Lecture 4

General Equivalent Positions

- A **general position** is an arbitrary (x, y) occupied by a motif
- Given (x, y), tells us which other positions are equivalent
  - e.g. for p2, (x, y) and $(\overline{x}, \overline{y})$ are equivalent
- Number of equivalent positions for a given point is called its **multiplicity**
- Special position: position where multiplicity is not at maximum
  - e.g. multiplicity of a general element in p4 is 4, but that of $(0, 0)$ is 1

Wyckoff Symbols

- Starts from a
- Increases with multiplicity

Terminology

- Chirality: property of a chemical whose mirror reflection **cannot** be produced by any combination of rotation and translation
- Enantiomer: object that demonstrates chirality. Comes in pairs

Centre of Symmetry

- Denoted by $\overline{1}$
- Does not exist in 2D as it simplifies to a mirror transformation
  - However it is unique in 3D

Rotoinversion

- Compound Inversion: a rotation then an inversion about the centre of symmetry
- also known as improper rotation
- n-fold rotoinversion: a $2\pi/n$ rotation about the axis, then an inversion about the centre of symmetry
- Denoted as $\overline{n}$

Rotoreflection

- Compound Inversion: a rotation then an inversion about the centre of symmetry
- also known as improper rotation
- n-fold rotoreflection: a $2\pi/n$ rotation about an axis **normal** to the mirror plane, then a reflection about the plane
- Denoted as $\tilde{n}$

3-D Point Group Symbol Nomenclature

Table 4.2 The order of the Hermann-Mauguin symbols in point groups

Crystal system	Primary	Secondary	Tertiary
Triclinic	–	–	–
Monoclinic	[010], unique axis **b** [001], unique axis **c**	–	–
Orthorhombic	[100]	[010]	[001]
Tetragonal	[001]	[100], [010]	[1$\bar{1}$0], [110]
Trigonal, Rhombohedral axes	[111]	[1$\bar{1}$0], [01$\bar{1}$], [$\bar{1}$01]	
Trigonal, Hexagonal axes	[001]	[100], [010], [$\bar{1}\bar{1}$0]	
Hexagonal	[001]	[100], [010], [$\bar{1}\bar{1}$0]	[1$\bar{1}$0], [120], [$\bar{2}\bar{1}$0]
Cubic	[100], [010], [001]	[111], [1$\bar{1}\bar{1}$], [$\bar{1}$1$\bar{1}$], [$\bar{1}\bar{1}$1]	[1$\bar{1}$0], [110], [01$\bar{1}$], [011], [$\bar{1}$01], [101]

3-D Point Groups

- Primary, Secondary, Tertiary axes in order
- Example: mP has a symbol of $\frac{2}{m}$, as along its primary axis, there is a 2-fold rotational symmetry and a mirror plane perpendicular to it

Crystallographic Point Groups

- 7 lattice symmetries
- Allowed point group operations: $1, 2, 3, 4, 6, \overline{1}, \overline{3}, \overline{4}, \overline{6}, m$
- 33 in total