

Crystal Symmetry

Space groups arranged in order of frequency in the Cambridge Crystallographic Data Base.

Laue Group : **-1** *Triclinic*
 Cell restrictions : $a \neq b \neq c$ $\alpha \neq \beta \neq \gamma \neq 90^\circ$
 Equivalent reflections : $I(h,k,l) = I(-h, -k, -l)$
 Unique Intensity Data Set : $\frac{1}{2}$ hemisphere
 $-h \rightarrow h$; $-k \rightarrow k$; $0 \rightarrow l$

Class	Space Groups
1	P1
-1	P -1 (P one-bar)

Laue Group : **2/m** *Monoclinic*
 Cell restrictions : $a \neq b \neq c$ $\alpha = \gamma = 90^\circ$ $\beta \neq 90^\circ$
 Equivalent reflections : $I(h,k,l) = I(-h, -k, -l)$
 $= I(-h, k, -l) = I(h, -k, l)$
 Unique Intensity Data Set : $\frac{1}{4}$ hemisphere :
 $0 \rightarrow h$; $0 \rightarrow k$; $-l \rightarrow l$

Class	Space Groups
2	P2₁ P2 C2
m	Pc Pm Cc Cm
2/m	P2₁/c (P2 ₁ /n; P2 ₁ /a) P2 ₁ /m P2/c P2/m C2/c C2/m

Laue Group : **mmm** *Orthorhombic*
 Cell restrictions : $a \neq b \neq c$ $\alpha = \beta = \gamma = 90^\circ$
 Equivalent reflections : $I(h,k,l) = I(-h, -k, -l)$
 $= I(-h, k, l) = I(h, -k, -l)$
 $= I(h, -k, l) = I(-h, k, -l)$
 $= I(h, k, -l) = I(-h, -k, l)$

Unique Intensity Data Set : $\frac{1}{8}$ hemisphere :
 $0 \rightarrow h$; $0 \rightarrow k$; $0 \rightarrow l$

Class	Space Groups
222	P2₁2₁2₁ P2 ₁ 2 ₁ 2 P222 ₁ P222 C222₁ C222 F222 I2₁2₁2₁ I222
mm2	Pna2₁ Pca2 ₁ Pnm2 ₁ Pnn2 Pmc2 ₁ Pba2 Pnc2 Pmm2 Pcc2 Pma2 Cmc2₁ Aba2 Ccc2 Abm2 Ama2 Amm2 Cmm2 Fdd2 Fmm2 Iba2 Ima2 Imm2
mmm	Pbca Pnma Pbcn Pccn Pbcm Pnmm Pnna Pmmm Pcca Pbam Pmna Pmma Pban Pnnn Pmmm Pccm Cmcm Cmca Ccca Cccm Cmmm Cmma Fddd Fmmm Ibam Ibca Imma Immm

Laue Group : **4/m** *Tetragonal*
 Cell restrictions : $a = b \neq c$ $\alpha = \beta = \gamma = 90^\circ$
 Equivalent reflections : $I(h,k,l) = I(-h, -k, -l)$
 $= I(-k, h, l) = I(k, -h, l)$
 $= I(-h, -k, l) = I(h, k, -l)$
 $= I(-k, h, -l) = I(k, -h, -l)$

Unique Intensity Data Set : $\frac{1}{8}$ hemisphere
 $0 \rightarrow h$; $0 \rightarrow k$; $0 \rightarrow l$

Class	Space Groups
4	P4₁ P4 ₃ P4 P4 ₂ I4₁ I4
-4	P -4 I -4
2/m	P4₂/n P4/n P4 ₂ /m P4/m I4/m I4/a

Laue Group : **4/mmm** *Tetragonal*
 Cell restrictions : $a = b \neq c$ $\alpha = \beta = \gamma = 90^\circ$
 Equivalent reflections : $I(h,k,l) = I(-h, -k, -l)$
 $= I(-k, h, l) = I(k, -h, -l)$
 $= I(-h, -k, l) = I(h, k, -l)$
 $= I(k, -h, l) = I(-k, h, -l)$
 $= I(h, k, -l) = I(-h, -k, l)$
 $= I(-k, h, -l) = I(k, -h, l)$
 $= I(k, -h, -l) = I(-k, h, l)$
 $= I(k, h, l) = I(-k, -h, -l)$

