Very Short Answer Questions: (3 points each)

1.   The electron configuration of Pb^{2+} is is [Xe] 6s^2 5d^{10} 4f^{14}.

2.   What is the border condition for the particle-in-a-box? V = 0 inside and V = ∞ outside

3.   The angular momentum quantum number represents the shape of the orbital.

4.   Orbitals within the same subshell shield each other not at all.

5.   Ionization energy is always endothermic (positive).

6.   *S* orbitals have no angular dependence.

7.   A point group is a collection of operations that describes the symmetry of an object.

8.   The T$_d$ point group has how many C_3 axes? 4

9.   A reaction that yields a thermodynamically less stable product is said to be kinetically controlled.

10. Which of the elements assigned for this test unexpectedly forms covalent bonds preferentially?
     beryllium

Discussion Questions: (You must show work to receive credit!)

1. Briefly discuss the origin of chemical explosions. (5 points)

    An explosion is the very rapid, violent expansion of a gas. They happen chemically when a reaction
    involving a solid or liquid material produces a gas. The reaction must occur very rapidly. As such, it
    probably will be very exothermic. Also, the reaction will typically produce several gas molecules for
    each reactant molecule.

2. Two different conditions give rise to atomic orbital nodes. What are they? What is the physical
    significance of a node? (10 points)

    One type of node arises from the radial portion of the wave equation. These nodes are the ones that
    lie within a particular orbital at varying distances from the nucleus. The other type of node is the
    angular node. This node arises from the shape of the orbital. For example all *p* orbitals have one
    nodal plane arising from the angular function. Nodes are places with zero electron density.

3. How can 3 of the following 4 be isolated from their naturally occurring sources: Al, He, Mg, Na? (9
    points)

    See handouts.

4.   The book notes that the alkali metals have favorable electron affinities.   In other words, it is
     energetically favorable for an alkali metal atom to add an electron. (10 points)

    a) Why?
       Normally the unfilled orbitals lying above a filled valence shell (inert gas configuration) are high in
       energy and not readily accessible. Since all alkali metals already have an electron in an *s* orbital
       this energy gap is not a problem. The negative energies the incoming electron will experience are
       electron-electron repulsions and the spin pairing energy. Nuclear charge partially offsets this and
       filled orbitals are very stable. Also, the nucleus is never completely shielded so that the incoming
       electron experiences the attraction of some positive nuclear charge.

b) Of course, in practice alkali metals always lose an electron when forming salts. If gaining electrons is favorable, then why do alkali metals always lose electrons when forming compounds?

At least one atom loses electrons because of the stability of the lattice energy released on forming a salt. The alkali metal always loses its electrons because of its lower electronegativity when compared with other atoms.

5. Effective nuclear charge (Z_{eff}) of the 2s orbital increases across the second period according to the table below. Comment on the uniformity of the increase and deviation(s) from uniformity. Is the dramatic increase in Z_{eff} that occurs on dropping to the third period expected or not? Why or why not?

Element	Li	Be	B	C	N	O	F	Ne	Na
Z_{eff} (2s)	1.28	1.91	2.58	3.22	3.85	4.49	5.13	5.76	6.57

The Z_{eff} of the 2s orbital increases uniformly (Δ = 0.63-0.64 per added electron) across the period with one exception. On going from Be to B, Δ = 0.67. The uniform increase arises from the fact that none of the electrons, regardless of whether they go into s or p orbitals, shields any of the other electrons well. The result is that each electron experiences a relatively constant increase in nuclear charge. The jump at Be-B arises from the fact that p orbitals penetrate more poorly than do s orbitals and the 2s orbital is shielded a little less well than an s electron would. Z_{eff} increases substantially for Na because the next electron goes into a 3s orbital which hardly shields the 2s at all. The result is that the 2s electron experiences much more of the new proton's positive charge.

6. Give point groups for each of the following (no work required): (16 points)

BCl_3: D_{3h}

 : C_{2h}
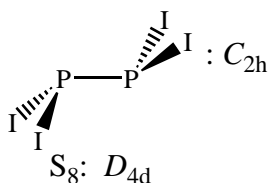
$Cl_2C=C=CCl_2$: D_{2d}

S_8: D_{4d}

7. Consider the molecule IF_3. What are the possible vibrational modes for this molecule? How many bands would one find in the infrared spectrum? In the Raman spectrum? (10 points)

	E	C_2	σ_v	σ_v'		
A_1	1	1	1	1	z	x^2, y^2, z^2
A_2	1	1	-1	-1	R_z	xy
B_1	1	-1	1	-1	x, R_y	xz
B_2	1	-1	-1	-1	y, R_x	yz
Γ_{red}	12	-2	4	2		

A_1: ¼[(1)(1)(12) + (1)(1)(-2) + (1)(1)(4) + (1)(1)(2)] = 4
A_2: ¼[(1)(1)(12) + (1)(1)(-2) + (1)(-1)(4) + (1)(-1)(2)] = 1
B_1: ¼[(1)(1)(12) + (1)(-1)(-2) + (1)(1)(4) + (1)(-1)(2)] = 4
B_2: ¼[(1)(1)(12) + (1)(-1)(-2) + (1)(-1)(4) + (1)(1)(2)] = 3

There are three translational modes (A_1, B_1, B_2) and three rotational modes (A_2, B_1, B_2) that must be subtracted from this list to obtain the full set of vibrational modes. The complete set of vibrational modes is thus: 3 A_1, 2 B_1, and 1 B_2. All are Raman active.