Homework 8

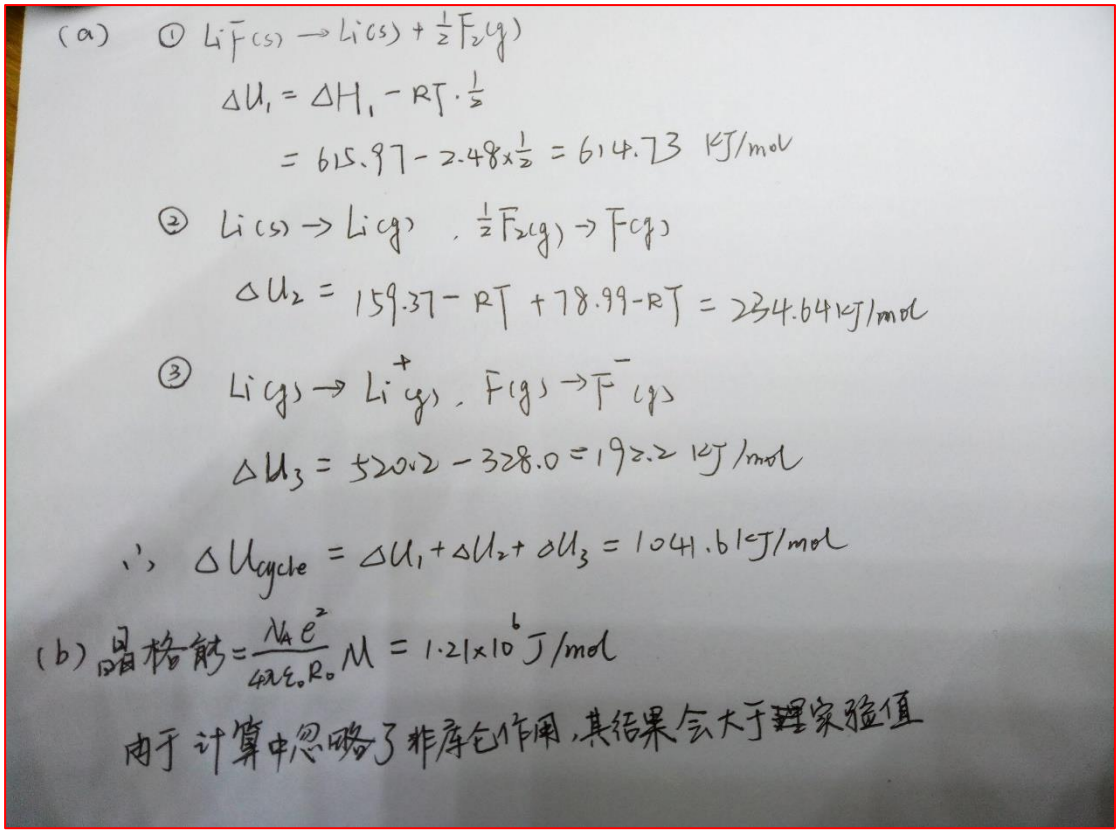
(0.6′)1. Calculate the energy needed to dissociate 1.00 mol of crystalline RbCl into its gaseous ions if the Madelung constant for its structure is 1.7476 and the radii of Rb^+ and Cl^- are

1.48 Å and 1.81 Å, respectively. Assume that the repulsive energy reduces the lattice energy by 10% from the pure Coulomb energy.

晶格能=$\frac{N_A e^2}{4\pi\varepsilon_0 R_0} M$ =738 kJ/mol，需要 738×90%=664 kJ/mol

(0.8′)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



(0.6′)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?

体对角线的四分之一，$\frac{\sqrt{3}}{4}$a=1.55 Å

(0.6′)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})?

(a) 2dsinθ=nλ，晶面间距 d=3.34 Å

(b) 简立方一个晶胞包含一个原子，$m=M/N_A$，$V=d^3$，$\rho=m/V=9.32\ g/cm^3$

(0.6′)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.

(a) x=0.84 (b) 84%的 Ti 位点被 Ti^{2+}和 Ti^{3+}占据，设其组分为 a ，b ，a+b=0.84,2a+3b=2，解得 a=0.5，b=0.34，故有 1-x=16%的 Ti^{2+}位点空着，有 34%的 Ti^{2+}被 Ti^{3+}取代

(0.8′)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?

(a) λ=1.499 Å

(b) a=晶面间距 $d=n\lambda/2\sin\theta$=4.817 Å

(c) L=1/2a=2.409 Å

(c) $r_1+r_2=L$，r_1=1.43 Å