TD03 An Atomic-Ion-in-Molecule Model for the $A^2\Pi$ and $C^2\Pi$ States of the CaX and MF Molecules [examples and interpretation]

- Atom in Molecule Models
- Back to the Periodic Table
- CaX $A^2\Pi$ and $C^2\Pi$ states and the spin-orbit constant of each X^- ion
- MF and M^+ npπ and n-1dπ orbitals
- Interpretation of the M^+ dependence of the trends in the A($A^2\Pi$) and A($C^2\Pi$) spin-orbit constants
- Ligand Field Theory: relative energies and mixing of npπ and
- n-1dπ M^+ orbitals
- Two Important References:
- R. W. Field, "Diatomic Molecule Electronic Structure beyond Simple Molecular Constants," Ber. Bunsenges. Phys. Chem. **86**, 771 (1982).
- S. F. Rice, H. Martin, and R. W. Field, "The Electronic Structure of the Calcium Monohalides. A Ligand Field Approach," J. Chem. Phys. **82**, 5023 (1985).
- ...a work in progress.