Symmetry Classification for Serial Crystallography Experiments

Groups with white backgrounds are merohedral and will exhibit indexing ambiguities. Move directly downwards to the nearest cell with a shaded background to find the corresponding "source symmetry". Chiral groups are shown in bold, centrosymmetric groups are underlined.

Point Groups		Space Groups	
Triclinic lattice			
$\bar{1}$	**1**	P$\bar{1}$	**P1**
Monoclinic lattice			
2	m	**P2, P2$_1$, C2**	Pm, Pc, Cm, Cc
	2/m		P2/m, P2$_1$/m, C2/m, P2/c, P2$_1$/c, C2/c
Orthorhombic lattice			
222	mm2	**P222, P222$_1$, P2$_1$2$_1$2, P2$_1$2$_1$2$_1$, C222$_1$, C222, F222, I222, I2$_1$2$_1$2$_1$**	Pmm2, Pmc2$_1$, Pcc2, Pma2, Pca2$_1$, Pnc2, Pmn2$_1$, Pba2, Pna2$_1$, Pnn2, Cmm2, Cmc2$_1$, Ccc2, Amm2, Aem2, Ama2, Aea2, Fmm2, Fdd2, Imm2, Iba2, Ima2
	mmm		Pmmm, Pnnn, Pccm, Pban, Pmma, Pnna, Pmna, Pcca, Pbam, Pccn, Pbcm, Pnnm, Pmmn, Pbcn, Pbca, Pnma, Cmcm, Cmce, Cmmm, Cccm, Cmme, Ccce, Fmmm, Fddd, Immm, Ibam, Ibca, Imma
Tetragonal lattice							
4	$\bar{4}$		4mm	4/m	**P4, P4$_1$, P4$_2$, P4$_3$, I4, I4$_1$**	P$\bar{4}$, I$\bar{4}$		P4/m, P4$_2$/m, P4/n, P4$_2$/n, I4/m, I4$_1$/a
422	$\bar{4}$2m	$\bar{4}$m2			**P422, P42$_1$2, P4$_1$22, P4$_1$2$_1$2, P4$_2$22, P4$_2$2$_1$2, P4$_3$22, P4$_3$2$_1$2, I422, I4$_1$22**	P$\bar{4}$2m, P$\bar{4}$2c, P$\bar{4}$2$_1$m, P$\bar{4}$2$_1$c, I$\bar{4}$2m, I$\bar{4}$2d	P$\bar{4}$m2, P$\bar{4}$c2, P$\bar{4}$b2, P$\bar{4}$n2, I$\bar{4}$m2, I$\bar{4}$c2	P4mm, P4bm, P4$_2$cm, P4$_2$nm, P4cc, P4nc, P4$_2$mc, P4$_2$bc, I4mm, I4cm, I4$_1$md, I4$_1$cd	
	4/mmm					P4/mmm, P4/mcc, P4/nbm, P4/nnc, P4/mbm, P4/mnc, P4/nmm, P4/ncc, P4$_2$/mmc, P4$_2$/mcm, P4$_2$/nbc, P4$_2$/nnm, P4$_2$/mbc, P4$_2$/mnm, P4$_2$/nmc, P4$_2$/ncm, I4/mmm, I4/mcm, I4$_1$/amd, I4$_1$/acd		

Trigonal lattice

3	$\underline{\bar{3}}$		**R3 (H3)**	$\underline{\text{R}\bar{3}\ (\text{H}\bar{3})}$	
32		3m	**R32 (H32)**		R3m (H3m), R3c (H3c)
	$\underline{\bar{3}\text{m}}$			$\underline{\text{R}\bar{3}\text{m}\ (\text{H}\bar{3}\text{m})}$, $\underline{\text{R}\bar{3}\text{c}\ (\text{H}\bar{3}\text{c})}$	

Hexagonal lattice

	3		$\underline{\bar{3}}$					**P3**, **P3$_1$**, **P3$_2$**			P$\bar{3}$							
				3m1		31m					P3m1, P3c1			P31m, P31c				
6					$\bar{6}$			**P6**, **P6$_1$**, **P6$_5$**, **P6$_2$**, **P6$_4$**, **P6$_3$**				P$\bar{6}$					$\underline{\text{P6/m}}$, $\underline{\text{P6}_3\text{/m}}$	
	312					$\underline{\bar{3}\text{1m}}$			**P312**, **P3$_1$12**, **P3$_2$12**						P$\underline{\bar{3}}$1m, P$\underline{\bar{3}}$1c			
		321	$\underline{\bar{3}\text{m1}}$							**P321**, **P3$_1$21**, **P3$_2$21**	P$\underline{\bar{3}}$m1, P$\underline{\bar{3}}$c1							
				$\bar{6}$m2	$\bar{6}$2m		6mm					P$\bar{6}$m2, P$\bar{6}$c2	P$\bar{6}$2m, P$\bar{6}$2c		P6mm, P6cc, P6$_3$cm, P6$_3$mc			
622			$\underline{6/\text{mmm}}$					**P622**, **P6$_1$22**, **P6$_5$22**, **P6$_2$22**, **P6$_4$22**, **P6$_3$22**			P6/mmm, P6/mcc, P6$_3$/mcm, P6$_3$/mmc							

