MATRL 218: Assignment 3

**Ram Seshadri (seshadri@mrl.ucsb.edu)**

1. 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. Also use VESTA if you wish.

   (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 crystal system and the centering in $OsAl_2$?

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

2. X-ray studies suggest that mineral Wickmanite (connectivity shown below) has corner-sharing octahedra of MnO_6 and SnO_6 with Mn–O and Sn–O bond lengths of 2.15 Å and 2.02 Å, respectively.

   Using the exponential bond-valence-sum relationship:

   $$s = \exp\left(\frac{R_0 - R}{B}\right),$$

   and the following values for R_0 and B (R_0 for Mn(II)–O is 1.790 Å; for Sn(IV)–O, it is 1.905 Å, and $B = 0.37$ Å), calculate the bond valence sums (BVS) for Mn, Sn, and O? What do the BVS tell you about the composition of the compound (hint: is this an oxide)?
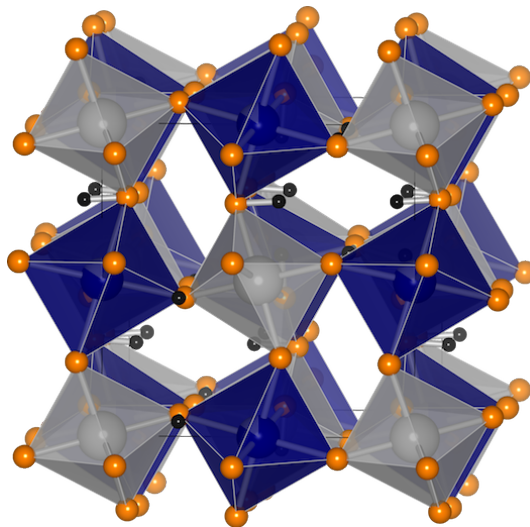
3. Use VESTA to sketch the structures of (i) graphite, (ii) diamond, (iii) NaCl, (iv) CsCl, (v) ZnS (wurtzite) and (vi) ZnS (zinc blende).