Homework 3
Due 20 September 2018
The numbers following each question give the approximate percentage of marks allocated to that question.

1. Briefly define/explain each of these terms. Add a sketch if convenient.

   (a) unit cell  
   (b) lattice parameters  
   (c) symmorphic space group  
   (d) abelian  

   2   
   2   
   2   
   2
2. Use the metric tensor to calculate the distance between atoms at 000 and $\frac{1}{2} \frac{3}{4}$ in a monoclinic unit cell with lattice constants $a = 1 \text{ Å}, b = 2 \text{ Å}, c = 3 \text{ Å}, \beta = 95^\circ$.

3. For each space group listed below, identify the point group and Bravais lattice.

- P6$_1$22
- P2$_1$/c
- Cmc2$_1$
- I4$_1$md
- Fd$\bar{3}$

4. Many space group notations are dependent upon the orientation of the axes which one chooses to describe a structure. In such cases there is a “standard” setting, but potentially many other “non-standard” ones as well. In the example of Pban (#50), if the axes were re-oriented such that $abc \rightarrow cab$, use what you know about symmetry operations and space-group notation to determine what the new notation would be, and explain your answer.
5. The structure of NaCl is usually described as face-centered cubic in space group \(Fm\bar{3}m\). The ionic positions are:

\[
\begin{align*}
\text{Na}^+ & \quad 4a & 0, 0, 0 \\
\text{Cl}^- & \quad 4b & \frac{1}{2}, \frac{1}{2}, \frac{1}{2}
\end{align*}
\]

Sketch one unit cell of this structure. How many ions comprise the basis? Annotate your drawing to show these ions.

A body-centered unit cell can be inscribed within the face-centered one. Sketch this new unit cell within a single fcc NaCl one and indicate its basis. What is the new Bravais lattice which is formed?

It is always possible to draw a primitive unit cell of any crystalline structure. Inscribe a primitive unit cell within a single fcc NaCl one and indicate its basis. What is the Bravais lattice now?
6. a. Draw a representation of $2/m$ point symmetry, including all the necessary symmetry elements and symmetry-related objects. Using this diagram, construct a multiplication table for this point group. Use either Schönflies or Hermann-Mauguin notation. 

*HINT: The order of the group is four.*

b. Draw a representation of $3m$ point symmetry, including all the necessary symmetry elements and symmetry-related objects, *uniquely labeling all of the mirror symmetry elements present*. Using this diagram, construct a multiplication table for this point group using the same labels. Use either Schönflies or Hermann-Mauguin notation. 

*HINT: The order of the group is six.*

c. Which, if either, of these two groups is/are abelian?
7. Draw schematics showing the positions of objects along a $3_1$ and a $4_3$ screw axis. For each case assume the screw axis is the $c$ axis and draw the axis in two ways, first parallel to the plane ($c$ axis to the right) then perpendicular to the plane ($c$ axis coming out of the plane), using the correct symbol for the symmetry element. Consider the implications of translational symmetry in each case.

For both $3_1$ and $4_3$, write out the resultant overall transformation (both rotation matrix and translation vector as well as their sum) in an appropriate axis system.

Demonstrate another way of describing the right-handed $4_3$ screw symmetry?