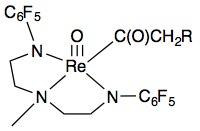
**Building Molecular Orbitals for a Square Pyramidal Oxorhenium(V)** **Complex**

1. Consider an octahedral complex of formula ML6. Assume for now that all ligands are σ-donors only.
   1. Label x,y and z axes (the z axis should be the vertical axis in the plane of the page). Draw the metal *d* orbitals.
   2. Which orbitals on the central metal will be affected by σ interactions with the ligands?
   3. Build a MO diagram for the orbitals of metal *d* character in this octahedral complex. Label the orbitals on your diagram. (You should have a set of orbitals of *eg* symmetry and another of *t2g* symmetry in this *Oh* point group*)*
2. Now remove a ligand L on the z axis to form a square pyramidal complex of formula ML5.
   1. How are the orbitals of metal *d* character affected in your MO diagram by the absence of a ligand L on the z axis?
   2. Redraw your MO diagram for orbitals of metal *d* character in a square pyramidal complex. Label the orbitals.
3. Now consider the oxorhenium(V) complex synthesized by Elon Ison’s group in *Organometallics* **2015**, *34,* 3152-3158. This complex is reported to have a “distorted” square pyramidal geometry. For the purpose of this exercise, first consider the structure to be an “ideal” square pyramid of formula M(L)3L’L”, then progressively add distortions by considering the differences between ligands.



* 1. Which ligands are also π-donors and/or π-acceptors?
  2. Which d orbitals on the central metal may be involved in π interactions with a ligand?
  3. Redraw a MO diagram for the square pyramidal oxorhenium(V) complex above that includes π interactions with the ligands. You should consider both the type of π interactions for the ligand (donor or acceptor) and the location of these ligands in the complex (xy plane or z axis).

1. Rhenium has an oxidation state of (V) in the complex above.
   1. What is the *dn* configuration of rhenium?
   2. Which *d* orbital(s) in your MO diagram above will contain these electrons?
   3. Are these electrons contained in *d* orbital(s) of bonding, nonbonding or antibonding character?
   4. Is the effect stabilizing or destabilizing for the complex? Explain.