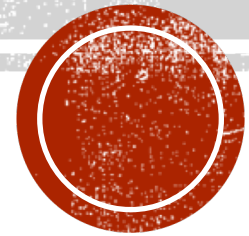


SPACE GROUPS



- After examining and understanding the symmetry elements and how they can be found in connection to the various Bravais 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 one 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
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HERMANN- MAUGUIN NOTATION

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

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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, $P1c1$, which is usually shortened to Pc ,

Direction	x	y	z
Lattice	a	b	c
Space group	$P1c1$		

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-grohhp 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
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General positions diagram

Figure 4.3
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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 reflections (spots) of differing intensities, while at certain points on the frame of data some reflections are missing or absent.

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 destructive interference of the incident X-rays. These absences are influenced by the positions of symmetry-related atoms or molecules within the crystal structure,

Figure 5.1
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- 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 file. The .hkl file contains Miller indices (hkl values) in the first three columns, followed by a numerical value of intensity (I) and a value of standard deviation (σ).



Figure 5.2
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