Symmetry and Space Groups

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

Laue Group : **-1** *Triclinic*
Cell restrictions : $a \neq b \neq c$ $\alpha \neq \beta \neq \gamma \neq 90^o$
Equivalent reflections : I (h,k,l) = I(-h, -k, -l)
Unique Intensity Data Set : ½ 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 : $a \neq b \neq c$ $\alpha = \gamma = 90^o$ $\beta \neq 90^o$
Equivalent reflections : I (h,k,l) = I(-h, -k, -l)
= I(-h, k, -l) = I(h, -k, l)
Unique Intensity Data Set : 1/4 hemisphere :
$0 \rightarrow h$; $0 \rightarrow k$; $-l \rightarrow l$

Class	Space Groups
2	**$P2_1$** P2
	C2
m	**Pc** Pm
	Cc Cm
2/m	**$P2_1/c$** ($P2_1/n$; $P2_1/a$) $P2_1/m$ P2/c P2/m
	C2/c C2/m

Laue Group : **mmm** *Orthorhombic*
Cell restrictions : $a \neq b \neq c$ $\alpha = \beta = \gamma = 90^o$
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 : 1/8 hemisphere :
$0 \rightarrow h$; $0 \rightarrow k$; $0 \rightarrow l$

Class	Space Groups
222	**$P2_12_12_1$** $P2_12_12$ $P222_1$ P222
	$C222_1$ C222
	F222
	$I2_12_12_1$ I222
mm2	**$Pna2_1$** $Pca2_1$ $Pnm2_1$ Pnn2 $Pmc2_1$ Pba2 Pnc2 Pmm2 Pcc2 Pma2
	$Cmc2_1$ Aba2 Ccc2 Abm2 Ama2 Amm2 Cmm2
	Fdd2 Fmm2
	Iba2 Ima2 Imm2
mmm	**Pbca** Pnma Pbcn Pccn Pbcm Pnnm Pnna Pmmn 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 : $a = b \neq c$ $\alpha = \beta = \gamma = 90^o$
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 : 1/8 hemisphere
$0 \rightarrow h$; $0 \rightarrow k$; $0 \rightarrow l$

Class	Space Groups
4	**$P4_1$** $P4_3$ P4 $P4_2$
	$I4_1$ I4
-4	**P -4**
	I -4
2/m	**$P4_2/n$** P4/n $P4_2/m$ P4/m
	I4/m $I4_1/a$

Laue Group : **4/mmm** *Tetragonal*
Cell restrictions : $a = b \neq c$ $\alpha = \beta = \gamma = 90^o$
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 : 1/16 hemisphere
$0 \rightarrow h$; $0 \rightarrow k$; $0 \rightarrow l$; $k >= h$

Class	Space Groups
422	**$P4_12_12$** $P4_32_12$ $P4_22_12$ $P4_122$ $P4_212$ P422 $P4_122$ $P4_322$
	$I4_122$ I422
4mm	**P4nc** $P4_2bc$ $P4_2nm$ $P4_2cm$ P4bm P4cc P4mm $P4_2mc$
	$I4_1cd$ $I4_1md$ I4cm I4mm
-42m	**$P-42_1c$** $P-42_1m$ P-4n2 P-4b2 P-42c P-42m P-4c2 P-4m2
	I-42d I-42m I-4c2 I-4m2
4/mmm	**P4/nmm** P4/ncc P4/mbm $P4_2/mnm$ P4/nnc P4/mmc P4/mmm $P4_2/mnc$ P4/mnc $P4_2/nnm$ $P4_2/ncm$ $P4_2/mbc$ $P4_2/nbc$ P4/nbm $P4_2/mmc$ $P4_2/mcm$
	$I4_1/acd$ $I4_1/amd$ I4/mmm I4/mcm

Laue Group : **-3** *Trigonal* (1)
Cell restrictions : $a = b \neq c$ $\alpha = \beta = 90^o$ $\gamma = 120^o$
Equivalent reflections : I(h,k,i,l) i = -(h + k)
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 : 1/6 hemisphere
$0 \rightarrow h$; $0 \rightarrow k$; $-l \rightarrow l$

Class	Space Groups
3	**$P3_1$ $P3_2$** P3
	R3
-3	**P-3**
	R-3

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

Cell restrictions : a = b ≠c α = β = 90° γ = 120°
Equivalent reflections I(h,k,i,l) i = -(h + k)
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)

Unique Intensity Data Set : 1/12 hemisphere
0 → h ; 0 →k; 0 →l

Class	Space Groups
32	**$P3_121$** $P3_221$ P321 $P3_212$ $P3_112$ 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 ≠c α = β = 90° γ = 120°
Equivalent reflections : I(h,k,i,l) i = -(h + k)
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)
= (k, -h-k, l) = I(-k, h+k, -l)
= (h+k, -h, l) = I(-h-k, h, -l)
= I(-h-k, h, l) = I(h+k, -h, -l)

Unique Intensity Data Set : 1/12 hemisphere :
0 → h ; 0 →k; 0 →l

Class	Space Groups
6	**$P6_5$** $P6_1$ $P6_2$ $P6_4$ $P6_3$ P6
-6	**P-6**
6/m	**$P6_3$/m** P6/m

Laue Group : **6/mmm** *Hexagonal*
Cell restrictions : a = b ≠ c α = β = 90° γ = 120°
Equivalent reflections : I(h,k,i,l) i = -(h + k)
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)

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

Class	Space Groups
622	**$P6_122$** $P6_522$ $P6_322$ $P6_422$ $P6_222$ P622
6mm	**$P6_3$mc** $P6_3$cm P6cc P6mm
-6m2	**P-62c** P-62m P-6c2 P-6m2
6/mmm	**$P6_3$/mmc** $P6_1$mmc P6/mmm $P6_3$/mcm

Laue Group : **m-3** *Cubic*
Cell restrictions : a = b = c α = β = γ = 90°
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, -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)

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

Class	Space Groups
23	**$P2_13$** P23
	F23
	I23 $I2_13$
m3	**Pa3** Pm3 Pn3
	Fd3 Fm3
	Im3 Ia3

Laue Group : **m-3m** *Cubic*
Cell restrictions : a = b = c α = β = γ = 90°
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, -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)

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

Class	Space Groups
432	**$P4_332$** $P4_132$ P432 $P4_232$
	$F4_132$ F432
	I432 $I4_132$
-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