CHEM-651 (F14)
Problem Set 1

1. DMA 1.12 – 1.14, 1.21 and 1.24

2. (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.

2. Predict the electronic configuration and multiplicity for each of the following atomic species. Indicate which electrons are core electrons and which are valence electrons.
   (a) Sc
   (b) Na
   (c) As
   (d) C^-
   (e) O^+
   (f) Fe^{2+}

3. Explain why the electron affinities of both silicon and sulfur are larger than that of phosphorus. Please provide electronic configurations for these atoms in the ground state and fully explain your reasoning

4. Provide Lewis structures for the molecules and ions listed below. Show resonance where appropriate and indicate all formal charges.

(a) FBr	(b) S_2	(c) Cl_2	(d) P_2
(e) NCO^-	(f) CNO^-	(g) $BeCl_2$	(h) CS_2
(i) BF_3	(j) SO_3	(k) CO_3^{2-}	(l) CF_4
(m) $SiBr_4$	(n) BF_4^-	(o) NCl_3	(p) PF_3
(q) CH_3^-	(r) SF_2	(s) XeO_3	(t) SO_2
(u) SF_6	(v) Na_2O	(w) ClO_2	(x) N_2F_2
(y) CsF	(z) SrO		

5. Provide Lewis structures for the following derivatives of xenon, showing resonance and formal charges where appropriate

   (a) XeO_4
   (b) XeO_3
   (c) XeF_8^{2-}
   (d) XeF_6
   (e) XeF_4
   (f) XeF_2
   (g) XeF^+

6. Predict the molecular shape and dipole moment for each of the following molecules.

(a) CS_2	(b) SO_3	(c) ICl_3	(d) BF_3
(e) CBr_4	(f) SiH_4	(g) SF_2	(h) SeF_6
(i) PF_3	(j) ClO_2	(k) IF_5	(l) OF_2
(m) H_2Te			