# THE MOLECULAR CONSTANTS OF THE X2Σ+, A2Π, B2Σ+, AND C2Π ELECTRONIC STATES OF THE CALCIUM MONOHALIDE RADICALS

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The alkaline earth monohalides are molecules of interest in fields such as astrophysics, high-temperature chemistry, chemiluminescent reactions, spectroscopy, computational chemistry, and cold molecule trapping. The electronic properties of the CaX molecules are well described by Ligand Field Theory. These properties include the relative energies of the X, A, B, and C states, their spin-orbit, spin-rotation, and lambda-doubling constants, and their spin-orbit and L-uncoupling perturbation matrix elements. In this talk we will present some Ligand Field Theory-based ideas: Schmidt orthogonalization, ligand-induced 4p-3d induced polarization, ligand-to-metal charge transfer, and molecular orbital-size based on effective principal quantum number $1/n^{*(3)}$ orbital radius scaling. This paper is dedicated to Joelle Rostas (deceased June 2019) who spent many years studying the alkaline earth monohalide molecules and discussing them with the authors of this talk.