Symmetry Classification for Serial Crystallography Experiments

Groups with white backgrounds are merohedral and will exhibit the "twinning ambiguity": the target point group should be the first shaded point group below. Chiral groups are shown in bold.

Laue Class	Point Groups			Centrosymmetric Space Groups	Non-Centrosymmetric Space Groups
$\bar{1}$	**1**			P$\bar{1}$	**P1**
2/m	**2**	m		P2/m, P2$_1$/m, C2/m, P2/c, P2$_1$/c, C2/c	**P2**, **P2$_1$**, **C2** ○ Pm, Pc, Cm, Cc
mmm	**222**	mm2		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	**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
4/m	**4**	$\bar{4}$		P4/m, P4$_2$/m, P4/n, P4$_2$/n, I4/m, I4$_1$/a	**P4**, **P4$_1$**, **P4$_2$**, **P4$_3$**, **I4**, **I4$_1$** ○ P$\bar{4}$, I$\bar{4}$
4/mmm	**422**	$\bar{4}$2m	4mm	P4/mmm, P4/mcc, P4/nbm, P4/nnc, P4/mbm, P4/mnc, P4/nmm, P4/ncc, P4$_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$/acd	**P422**, **P42$_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$c, P$\bar{4}$m2, P$\bar{4}$c2, P$\bar{4}$b2, P$\bar{4}$n2, I$\bar{4}$m2, I$\bar{4}$c2, I$\bar{4}$2m, I$\bar{4}$2d ○ P4mm, P4bm, P4$_2$cm, P4$_2$nm, P4cc, P4nc, P4$_2$mc, P4$_2$bc, I4mm, I4cm, I4$_1$md, I4$_1$cd
$\bar{3}$	**3**			R$\bar{3}$ (H$\bar{3}$)	**R3 (H3)**
$\bar{3}$m	**32**	3m		R$\bar{3}$m (H$\bar{3}$m), R$\bar{3}$c (H$\bar{3}$c)	**R32 (H32)** ○ R3m (H3m), R3c (H3c)
$\bar{3}$	**3**			P$\bar{3}$	**P3**, **P3$_1$**, **P3$_2$**
$\bar{3}$1m	**312**	31m		P$\bar{3}$1m, P$\bar{3}$1c	**P312**, **P3$_1$12, P3$_2$12** ○ P31m, P31c
$\bar{3}$m	**32**	3m		P$\bar{3}$m1, P$\bar{3}$c1	**P321**, **P3$_1$21, P3$_2$21** ○ P3m1, P3c1
6/m	**6**	$\bar{6}$		P6/m, P6$_3$/m	**P6**, **P6$_1$**, **P6$_5$**, **P6$_2$**, **P6$_4$**, **P6$_3$** ○ P$\bar{6}$
6/mmm	**622**	$\bar{6}$2m	6mm	P6/mmm, P6/mcc, P6$_3$/mcm, P6$_3$/mmc	**P622**, **P6$_1$22**, **P6$_5$22**, **P6$_2$22**, **P6$_4$22**, **P6$_3$22** ○ P$\bar{6}$m2, P$\bar{6}$c2, P$\bar{6}$2m, P$\bar{6}$2c ○ P6mm, P6cc, P6$_3$cm, P6$_3$mc
m$\bar{3}$	**23**			Pm$\bar{3}$, Pn$\bar{3}$, Fm$\bar{3}$, Fd$\bar{3}$, Im$\bar{3}$, Pa$\bar{3}$, Ia$\bar{3}$	**P23**, **F23**, **I23**, **P2$_1$3**, **I2$_1$3**
m$\bar{3}$m	**432**	$\bar{4}$32		Pm$\bar{3}$m, Pn$\bar{3}$n, Pm$\bar{3}$n, Pn$\bar{3}$m, Fm$\bar{3}$m, Fm$\bar{3}$c, Fd$\bar{3}$m, Fd$\bar{3}$c, Im$\bar{3}$m, Ia$\bar{3}$d	**P432**, **P4$_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

Symmetry Classification for 2D Serial Crystallography

Groups with white backgrounds are 'merohedral' and hence data will appear 'twinned'.

Laue Class	Point Groups	Centrosymmetric Plane Groups	Non-Centrosymmetric Plane Groups
2	1	p2	p1
2mm	m	p2mm, p2mg, p2gg, c2mm	pm, pg, cm
4	—	p4	—
4mm	—	p4mm, p4gm	—
6	3	p6	p3
6mm	3m	p6mm	p3m1, p31m

How To Use These Tables

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 Laue class should be located by moving down to the next shaded row, and all the way to the left of the table. This is the point group which must be used when merging intensities from serial crystallography in the absence of a mechanism to resolve the ambiguity. If such a mechanism is available, then the original point group may be used.

Apart from a few very rare 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.