

CHEM-457 (S14)
Problem Set 1

- (a) Using a common set of Cartesian coordinates that is consistent for each wavefunction, draw and label all of the possible atomic orbitals with principal quantum number, $n = 3$ and angular momentum, $l = 0 - 2$. Indicate the angular momentum for each orbital. (b) Indicate whether each orbital is gerade or ungerade.
- Miessler, Fischer and Tarr #2.9 and #2.29
- Predict the electronic configuration and multiplicity for each of the following atomic species. Indicate which electrons are core electrons and which are valence electrons.
 - Sc
 - Os
 - Cd
 - Cl
 - Tc⁺
 - Fe²⁺

- Predict whether potassium or calcium should have an electron affinity closer to zero. Provide your reasoning for this prediction.
- Consider the following possible electron arrangements for a $3p^3$ configuration.



Enumerate the Coulomb repulsion energy (Π_c) and exchange energy (Π_e) for each configuration, and indicate which is the ground configuration. Recall that electrons must share the same m_s value to exchange.

- Should phosphorus or sulfur have a higher first ionization energy? Please provide electronic configurations for each atom in the ground state and fully explain your reasoning.

6. Using the electronegativity data shown in class, determine which of the following bonding interactions are polar. Indicate the direction of the dipole where appropriate.
- (a) C—Si
 - (b) C—N
 - (c) C—Au
 - (d) Ru—Os
 - (e) F—Si
 - (f) N—Br