Unique Intensity Data Set : $\frac{1}{16}$ hemisphere
 $0 \rightarrow h$; $0 \rightarrow k$; $0 \rightarrow l$; $k > = h$

Class	Space Groups
422	P4₃2₁2 P4 ₃ 2 ₁ 2 P4 ₂ 2 ₁ 2 P4 ₁ 22 P42 ₁ 2 P422 P4 ₁ 22 P4 ₃ 22 I4₁22 I422
4mm	P4₁nc P4 ₂ bc P4 ₂ nm P4 ₂ cm P4bm P4cc P4mm P4 ₂ mc I4₁cd I4 ₁ md I4cm I4mm
-42m	P-42₁c P-42 ₁ m P-4n2 P-4b2 P-42c P-42m P-4c2 P-4m2 I-42d I-42m I-4c2 I-4m2
4/mmm	P4/mmm P4/ncc P4/mbm P4 ₂ /mnm P4/nnc P4/mmc P4/mmm P4 ₂ /mnc P4/mnc P4 ₂ /nmm P4 ₂ /ncm P4 ₂ /mbc P4 ₂ /nbc P4 ₂ /nbm P4 ₂ /mmc P4 ₂ /mcm I4₁/acd I4 ₁ /amd I4/mmm I4/mcm

Laue Group : **-3** *Trigonal (1)*
 Cell restrictions : $a = b \neq c$ $\alpha = \beta = 90^\circ$ $\gamma = 120^\circ$
 Equivalent reflections : $I(h,k,i,l) = I(-h + k, -l)$
 $I(h,k,l) = I(-h, -k, -l)$
 $= I(-h-k, h, l) = I(h+k, -h, -l)$
 $= I(k, -h-k, l) = I(-k, h+k, -l)$

Unique Intensity Data Set : $\frac{1}{6}$ hemisphere
 $0 \rightarrow h$; $0 \rightarrow k$; $-l \rightarrow l$

Class	Space Groups
3	P3₁ P3 ₂ P3 R3
-3	P -3 R -3

Laue Group : **-3m** *Trigonal*

Cell restrictions : $a = b \neq c$ $\alpha = \beta = 90^\circ$ $\gamma = 120^\circ$

Equivalent reflections $I(h,k,l)$ $i = -(h+k)$

$$\begin{aligned} I(h,k,l) &= I(-h, -k, -l) \\ &= I(-h-k, h, l) = I(h+k, h, l) \\ &= I(k, -h-k, l) = I(-k, h+k, -l) \\ &= I(k, h, -l) = I(-k, -h, l) \\ &= I(-h-k, k, -l) = I(h+k, -k, l) \\ &= I(h, -h-k, -l) = I(-h, h+k, l) \end{aligned}$$

Unique Intensity Data Set : 1/12 hemisphere
 $0 \rightarrow h$; $0 \rightarrow k$; $0 \rightarrow l$

Class	Space Groups
32	P3₁21 P3 ₂ 21 P3 ₁₂ 12 P3 ₁₂ 1 P312
	R32
3m	P31c P3c1 P31m P3m1
	R3c R3m
-3m	P-3c1 P-31c P-3m1 P-31m
	R-3c R-3m

Laue Group : **6/m** *Hexagonal*

Cell restrictions : $a = b \neq c$ $\alpha = \beta = 90^\circ$ $\gamma = 120^\circ$

Equivalent reflections : $I(h,k,i,l)$ $i = -(h+k)$

$$\begin{aligned} I(h,k,l) &= I(-h, -k, -l) \\ &= I(-h, -k, l) = I(h, k, -l) \\ &= I(-k, h+k, l) = I(k, -h-k, -l) \\ &= I(k, -h-k, l) = I(-k, h+k, -l) \\ &= I(h+k, -h, l) = I(-h-k, h, -l) \\ &= I(-h-k, h, l) = I(h+k, -h, -l) \end{aligned}$$

Unique Intensity Data Set : 1/12 hemisphere :
 $0 \rightarrow h$; $0 \rightarrow k$; $0 \rightarrow l$

Class	Space Groups
6	P6₅ P6 ₁ P6 ₂ P6 ₄ P6 ₃ P6
-6	P-6
6/m	P6₃/m P6/m

Laue Group : **6/mmm** *Hexagonal*

Cell restrictions : $a = b \neq c$ $\alpha = \beta = 90^\circ$ $\gamma = 120^\circ$

