SYMMETRY ELEMENTS

TYPES OF SYMMETRY ELEMENT

- The types of symmetry element that occur in crystal lattices can broadly be divided into two large groups: non-translational and translational symmetry elements. In diffraction data, these can be differentiated by the occurrence of absences. Absences in diffraction data occur when the intensity corresponding to a specific Miller index (hkl value) is zero.
- Translational symmetry elements can be identified by a translation. A translation of an object can be defined as moving an object in a direction (a, b, c) without rotating or reflecting the object.
- For example an object located at (x, y, z) when translated by (a, b, c) will be located at (x + a, y + b, z + c). These types of symmetry elements will cause absences within diffraction data. These are screw axes and glide planes.
- Nontranslational symmetry elements do not cause absences in crystal data. These are centre of symmetry (inversion centre), reflection, rotation (only two-, three-, four-, or six-fold), and rotary inversion. The following sections describe these symmetry elements in detail.

NON-TRANSLATIONAL SYMMETRY ELEMENTS

- The inversion centre: An inversion centre or a centre of symmetry is typically identified by a bold or darkened point. It is also denoted in writing with a bar across the top of a number, e.g., $\bar{1}$.

Figure 3.2 Principles of Xray Crystallography, L.Ooi, Oxford Uni. Press

Reflection: A reflection, like the most common reflections that we know of, takes place across a mirror plane. The mirror plane is denoted by the letter **m** and by a dark horizontal line in the perpendicular view (**-**) while in the plane view it is denoted by a top-right corner (ᒣ)

Figure 3.3 Principles of Xray Crystallography, L.Ooi, Oxford Uni. Press

Rotation (only one-, two-, three, four. or six-fold)

All rotations in crystallography occur counterkwise, as a fraction of the circle upon which that rotation occurs. There are only five types of rotation; one-, two-, three-, four-. and sixfold. Rotations are denoted by an integer, n, (n-fold) and by the symbols given in Table.

Table 3.1 Principles of Xray Crystallography, L.Ooi, Oxford Uni. Press

Figure 3.4 Principles of Xray Crystallography, L.Ooi, Oxford Uni. Press

Rotation-inversion

A rotation-inversion consists of a combination of two symmetry elements; a rotation followed by an inversion. Here again the rotations occur in a *counterclockwise* fashion, and are considered as a fraction of a full circle. A rotation-inversion is denoted by a bar across the top of the allowed rotations, $\bar{2}$, $\bar{3}$, $\bar{4}$, or $\bar{6}$, and by the symbols in Table 3.2.

TABLE 3.2 Typical rotation-inversions and symbols, where axes are normal to plane

Name of rotation-inversion	Notation	Symbol
Diad	2-fold	⬯
Triad	3-fold	△
Tetrad	4-fold	◇
Hexad	6-fold	⬡

Figure 3.5 Principles of Xray Crystallography, L.Ooi, Oxford Uni. Press

TRANSLATIONAL SYMMETRY ELEMENTS

There are only two types of translational symmetry in crystaJlography; the screw axis and the glide plane. Both of these can be identified in diffraction data by absences caused.

Screw axis

A screw axis consists of a combination of two symmetry operations; a translation followed by a rotation.

This can be written generally as $M_{n,}$ where each object is rotated by 360/M degrees. then translated upwards by a fraction n/M of the unit cell.

Table 3.3 Principles of Xray Crystallography, L.Ooi, Oxford Uni. Press

Figure 3.6 Principles of Xray Crystallography, L.Ooi, Oxford Uni. Press

The example shown in Fig. represents two possible types of three-fold screw axis;
(a) 3_1 and (b) 3_2,

Figure 3.6 Principles of Xray Crystallography, L.Ooi, Oxford Uni. Press

The example shown in Fig. represents two possible types of three-fold screw axis;
(a) 3_1 and (b) 3_2,

- **Glide plates :** A glide plane also consists of a combination of two symmetry operations, in this case a translation followed by a reflection.
- Glide planes are denoted by the planes along which the glide occurs, most commonly a, b, c, or n (an n glide typically refers to a diagonal direction within the unit cell).

Figure 3.7 Principles of Xray Crystallography, L.Ooi, Oxford Uni. Press

LATTICE TYPES AND SYMMETRY ELEMENTS

- In this section, we will see how we can determine the types of symmetry operations that may occur in the different lattice types.

Triclinic lattices ($a \neq b \neq c$; $\alpha \neq \beta \neq \gamma \neq 90°$)

Figure 3.7 Principles of Xray Crystallography, L.Ooi, Oxford Uni. Press

Monoclinic lattices ($a \neq b \neq c$; $\alpha = \gamma = 90°, \beta \neq 90°$)

Figure 3.8 Principles of Xray Crystallography, L.Ooi, Oxford Uni. Press

Trigonal lattices ($a = b \neq c$; $\alpha = \beta = 90°, \gamma = 120°$)

Figure 3.9 Principles of Xray Crystallography, L.Ooi, Oxford Uni. Press

Hexagonal lattices ($a = b \neq c$; $\alpha = \beta = 90°$, $\gamma = 120°$)

Figure 3.9 Principles of Xray Crystallography, L.Ooi, Oxford Uni. Press

Orthorhombic lattices ($a \neq b \neq c$; all angles $= 90°$)

Figure 3.9 Principles of Xray Crystallography, L.Ooi, Oxford Uni. Press

Tetragonal lattices ($a = b \neq c$; all angles = 90°)

Figure 3.9 Principles of Xray Crystallography, L.Ooi, Oxford Uni. Press

Cubic lattices ($a = b = c$; all angles = 90°)

Figure 3.9 Principles of Xray Crystallography, L.Ooi, Oxford Uni. Press