

# 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	<b>P1</b>
-1	<b>P-1 (P one-bar)</b>

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	<b>P2<sub>1</sub></b> P2 <b>C2</b>
m	<b>Pc</b> Pm <b>Cc</b> Cm
2/m	<b>P2<sub>1</sub>/c</b> (P2 <sub>1</sub> /n; P2 <sub>1</sub> /a) P2 <sub>1</sub> /m P2/c P2/m <b>C2/c</b> 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	<b>P2<sub>1</sub>2<sub>1</sub>2<sub>1</sub></b> P2 <sub>1</sub> 2 <sub>1</sub> 2 P222 <sub>1</sub> P222 <b>C222<sub>1</sub></b> C222 <b>F222</b> <b>I2<sub>1</sub>2<sub>1</sub>2<sub>1</sub></b> I222
mm2	<b>Pna2<sub>1</sub></b> Pca2 <sub>1</sub> Pnm2 <sub>1</sub> Pnn2 Pmc2 <sub>1</sub> Pba2 Pnc2 Pmm2 Pcc2 Pma2 <b>Cmc2<sub>1</sub></b> Aba2 Ccc2 Abm2 Ama2 Amm2 Cmm2 <b>Fdd2</b> Fmm2 <b>Iba2</b> Ima2 Imm2
mmm	<b>Pbca</b> Pnma Pbcn Pccn Pbcm Pnmm Pnna Pmmm Pcca Pbam Pmna Pmma Pban Pnnn Pmmm Pccm <b>Cmcm</b> Cmca Ccca Cccm Cmmm Cmma <b>Fddd</b> Fmmm <b>Ibam</b> 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	<b>P4<sub>1</sub></b> P4 <sub>3</sub> P4 P4 <sub>2</sub> <b>I4<sub>1</sub></b> I4
-4	<b>P-4</b> <b>I-4</b>
2/m	<b>P4<sub>2</sub>/n</b> P4/n P4 <sub>2</sub> /m P4/m <b>I4/m</b> 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	<b>P4<sub>3</sub>2<sub>1</sub>2</b> P4 <sub>3</sub> 2 <sub>1</sub> 2 P4 <sub>2</sub> 2 <sub>1</sub> 2 P4 <sub>1</sub> 22 P42 <sub>1</sub> 2 P422 P4 <sub>1</sub> 22 P4 <sub>3</sub> 22 <b>I4<sub>1</sub>22</b> I422
4mm	<b>P4<sub>1</sub>nc</b> P4 <sub>2</sub> bc P4 <sub>2</sub> nm P4 <sub>2</sub> cm P4bm P4cc P4mm P4 <sub>2</sub> mc <b>I4<sub>1</sub>cd</b> I4 <sub>1</sub> md I4cm I4mm
-42m	<b>P-42<sub>1</sub>c</b> P-42 <sub>1</sub> m P-4n2 P-4b2 P-42c P-42m P-4c2 P-4m2 <b>I-42d</b> I-42m I-4c2 I-4m2
4/mmm	<b>P4/mmm</b> P4/ncc P4/mbm P4 <sub>2</sub> /mnm P4/nnc P4/mmc P4/mmm P4 <sub>2</sub> /mnc P4/mnc P4 <sub>2</sub> /nmm P4 <sub>2</sub> /ncm P4 <sub>2</sub> /mbc P4 <sub>2</sub> /nbc P4 <sub>2</sub> /nbm P4 <sub>2</sub> /mmc P4 <sub>2</sub> /mcm <b>I4<sub>1</sub>/acd</b> I4 <sub>1</sub> /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	<b>P3<sub>1</sub></b> P3 <sub>2</sub> P3 <b>R3</b>
-3	<b>P-3</b> <b>R-3</b>

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	<b>P3<sub>1</sub>21</b> P3 <sub>2</sub> 21 P3 <sub>1</sub> 2 P3 <sub>1</sub> 12 P312
	<b>R32</b>
3m	<b>P31c</b> P3c1 P31m P3m1
	<b>R3c</b> R3m
-3m	<b>P-3c1</b> P-31c P-3m1 P-31m
	<b>R-3c</b> 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	<b>P6<sub>5</sub></b> P6 <sub>1</sub> P6 <sub>2</sub> P6 <sub>4</sub> P6 <sub>3</sub> P6
-6	<b>P-6</b>
6/m	<b>P6<sub>3</sub>/m</b> 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	<b>P6<sub>1</sub>22</b> P6 <sub>5</sub> 22 P6 <sub>3</sub> 22 P6 <sub>4</sub> 22 P6 <sub>2</sub> 22 P622
6mm	<b>P6<sub>3</sub>mc</b> P6 <sub>3</sub> cm P6cc P6mm
-6m2	<b>P-62c</b> P-62m P-6c2 P-6m2
6/mmm	<b>P6<sub>3</sub>/mmc</b> P6 <sub>1</sub> mmc P6/mmm P6 <sub>3</sub> /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	<b>P2<sub>1</sub>3</b> P23
	<b>F23</b>
	<b>I23</b> I2 <sub>1</sub> 3
m3	<b>Pa3</b> Pm3 Pn3
	<b>Fd3</b> Fm3
	<b>Im3</b> 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	<b>P4<sub>3</sub>32</b> P4 <sub>1</sub> 32 P432 P4 <sub>2</sub> 32
	<b>F4<sub>3</sub>32</b> F432
	<b>I432</b> I4 <sub>1</sub> 32
-43m	<b>P-43n</b> P-43m
	<b>F-43c</b> F-43m
	<b>I-43m</b> I-43d
m3m	<b>Pm-3m</b> Pn-3n Pm-3n Pn-3m
	<b>Fm-3m</b> Fd-3m Fd-3c Fm-3c
	<b>Im-3m</b> Ia-3d