MATRL 218/CHEM 277: Assignment 3

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1. The accompanying figure shows a two dimensional crystal structure formed by A, B, and C atoms.

   (a) What is the formula of the compound ?

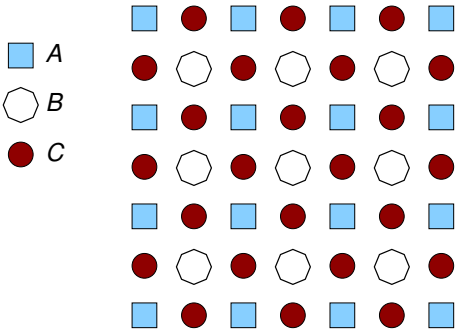
   (b) Identify the mirrors and rotation axes at the different atom sites.

   (c) Outline the unit cell.

   (d) What is the centering in the crystal ?

   (e) Can you suggest the name of the plane group.

   (f) Provide the complete minimal crystal structure description in terms of the plane group, cell parameters and the atom positions.



2. The compound OsAl has the following structure: SG = $Pm\bar{3}m$, a = 3.00 Å , Os at (1/2, 1/2, 1/2) and Al at (0,0,0).

   (a) Sketch the structure as sections, and within a cube.

   (b) What is this structure type called ?

   (c) $OsAl_2$ is formed by successively stacking OsAl cubes, but every new stack is created from the old one by adding (1/2, 1/2, ≈1.5) Sketch $OsAl_2$ as sections after generating its coordinates. Is $OsAl_2$ cubic ? What are the cell parameters.

   (d) Can you guess the space group of $OsAl_2$?

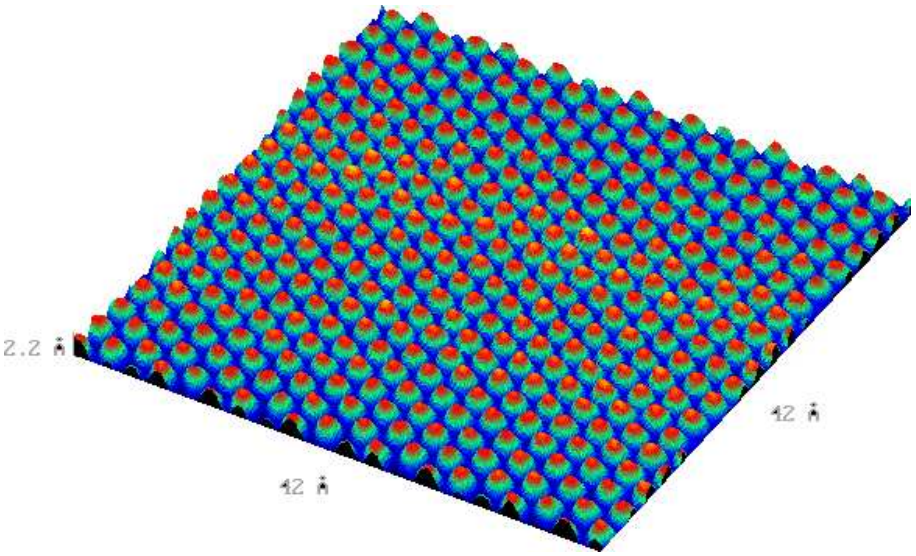
   (e) Can you guess how Os_2Al_3 is built up ?

3. Sketch the ideal perovskite ABO_3 structure with A atoms at the corners of the cell and the B atom in the middle. What are the coordinates of A, B and O ? Remember to provide the minimal, crystallographic description. How many nearest neighbors do A, B, and O each have ?

4. Sketch the perovskite structure as projections and then sketch the rock salt structure as projections. Compare the layers. Are there any structural relationships ? Show that the perovskite structure can be considered as alternate stackings of AO rock salt layers and BO_2 layers.

5. A compound is described with three kinds of atoms in the unit cell, A, B and C. A is in the Wyckoff position 2a, (for the specific space group) B is in the Wyckoff position 8c and C in 24f. What is the formula of the compound.

6. Given below is an STM image of the surface of a highly oriented graphite crystal. Given what you know about the graphite crystal structure, can you tell what the blimps are ? Are they atoms ?



The image is from `http://www.physics.louisville.edu/`

7. Carbon nanotubes are formed by rolling up single graphite sheets. Show using a suitable sketch that some carbon nanotubes can possess chiral[1] screw axes along the tube direction. Extra points for making models !!!

8. The electrostatic valence rule of Pauling states:

$$\Sigma s = -V_- \text{ and } s = V_+/Z$$

where s is the bond valence, V_+ is the charge (valence) of the cation, V_- is the charge of the anion, and Z is the coordination number of the cation. If $Z = 4$ in amorphous SiO_2, how many Si is each O bonded to.

   (a) Assign charges on Si and O in SiO_2.
   Describe the Si-O network in amorphous SiO_2 with a sketch.
   Verify that the valence rule works for amorphous SiO_2
   The addition of H_2O to SiO_2 (as happens in certain hydrothermal processes in geology) results in the Si-O-Si network of silica being broken. Use electrostatic valence to determine the H_2O:SiO_2 ratio required so that all SiO_4 tetrahedra are *isolated*, *ie.* no two tetrahedra share O atoms.

   (b) If Z were 6 in SiO_2 (giving SiO_6 octahedra as in stishovite SiO_2) how many Si would O be bonded to ?

   (c) TiO and TiN crystallizes in the rock-salt structure. Apply the electrostatic valence rule (you will have to chose charges). If the rule fails, attempt an explanation for why it does ?

[1] Meaning that there are left and right handed versions such as the screws 6_1 and 6_5