Assignment 1

Symmetry operations, point groups, crystal systems

Please no AI generated solutions. Would be your loss!

Question 1

Show the location of the **6** rotation axis on the hexagonal unit cell.

Question 2

(a) Why is there no base-centered (C-centered) cubic lattice? Describe your response using appropriate geometrical drawings.

(b) Why is there no f-centred tetragonal Bravais lattice?

(c) Why is it not possible to centre two, instead of three, faces of a cubic unit cell?

Question 3

(a) The point group D_{4h} or $\mathbf{4/mmm}$ is developed from the point group C_{4h} or $\mathbf{4/m}$ by introducing a **2** rotation axis perpendicular to the principal 2 axis of the $\mathbf{2/m}$ point group. This construction can be written as:

$$D_{4h} = \{1, 2'\} \circ C_{4h}.$$

Draw the stereograms of $C_4 \equiv \mathbf{4}$, $C_{4h} \equiv \mathbf{4/m}$, $D_{4h} \equiv \mathbf{4/mmm}$, evolving them in a step-by-step fashion.

(b) Could you repeat this line of argument and show the development of the $D_{2d} \equiv \bar{\mathbf{4}}\mathbf{2m}$ point group starting from $\bar{\mathbf{4}}$ point group?

Question 4

The monoclinic unit cell is compatible with the point group **2**, **m** and **2/m**. They are described by the symmetry elements:

2	a lone two rotation axis
m	a single mirror plane
2/m	a two fold axis with a perpendicular mirror plane

Diagrammatically, these are represented as follows:

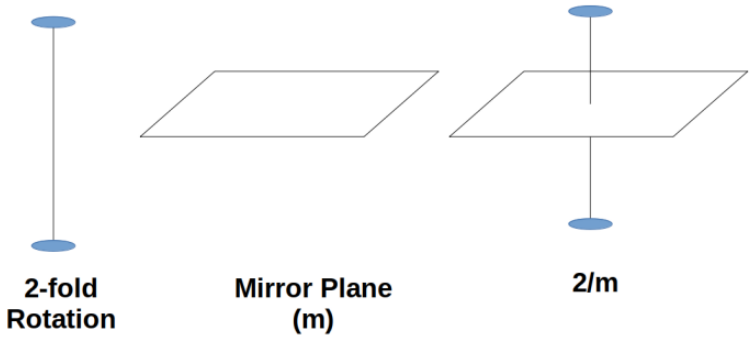

Figure 1: Diagrams of the symmetry elements.

Draw similar diagrams for the group **222**, **mm**, and **mmm** compatible with the orthorhombic system.

Question 5

Show that in the hexagonal unit cell, if we accidentally set $a = b$, $\gamma = 120°$, we in fact generate another Bravais lattice. What is that Bravais lattice and what are its cell dimensions?

Question 6

(a) In a unit cell, Au has atoms at 000, $0\frac{1}{2}\frac{1}{2}$, $\frac{1}{2}0\frac{1}{2}$, $\frac{1}{2}\frac{1}{2}0$. What is the Bravais lattice for Au? Identify the basis/motif?

(b) Au_3Cu has:

$$\begin{array}{ll} \text{Au} & 000 \\ \text{Cu} & 0\frac{1}{2}\frac{1}{2}, \quad \frac{1}{2}0\frac{1}{2}, \quad \frac{1}{2}\frac{1}{2}0 \end{array}$$

What is its Bravais lattice? Identify the basis/motif?

Question 7

The compound La_2CuO_4 was discovered to be a superconductor at $T_c \sim 30K$. Its system is tetragonal with $a = 3.8$Å, $c = 13.3$Å. The approximate coordinates of atoms in the ratio 2:1:4 are:

Au	$00\frac{3}{8}$,	$\frac{1}{2}\frac{1}{2}\frac{7}{8}$		
Cu	000,	$\frac{1}{2}\frac{1}{2}\frac{1}{2}$		
O	$00\frac{1}{6}$,	$0\frac{1}{2}0$,	$\frac{1}{2}\frac{1}{2}\frac{2}{3}$,	$\frac{1}{2}0\frac{1}{2}$

Identify the Bravais lattice and the motif.