OF CrCN

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The spin-orbit-induced vibronic coupling interactions in the $^6\Sigma^+$ electronic ground state of the linear CrCN molecule are investigated, employing the microscopic (Breit-Pauli) spin-orbit (SO) coupling operator. The $6\times6$ Hamiltonian matrix is derived in a diabatic spin-orbital electronic basis set including terms up to second order in the expansion of the molecular Hamiltonian in the bending normal coordinate. \textit{Ab initio} calculations of the potential energies of the $^6\Sigma^+$ state are performed as a function of the bending normal coordinate. The fitting of the spin degeneracy of the $^6\Sigma^+$ state via various SO coupling terms is investigated. The predicted electronic structure of the $X^6\Sigma^+$ electronic state of CrCN shows a good agreement with the experimentally determined Cr-C bond length but less so for the C-N bond length. The nature of the metal-ligand bonding is also discussed.