Inorganic Chemistry 1 – Chem. 2233

Problem Set 3 (15 points)

Name: Answer key

ID #: ______________________________

Please place final answers in the space provided for each question. There is no partial credit so make your final answer is clear.

The due date is: 9/27/2016

1pt. each

1. State the coordination number of a sphere in each of the following arrangements:
(a) *ccp* 12, (b) *hcp* 12, (c) *bcc* 8, (d) *fcc* 12

2. Beryllium has a hexagonal crystal structure, with a = 0.22858 nm and c = 0.35842 nm. The atomic radius is 0.1143 nm, the density is 1.848 g/cm^3, and the atomic weight is 9.01 g/mol. Determine: See p.2 for work

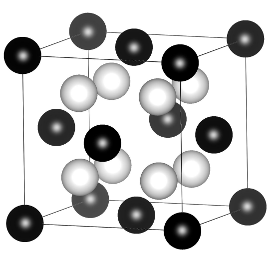
1pt. a. The number of atoms in each unit cell: 2

1pt. b. The packing density (as a percentage) in the unit cell: 77%

1 pt. 3. Nickel has the *fcc* crystal structure and a lattice parameter of a = 0.3517 nm. Using this information, determine the atomic radius of Ni in angstroms: 1.243 Å see p.2

1 pt. 4. A compound is formed by two elements M and N. The element N forms *ccp* lattice and atoms of M occupy 1/3rd of the tetrahedral voids. What is the formula? M_2N_3 see p.2

5. Given the following unit cell:



1pt. a. What is the composition of the unit cell? BA_2

1pt. b. What is the most likely "*Z* value"? 4

1pt. c. What is the coordination environment of the "white" atoms? tetrahedral

Black = B → $(\frac{1}{8}\times 8)+(\frac{1}{2}\times 6) = 4$ ⇒ B_4A_8 = BA_2

white = A → 8

A are in Td holes of a fcc lattice of B, so there are 2 holes per atom of B.

2 pt. 6. The equilibrium distance in diatomic LiF is 1.52 Å. Assuming ionic bonding between the two atoms, calculate the (lattice) energy required to separate them: $Li^+ – F^- \rightarrow Li^+ + F^-$

answer: 1.60×10^3 kJ/mol

2pt. 7. Use the data given below to construct a Born-Haber cycle to determine the lattice energy of CaO following the reaction: Ca(s) + O_2 --> CaO

Reaction	ΔH°(kJ/mol)
Sub. of Ca	+193
IE1 of Ca	+590
IE2 of Ca	+1010
BDE of O2	+498
EA1 of O	–141
EA2 of O	+878
ΔH°_f[CaO(s)]	–635

answer: -3.41×10^3 kJ/mol

2. Volume of the hexagonal unit cell

$V = (0.22858\text{ nm})^2 (0.35842\text{ nm}) \cos 30 = 0.01622\text{ nm}^3 = 1.622 \times 10^{-23}\text{ cm}^3$

(a) from the density equation

$$1.848 \frac{g}{cm^3} = \frac{(x \text{ atoms/cell})(9.01\text{ g/mol})}{(1.622\times10^{-23}\text{cm}^3)(6.022\times10^{23}\text{atoms/mol})}$$

$x = 2$ atoms/cell

(b) the packing density is

$$PD = \frac{(2\text{atoms/cell})(\frac{4}{3}\pi)(0.1143\text{ nm})^3}{0.01622\text{ nm}^3} = 0.77$$

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3. $r = \frac{a}{\sqrt{8}} = 0.124\text{nm}$ (see lecture 7)

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4. Count the N atoms in ccp lattice: $\left(\frac{1}{8}\times8\right) + \left(\frac{1}{2}\times6\right) = 4$

M atoms are in 1/3 of the tetrahedral holes. There are two tetrahedral holes per atom in the ccp lattice.

