MATRL 218: Assignment 3

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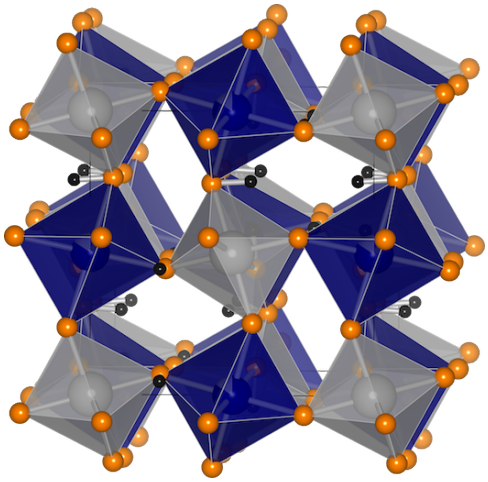
1. The compound OsAl has the following structure: SG = $Pm\bar{3}m$, a = 3.00 Å, Os at (1/2,1/2,1/2) and Al at (0,0,0).
   (a) Sketch the structure as sections, and within a cube. Also use VESTA if you wish.
   (b) What is this structure type called ?
   (c) $OsAl_2$ is formed by successively stacking 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? What is the issue with the use of X-rays?



3. Use VESTA to sketch the structures of (i) graphite (connect the carbons), (ii) diamond (connect the carbons), (iii) NaCl, (iv) CsCl.

4. Use VESTA to sketch the structures of CuO and NbO using the provided CIF files that can be directly opened by VESTA. Can you describe how these are derived from the structure of NaCl.