SPACE GROUPS

- After examining and understanding the symmetry elements and how they can be found in connection to the various Sravais lattice types in previous chapter, we now need to consider how this information may be easily shared or transmitted.
- Crystallographers use a simple and concise mathematical representation of lattice types and symmetry operators, known as space groups. Here, we will look at the concept of space groups and examine why there are 230 space groups. We will learn the use of the Hermann-Mauguin notation and space group symbols in representing symmetry operations.

- we examined how not all symmetry operators could occur in all of the Bravais lattice types. We found that the higher the symmetry of the Bravais lattice, the more likely it was to contain onc or more symmetry elements.
- The type of centring of the Bravais lattice (primitive, body-centred, or face-centred) also contributes significantly to the symmetry elements that may be found within that lattice type. Various combinations of the six symmetry operations with the different lattice types produce 230 unique arrangements of objects that fill space; hence the 230 space groups distributed across seven crystal systems.

Table 4.1
Principles of Xray Crystallography, L.Ooi, Oxford Uni. Press

HERMANN- MAUGUIN NOTATION

- The Hermann-Mauguin nolation is written with the first letter representing the lattice type and the follow ing three notations representing the lype of symmetry operation or operations along the corresponding axes of x, y, and z.

Table 4.2
Principles of Xray Crystallography, L.Ooi, Oxford Uni. Press

In the case of glide planes, however, the notation is such that the named glide plane runs *perpendicularly to* the axis.

For example in the monoclinic space group, *P* 1*c* 1, which is usually shortened to *P c*,

Direction	*x*	*y*	*z*
Lattice	*a*	*b*	*c*
Space group	*P* 1*c* 1		

explains that the lattice is a primitive lattice with a c glide plane perpendicular to the b-direction while there are no other symmetry elements along the other directions.

- A space-grollp diagram is a two-dimensional projection of a 3D unit cell.
- Figure shows a 3D view of a unit cell in solid black lines. with the dotted boxes dividing the unit cell along each of the axes into two equal halves. The positionai coordinates of this object are (a, b, c), which can be described as a value of a along x, a value of b along y. and a value of c along z.

Figure 4.2
Principles of Xray Crystallography, L.Ooi, Oxford Uni. Press

General positions diagram

Figure 4.3
Principles of Xray Crystallography, L.Ooi, Oxford Uni. Press

SYSTEMATIC ABSENCES IN CRYSTAL DATA

- When a diffraction pattern is collected either on photographic film or on an X~ray diffractometer, each 'frame' of data (Fig.) contains reflec tions (spots) of differing intensities, while at certain points on the frame of data some reflections are missing or absent.

Figure 5.1
Principles of Xray Crystallography, L.Ooi, Oxford Uni. Press

Some of these absent reflections have intensities close to zero because only very few electrons in the crystal structure are contributing to diffraction from the associated plane, while other reflections are precisely zero because of the dest ructive interference of the incident X-rays. These absences are influenced bylhe positions of symmetry-related atoms or molecules within the crystal st ructure,

- During the course of a data collection, multiple frames of data are collected, in order to accumulate sufficient data to cover the reciprocal space of the entire crystal lattice.
- Within each frame of data, each reflection is related to a specific Miller plane (h, k, l) with a specific value of'observed' intensity I_{hkl}^{obs} used to define it.
- An absellce occurs when $I_{hkl}^{obs} = 0$

- Each integrated value of intensity is proportional to the square of the observed **structure factor** (F_{hkl}^{obs}) for the associated Miller index;

- $I_{hkl}^{corr} \propto (F_{hkl}^{obs})^2$

- After integration, scaling, and various corrections for background are applied, culminating in the output of a text-based computer file of diffraction data representative of the Single crystal. This is known as the .hkl fi le. The .hkl file contains Miller indices (hkl values) in the first th ree columns, followed by a numerical value of intensity (I) and a value of standard deviation (σ).

Figure5.2
Principles of Xray Crystallography, L.Ooi, Oxford Uni. Press