So $4\times2 = 8$ tetrahedral holes

and $8 \times \frac{1}{3} = \frac{8}{3}$ M

$N:M = 4:\frac{8}{3} = 12:8 \rightarrow \overset{N}{3}:\overset{M}{2}$, M_2N_3

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6. $r_{AB} = 1.52$ Å, $A = 1.7476$ (NaCl-type structure) $\quad \varepsilon_0 = 8.854\times10^{-12}\text{ Fm}^{-1} = C^2/Jm$

$$\Delta U = -A\left(\frac{z_+ z_- e^2}{4\pi\varepsilon_0 r_{AB}}\right)L$$

$\rightarrow$ (equation from Lecture 8 for solids)

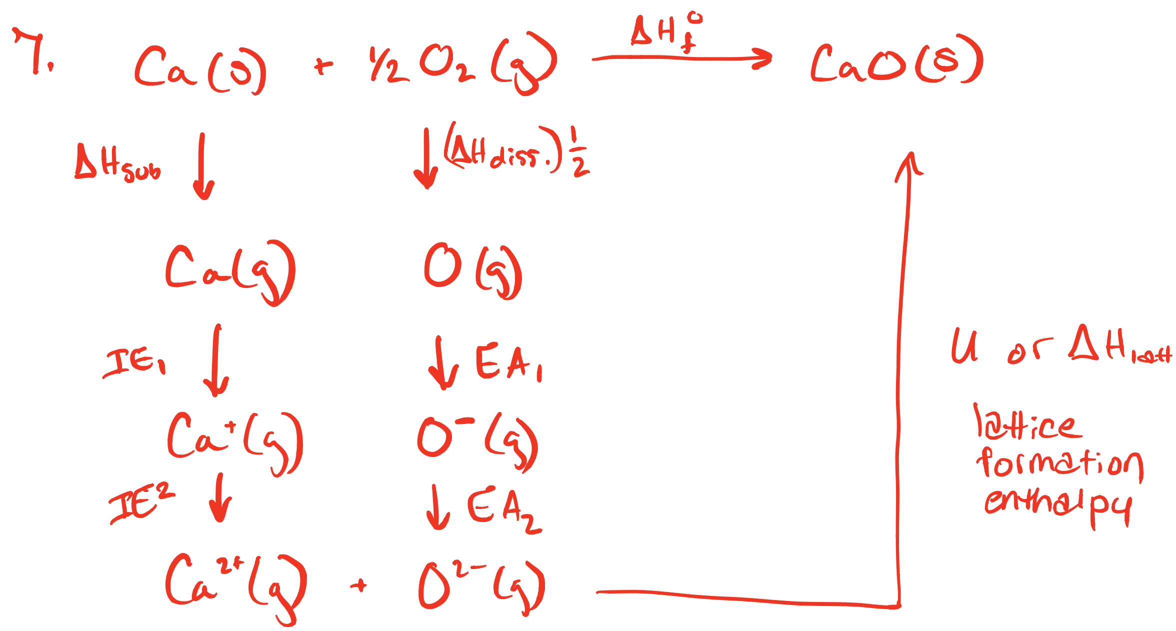
$$= -1.7476\left(\frac{(1.602\times10^{-19}\,C)^2 \times 1 \times 1}{4\pi\cdot 8.854\times10^{-12}\,F\,m^{-1}\cdot 1.52\times10^{-10}\,m}\right)\times 6.022\times10^{23}\,mol^{-1}$$

$$= -1.597\times10^{6}\ J/mol$$

$$= -1.60\times10^{3}\ kJ/mol \quad \text{(lattice formation)}$$

$$\hookrightarrow +1.60\times10^{3}\ kJ/mol \quad \text{(lattice separation)}$$

7.



$$\Delta H_f^\circ = \Delta H_{sub} + IE_1 + IE_2 + \frac{1}{2}\Delta H_{diss} + EA_1 + EA_2 + U$$

$$U = \Delta H_f^\circ - \Delta H_{sub} - IE_1 - IE_2 - \Delta H_{diss} - EA_1 - EA_2$$

$$= -3.41\times10^{3}\ kJ/mol$$