

## THE MOLECULAR CONSTANTS OF THE $X^2\Sigma^+$ , $A^2\Pi$ , $B^2\Sigma^+$ , AND $C^2\Pi$ ELECTRONIC STATES OF THE CALCIUM MONOHALIDE RADICALS

CHIHEB BAHIRINI, *Department of Physics, Tunis Preparatory Engineering Institute (IPEIT), Tunis, Tunisia*; ROBERT W FIELD, *Department of Chemistry, MIT, Cambridge, MA, USA*; GUY TAIEB, *Institut des Sciences Moléculaires d'Orsay, Université Paris-Sud, Orsay, France*.

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  $\text{CaX}$  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. The lambda doublings definitely prove that the spin-orbit splitting in the C-state is 1/2 below 3/2 (i.e. regular). Finally, the simultaneous use of both laser techniques Laser Induced Fluorescence (LIF) and Cavity Ring Down Spectroscopy (CRDS), allowed the extension of previous measurements to high vibrational levels and provided accurate vibrational parameters <sup>a</sup>.

---

<sup>a</sup>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.