Homework 8

1. Calculate the energy needed to dissociate 1.00 mol of crystalline RbCl into its gaseous ions if the Madelung constant for its structure is 1.7476 and the radii of Rb^+ and Cl^- are 1.48 Å and 1.81 Å, respectively. Assume that the repulsive energy reduces the lattice energy by 10% from the pure Coulomb energy.

2. (a) Use the Born–Haber cycle, with data from Appendices D and F, to calculate the lattice energy of LiF.

(b) Compare the result of part (a) with the Coulomb energy calculated by using an Li-F separation of 2.014 Å in the LiF crystal, which has the rock-salt structure

3. The crystal structure of diamond is fcc, and the atom coordinates in the unit cell are

(0 , 0 , 0) , (½ , ½ , 0) , (½ , 0 , ½) , (0 , ½ , v) , (¼ , ¼ , ¼) , (¾ , ¼ , ¾) , (¾ , ¾ , ¼) , (¼ ,¾ ,¾). The lattice parameter is a= 3.57 Å. What is the C-C bond distance in diamond?

4. Polonium is the only element known to crystallize in the simple cubic lattice.

(a) What is the distance between nearest neighbor polonium atoms if the first-order diffraction of X-rays with λ= 1.785 Å from the parallel faces of its unit cells appears at an angle of 2θ = 30.96° from these planes?

(b) What is the density of polonium in this crystal (in g cm^{-3})?

5. A compound of titanium and oxygen contains 28.31% oxygen by mass.

(a) If the compound's empirical formula is Ti_xO, calculate x to four significant figures.

(b) The nonstoichiometric compounds Ti_xO can be described as having a Ti^{2+}-O^{2-} lattice

in which certain Ti^{2+} ions are missing or are replaced by Ti^{3+} ions. Calculate the fraction

of Ti^{2+} sites in the nonstoichiometric compound that are vacant and the fraction that

are occupied by Ti^{3+} ions.

6. Sodium hydride (NaH) crystallizes in the rock-salt structure, with four formula units

of NaH per cubic unit cell. A beam of monoenergetic neutrons, selected to have a

velocity of 2.639×10^3 m s^{-1}, is scattered in second order through an angle of $2\theta = 36.26°$

by the parallel faces of the unit cells of a sodium hydride crystal.

(a) Calculate the wavelength of the neutrons.

(b) Calculate the edge length of the cubic unit cell.

(c) Calculate the distance from the center of an Na$^+$ ion to the center of a neighboring

H$^-$ ion.

(d) If the radius of an Na$^+$ ion is 0.98 Å, what is the radius of an H$^-$ ion, assuming the two

ions are in contact?