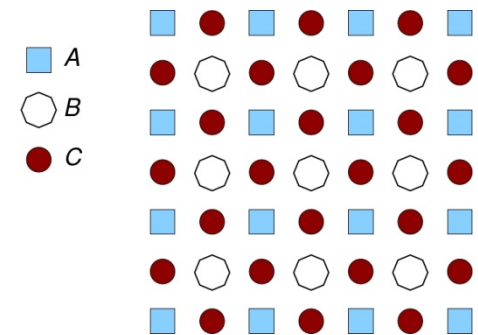


Assignment 3: Due Thursday February 4th 2010

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

- What is the formula of the compound ?
- Identify the mirrors and rotation axes at the different atom sites.
- Outline the unit cell.
- What is the centering in the crystal ?
- Can you suggest the name of the plane group.
- Provide the complete minimal crystal structure description in terms of the plane group, cell parameters and the atom positions. (just as structures are described in your notes)



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

- Sketch the structure as sections, and within a cube.
- What is this structure type called ?
- OsAl₂ is formed by successively stacking OsAl cubes, but every new stack is created from the old one by adding $(1/2, 1/2, \sim 1.5)$ Sketch OsAl₂ as sections after generating its coordinates. Is OsAl₂ cubic ? What are the cell parameters.
- Can you guess the space group of OsAl₂ ?
- Can you guess how Os₂Al₃ is built up ?

Note that OsAl, OsAl₂, and Os₂Al₃ VESTA files are posted.

3. Use the bond valence values from the PDF file provided on the course website, and the exponent formula (not the power-law formula; formula in PDF file) to estimate the cell parameters of NaCl, CsCl, and CaF₂. Compare these values with values you would obtain using the appropriate ionic radii (also to be found on the Seshadri group website). Finally compare these with the values in your notes.