MATRL 218: Assignment 3

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1. The compound OsAl has the following structure: SG = $Pm\bar{3}m$, $a = 3.00\,\text{Å}$, 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, $\approx$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 ?

2. The 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 $B = 0.37\,\text{Å}$), 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)?
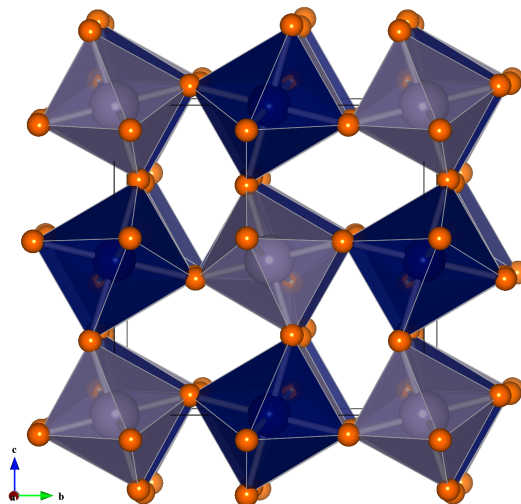
3. Use VESTA to draw all of the binary structures discussed in class.