CHEM 245
PROBLEM SET III

1. Which of the following schemes in the packing of atoms (or spheres) will produce a close-packed structure?

    a) ABCABC.....

    b) ABBA.....

    c) ABCBC.....

2. The interstitial alloy tungsten carbide, WC, has the rock-salt (i.e. NaCl) structure. Describe the occupancy of the holes (sites) in this structure.

3. Consider the cesium chloride (CsCl) structure.
    a) What is the coordination number of the anion?
    b) What is the coordination number of the cation?
    c) How many Cs^+ ions occupy the second-nearest neighbour locations of a Cs^+ ion?

4. The ionic radii of Na^+ and Cl^- ions in NaCl are 95 and 181 pm, respectively. What is the length of the unit cell in this structure?

5. At room temperature, iron (Fe) crystallizes in a body-centred cubic (BCC) structure. The edge of this BCC cell is determined to be 287 pm. What is the radius of an Fe atom?

6. Using the data in question 5 above, and given that the atomic weight of Fe = 55.85 g/mol and that Avogadro's number = 6.022×10^{23} atoms/mol, calculate the density of Fe.

7. What is the name of the mineral with the formula $MgAl_2O_4$? What other cation charges can exist in mixed oxides of this structure?

8. For the perovskite structure to occur, what must be the true size of the cations?

9. Design a cycle of the Born-Haber type to evaluate the enthalpy of the reaction:,

$$NH_3(g) + H^+(g) \rightarrow NH_4^+(g)$$