Cubic lattice

23		$\underline{\text{m}\bar{3}}$	**P23**, **F23**, **I23**, **P2$_1$3**, **I2$_1$3**		$\underline{\text{Pm}\bar{3}}$, $\underline{\text{Pn}\bar{3}}$, $\underline{\text{Fm}\bar{3}}$, $\underline{\text{Fd}\bar{3}}$, $\underline{\text{Im}\bar{3}}$, $\underline{\text{Pa}\bar{3}}$, $\underline{\text{Ia}\bar{3}}$
432	$\bar{4}$32		**P432**, **P4$_2$32**, **F432**, **F4$_1$32**, **I432**, **P4$_3$32**, **P4$_1$32**, **I4$_1$32**	P$\bar{4}$3m, F$\bar{4}$3m, I$\bar{4}$3m, P$\bar{4}$3n, F$\bar{4}$3c, I$\bar{4}$3d	
	$\underline{\text{m}\bar{3}\text{m}}$				$\underline{\text{Pm}\bar{3}\text{m}}$, $\underline{\text{Pn}\bar{3}\text{n}}$, $\underline{\text{Pm}\bar{3}\text{n}}$, $\underline{\text{Pn}\bar{3}\text{m}}$, $\underline{\text{Fm}\bar{3}\text{m}}$, $\underline{\text{Fm}\bar{3}\text{c}}$, $\underline{\text{Fd}\bar{3}\text{m}}$, $\underline{\text{Fd}\bar{3}\text{c}}$, $\underline{\text{Im}\bar{3}\text{m}}$, $\underline{\text{Ia}\bar{3}\text{d}}$

Detailed Description

Each space group or plane group (hereafter, “space group” should be interpreted as “plane group” for the 2D case) is associated with a single point group. If the space group is centrosymmetric, then the point group must also be centrosymmetric. A centrosymmetric point group can alternatively be called a “Laue class”, and every non-centrosymmetric point group belongs to a single Laue class. The Laue class describes the point symmetry of the structure if a centre of symmetry were to be added. For each Laue class, the centre of symmetry could be removed to produce a non-centrosymmetric point group. For many Laue classes, there are multiple ways in which this could be done, and so multiple non-centrosymmetric point groups belong to that same Laue class.

Each row of these tables shows all the space groups associated with the Laue class at the far left of the row. To the right of the Laue class are listed the non-centrosymmetric point groups which belong to that Laue class. To the right of the double ruled line are found the space groups: centrosymmetric space groups to the left (whose corresponding point group is centrosymmetric, and so is the Laue class for the row), and non-centrosymmetric space groups to the right. Each non-centrosymmetric space group corresponds to one of the non-centrosymmetric point groups found in the second column in the row. Where there are multiple non-centrosymmetric point groups, the space groups belonging to each point group are separated by a circle “○”. This means that the corresponding point group can be determined from the tables for any space group.

The point group describes how diffracted intensities from the structure would be merged. The only relevant additional information given by the space group is about which reflections must be absent (or centric). Since the Laue class is the point group including a centre of symmetry, it describes the symmetry of the diffracted intensities if absorption is negligible.

Serial crystallography introduces the additional problem that intensities must be merged from unrelated orientations, where the only information about the orientation comes from the indexing procedure. Since indexing algorithms are primarily based on the positions of reflections *but not their intensities*, an ambiguity can arise. If the structure has the same point symmetry as the lattice, then there is no problem. Symmetry groups satisfying this condition are described as *holohedral*, and are shaded in grey in these tables. However, if the symmetry of the structure is lower than that of the lattice, then there will be more than one choice of relative orientation when, for example, merging intensities from two patterns. Symmetry groups with this problem are described as *merohedral*, and are unshaded in the tables. For macroscopic crystals, there would exist in this case the additional possibility of the crystals being physically twinned.

To determine the correct point group to use for merging data, first locate the point group corresponding to the given space group. If it has a white background, the corresponding holohedral point group should be located by moving directly downwards to the next shaded row. You will arrive at the point group which must be used when merging intensities from serial crystallography in the absence of a mechanism to resolve the ambiguity (the “source symmetry”). If such a mechanism is available, then the original point group may be used. In either case, if you are not interested in the differences between Friedel pairs, you may move all the way to the left of the table to find the corresponding Laue class and merge according to that.

If the crystal symmetry is trigonal, a rhombohedral lattice is used for some space groups (those beginning with the letter R), and a hexagonal lattice for others (beginning with the letter P). Different ambiguities arise in these two distinct cases, leading to some of the trigonal point groups appearing in the table twice. If the “H centered” hexagonal unit cell is used to represent a rhombohedral structure, no further ambiguity is introduced since the great many systematically absent reflections provide sufficient constraints.

Apart from a few very rare and specialised cases, only the chiral groups (shown in bold) are acceptable for 3D crystals of biological macromolecules such as proteins. This restriction does not apply in 2D.