F orbitals and Metal-Ligand Bonding in Lanthanide Octahedral Complexes

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The independent study will compare metal-ligand bonding in octahedral complexes with rare lanthanide metals such as Ce$^{3+}$ to Yb$^{3+}$ and describe how f-orbital interactions in hexachloro complexes differ from the 3d metal complexes using experimental and theoretical evidence. The f-f and ligand to metal charge transfer transitions will be defined using electronic absorption spectroscopy and molecular orbital theory. The extent of the metal 4f-ligand 3p orbital mixing and interactions and ligand to metal covalency will be estimated. The electrostatic interactions of ligand-ligand repulsion, and metal-ligand attraction will be explored as well as bond lengths and bond energies for 4f orbital complexes as compared to that of 3d orbital complexes. With the use of molecular orbital theory a molecular orbital diagram, shapes of the orbitals, and the interactions of ligand orbitals to metal orbitals will be discussed. From crystal field theory an estimate of f orbital splitting and ligand field stabilization energies can be estimated.

References:
