Problem 1 (Extension of Last Year)) Difference Between Wurtzite, Rhombohedral and Zinc Blend Structures

a) Problem 5 - Chapter 3 of the text. When the problem asks "Discuss the difference..." do this in terms of the relative orientations of neighboring tetrahedral arrangements of the atoms. Also, how does the wurtzite structure differ from the rhombohedral structure.
b) The space group of the wurtzite structure is $P6_3mc$. Explain the notation. What is the point symmetry associated with the space group. Is the structure symorphic or non-symorphic?

Problem 2) Symmetry Operations of a Space Group (Gave this last year)

a) Compare Fig 3-3 with Fig 3-4 and Fig 3-5 (space groups for Si and GaAs ). Why are there 1 a) position in the first, 2 in the second and 4 in the later?
b) Explain why there are 48 general points listed in the three Figs. but the respective numbers stated are 48,96, and 192 respectively. Why is the site symmetry of the general point 1?
c) For the c) site in Si, the site symmetry is $\bar{4}3m$. What symmetries are lost? Does the site symmetry imply that the points transform into themselves or more generally into each other?
d) Problem 2.2 of Burns. Only do this for the cubic or the tetragonal structure if you wish (that is a or b of this problem).

Problem 3) (New: Taken from Sands)
Palladium sulfide has a tetragonal structure with a= 6.429 Angstroms, and c= 6.608 Angstroms. The space group is $P4_2/m$. and there are eight palladium and eight sulfur atoms per unit cell. The sulfur atoms occupy the general positions (8k) with x= .19, y = .32 and z = .23 .

a) What are the other positions of the sulfur atoms in the unit cell?
b) What are the positions of the Pd atoms in the unit cell?
c) Draw the unit cell with a and b in the plane of the paper and c out of the paper. Indicate the distance in the c direction beside each atom. (That is the projection onto (001)).

Problem 4) Reciprocal Lattices (again)
a) Problem 6 - Chapter 4 of the text.
b) Obtain the Wigner-Seitz lattices of the direct and reciprocal lattices.
c) Refer to Fig.(10-15) for the reciprocal lattice of the face centered cubic lattice. The Brillouin zone is the Wigner-Seitz lattice of the reciprocal lattice. Determine the distance from
the Γ point to the X point in terms of the unit cell length a; also between Γ and the L point (the answer to this is just below Eq.(10-44))

Problem 5) (Modification of last years) Basic Conservation of Momentum and Energy in Elastic Scattering
a) Problem 2 - Chapter 4 of the text. Basically give the same conservation of energy and momentum arguments discussed in class.
b) Show that strong X-ray scattering occurs at the edge of the Brillouin zone.

Problem 6) (Extension of last years)
The polarization associated with a linear electro-optic material is given by $P_i = \chi_{ijk}E_jE_k$ where $\chi_{ijk}$ is a third order "tensor".
a) State the convention which allows $\chi$ to be written as a 3 by 6 matrix.
b) Obtain the non-zero elements and their mutual relationships for m3m and 43m symmetries.
c) Argue that the same relationships must hold for the piezo-electric coefficients.
d) Show that the linear susceptibility of a lossless material is symmetric. Does this hold for the conductivity (the Onsager hypothesis)?
d) (Extra for optical interests). Give one possible configuration for an optical modulator using GaAs.

Problem 8- Character Analysis (New)
a) Show using the character table of the equilateral triangle that Eq. (8-13) is correct for $s p^2$ superposition (hybridization). In fact should find $c = \sqrt(3)b$. a and b can then be uniquely determined by normalizing the wave functions to 1 and requiring different hybrids be orthogonal. I believe a should be $1/\sqrt{3}$ (and b = $\sqrt{2}a$)

Problem 9- Bonding
Show that the result Eq.(6-5) of Burns is correct.