5.04 Principles of Inorganic Chemistry II
Fall 2008

Due: Friday, 10 October

1. The octahedral molecular orbital (MO) diagram provides the starting point for the construction of the electronic structure of several metal complexes. But not all complexes are conveniently referenced to octahedral geometry. Other important geometries include tetrahedral, square planar, trigonal bipyramidal and pyramidal. Construct MO diagrams for each in the σ-only ligand framework. For the tetrahedral complex, also show the MO diagram for π- and π*-bonding ligands.

2. Derive the MO diagram for trigonal prismatic WH_6. The ReH_9^{2-} complex has hydride ligands capping the trigonal prismatic faces. Construct the MO diagram for The ReH_9^{2-}.

    a. Make a LCAO of two H_3 molecules interacting face-to-face.

    b. Place W between the two H_3 faces and then perturb the orbitals.

    c. Mix another set of H_3 orbitals into the MO diagram you made in (b) to arrive at the MO diagram for.

3. Consider a one-dimensional chain of orbitals, for example polyacetylene. (a) Use Hückel theory to generate the energy bands for a geometry in which all C–C distances are equal. (b) Now generate the energy bands a geometry with alternating long and short C–C bonds. Use β for the H_{ij} across short bonds and $\beta/2$ across long bonds. (c) Will polyacetylene in either one or both geometries be a metal or an insulator?