MATRL 218 / CHEM 277: Assignment 1

1. The cubic crystal structure of double perovskite $\text{Ba}_2\text{MgWO}_6$ is presented in the Oxides Structures slides. Sketch the appropriate bond-valence map for this structure. The charges are $\text{Ba}^{2+}$, $\text{Mg}^{2+}$, $\text{W}^{6+}$ and $\text{O}^{2-}$. Assign charges for all the lines in the graph (as illustrated for other structures) and verify that the second Paulings rule is applicable by counting all the charges reaching $\text{O}$, as also described in the structures slides.

2. Use the bond valence formula:

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

and the values, $B = 0.37 \text{ Å}$, $R_0 = 1.693 \text{ Å}$ ($\text{Mg}^{2+}$ and $\text{O}$) and $1.917 \text{ Å}$ ($\text{W}^{6+}$ and $\text{O}$) to estimate $R$ for the two pairs, and thereby the unit cell parameter for $\text{Ba}_2\text{MgWO}_6$. The experimental value is close to $8.10 \text{ Å}$.

3. You have seen the glide $g$ in 1D and 2D. What do the $n$ and $d$ glides in 3D crystals do? Depict them with appropriate sketches.

4. Cubic cells always have a $\bar{3}$ or 3 in the space group label. What is the $\bar{3}$ symmetry element in a cube?

5. Show that $\bar{6}$ also implies a 3-fold rotation.

6. Sketch the $6_1$ and $6_5$ mirror pairs of symmetry operations and the $6_2$ and $6_4$ mirror pairs. Use a low-symmetry motif of the letter “R” for your illustration.

7. Sketch 2D objects with the following symmetries: (i) $2m'$ and (ii) $4mm$. Indicate the mirror lines. Also, mention any other symmetry operations that you find.

8. The plane groups $p31m$ and $p3m1$ differ in that, in one of them but not the other, all rotation axes are on mirrors. Sketch examples of the two plane groups, indicating rotation axes and mirrors.