Equivalent reflections : $I(h,k,i,l)$ $i = -(h+k)$

$$\begin{aligned} I(h,k,l) &= I(-h, -k, -l) \\ &= I(-k, h+k, l) = I(k, -h-k, -l) \\ &= I(-h-k, h, l) = I(h+k, -k, -l) \\ &= I(-h, -k, l) = I(h, k, -l) \\ &= I(k, -h-k, l) = I(-k, h+k, -l) \\ &= I(h+k, -h, l) = I(-h, -k, h, -l) \\ &= I(k, h, l) = I(-k, -h, -l) \\ &= I(h+k, -k, l) = I(-h-k, k, -l) \\ &= I(h, -h-k, l) = I(-h, h+k, -l) \\ &= I(-k, -h, l) = I(k, h, -l) \\ &= I(-h-k, k, l) = I(h+k, -k, -l) \\ &= I(-h, h+k, l) = I(h, -h-k, -l) \end{aligned}$$

Unique Intensity Data Set : 1/24 hemisphere
 $0 \rightarrow h$; $0 \rightarrow k$; $0 \rightarrow l$ $k >= h$

Class	Space Groups
622	P6₁22 P6 ₅ 22 P6 ₃ 22 P6 ₄ 22 P6 ₂ 22 P622
6mm	P6₃mc P6 ₃ cm P6cc P6mm
-6m2	P-62c P-62m P-6c2 P-6m2
6/mmm	P6₃/mmc P6 ₁ mmc P6/mmm P6 ₃ /mcm

Laue Group : **m-3** *Cubic*

Cell restrictions : $a = b = c$ $\alpha = \beta = \gamma = 90^\circ$

Equivalent reflections : $I(h,k,l) = I(-h, -k, -l)$

$$\begin{aligned} &= I(-h, k, l) = I(h, -k, -l) \\ &= I(h, -k, l) = I(-h, k, -l) \\ &= I(h, k, -l) = I(-h, -l, l) \\ &= I(l, h, k) = I(-l, -h, -k) \\ &= I(-l, h, k) = I(l, -h, -k) \\ &= I(l, -h, k) = I(-l, h, -k) \\ &= I(l, h, -k) = I(-l, -h, k) \\ &= I(k, l, h) = I(-k, -l, -h) \\ &= I(-k, l, h) = I(k, -l, -h) \\ &= I(k, -l, h) = I(-k, l, -h) \\ &= I(k, l, -h) = I(-k, -l, h) \end{aligned}$$

Unique Intensity Data Set : 1/24 hemisphere
 $0 \rightarrow h$; $0 \rightarrow k$; $0 \rightarrow l$ $k >= h$

Class	Space Groups
23	P2₁3 P23
	F23
	I23 I2 ₁ 3
m3	Pa3 Pm3 Pn3
	Fd3 Fm3
	Im3 Ia3

Laue Group : **m-3m** *Cubic*

Cell restrictions : $a = b = c$ $\alpha = \beta = \gamma = 90^\circ$

Equivalent reflections : $I(h,k,l) = I(-h, -k, -l)$

$$\begin{aligned} &= I(-h, k, l) = I(h, -k, -l) \\ &= I(h, -k, l) = I(-h, k, -l) \\ &= I(h, k, -l) = I(-h, -l, l) \\ &= I(l, h, k) = I(-l, -h, -k) \\ &= I(-l, h, k) = I(l, -h, -k) \\ &= I(l, -h, k) = I(-l, h, -k) \\ &= I(l, h, -k) = I(-l, -h, k) \\ &= I(k, l, h) = I(-k, -l, -h) \\ &= I(-k, l, h) = I(k, -l, -h) \\ &= I(k, -l, h) = I(-k, l, -h) \\ &= I(k, l, -h) = I(-k, -l, h) \end{aligned}$$

Unique Intensity Data Set : 1/48 hemisphere
 $0 \rightarrow h$; $0 \rightarrow k$; $0 \rightarrow l$ $l >= k >= h$

Class	Space Groups
432	P4₃32 P4 ₁ 32 P432 P4 ₂ 32
	F4₃32 F432
	I432 I4 ₁ 32
-43m	P-43n P-43m
	F-43c F-43m
	I-43m I-43d
m3m	Pm-3m Pn-3n Pm-3n Pn-3m
	Fm-3m Fd-3m Fd-3c Fm-3c
	Im-3m Ia-3d