

MATRL 218: Assignment 3

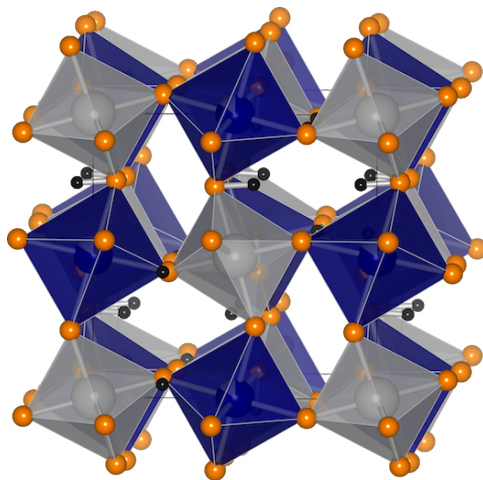
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- Use VESTA to sketch the structures of (i) diamond Si (connect the Si), (ii) graphite (connect the carbons), (iii) NaCl, (iv) CsCl.
- The compound OsAl has the following structure: $SG = Pm\bar{3}m$, $a = 3.00 \text{ \AA}$, Os at $(1/2, 1/2, 1/2)$ and Al at $(0, 0, 0)$.
 - Sketch the structure as sections, and within a cube. Also use VESTA if you wish.
 - What is this structure type called ?
 - 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?
 - Can you guess the crystal system and the centering in OsAl_2 ?
 - Can you guess how Os_2Al_3 is built up ?
- 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 \AA and 2.02 \AA , respectively.

Use the exponential bond-valence-sum relationship:

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

and the following values: R_0 for Mn(II)–O is 1.790 \AA and for Sn(IV)–O, it is 1.905 \AA ; $B = 0.37 \text{ \AA}$. Calculate the bond valence sums (BVS) for Mn, Sn, and O (by adding all the individual valences reaching the atom). 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?



- 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.