Space Groups

Andriy Zhugayevych (ORCID: 0000-0003-4713-1289)

May 9, 2026

§1. Symmetry elements of crystallographic groups

Spatial symmetry elements (i.e., elements of the Euclidean group $E(n)$) in three-dimensional space are a combination of a point transformation and a translation. The basic non-point elements of spatial symmetry include translation, screw axis, and glide plane. Any element of a crystallographic group can be represented as

$$\boldsymbol{r} \to \mathbf{R}\boldsymbol{r} + \boldsymbol{v}(\mathbf{R}) + \boldsymbol{t}, \tag{1.1}$$

where $\mathbf{R}$ is the linear part of the transformation (point symmetry element), $\boldsymbol{t}$ is the primitive (lattice) translation, i.e. translation by integer linear combinations of lattice translation vectors, and $\boldsymbol{v}(\mathbf{R})$ is the fractional translation. See Fig. 1 for the notation of symmetry elements. A screw axis n_k denotes rotation by $2\pi/n$ combined with translation along the axis by k/n. Glide planes are denoted by {a,b,c,n,d}: axial glides {a,b,c} denote a shift by 1/2 along the corresponding axis combined with a reflection in the plane parallel to this axis, diagonal glide {n} denotes a shift by 1/2 along any diagonal, diamond glide {d} denotes a diagonal shift by 1/4 (see the example in Fig. 4). For crystallographic groups, rotation axes can only have order 1, 2, 3, 4, or 6. In lattice coordinates, the matrix $\mathbf{R}$ and the vector $\boldsymbol{t}$ are integer, and the components of the vector $\boldsymbol{v}(\mathbf{R})$ are fractions with possible denominator of 2, 3, 4, 6.

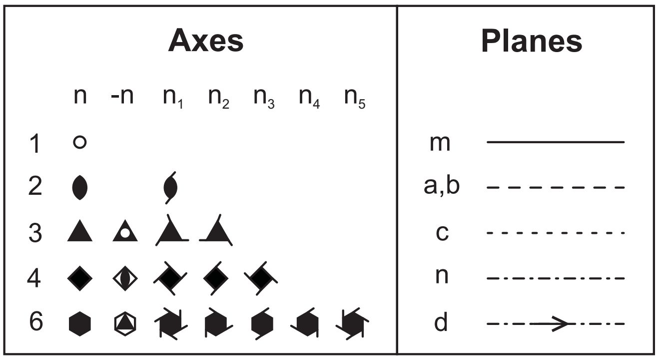


Figure 1: Graphical notation of symmetry elements.

Vectors and planes in crystals are denoted by crystallographic indices. A vector with lattice coordinates n_i is denoted by $[n_1 n_2 n_3]$, a plane $hx + ky + lz = \text{const}$ is denoted by (hkl). The indices of a plane passing through two given vectors can be found by taking their cross product.

§2. Bravais lattice

Translation group of a crystal (the group of translations that leave the crystal invariant) is an invariant subgroup of the crystallographic group. *Unit cell* is a part of a crystal, from which the entire crystal can be obtained by translations. *Primitive cell* is a unit cell of minimal volume. If the latter is spanned by primitive translation vectors, it is called a primitive parallelepiped. The choice is still non-unique, so that primitive vectors of minimal length are usually chosen.

Lattice system	Conventional cell shape	Parameters	Symmetry	HM
anorthic (triclinic)		$a, b, c, \alpha, \beta, \gamma$	P-1	aP
monoclinic	$\alpha = \gamma = \pi/2$	a, b, c, β	P2/m	mP
			C2/m	mC
orthorhombic	$\alpha = \beta = \gamma = \pi/2$	a, b, c	Pmmm	oP
			Cmmm	oC
			Fmmm	oF
			Immm	oI
tetragonal	$a = b,\ \alpha = \beta = \gamma = \pi/2$	a, c	P4/mmm	tP
			I4/mmm	tI
rhombohedral	$a = b = c,\ \alpha = \beta = \gamma$	a, α	R-3m	hR
hexagonal	$a = b,\ \alpha = \beta = \pi/2,\ \gamma = 2\pi/3$	a, c	P6/mmm	hP
cubic	$a = b = c,\ \alpha = \beta = \gamma = \pi/2$	a	Pm-3m	cP
			Fm-3m	cF
			Im-3m	cI

Table 1: Bravais lattice types. The last two column gives Hermann–Mauguin notations. Possible lattice centerings are primitive (P), face-centered in the ab-plane (C), face-centered in the bc-plane (A), face-centered (F), body-centered (I), rhombohedral (R).

A lattice constructed by translations of a primitive parallelepiped with points at its vertices (i.e., the set of points $\sum_{n_i \in \mathbb{Z}} \sum_{i=1}^{3} n_i \boldsymbol{a}_i$) is called the *Bravais lattice* of the crystal. Thus, the Bravais lattice describes the symmetry of the primitive parallelepiped (lattice symmetry) independently of the actual arrangement of atoms within it. The arrangement of atoms within the unit cell is called the *motif.*

There are 14 types of Bravais lattices distinguished by their symmetry (*Bravais groups*), see Table 1 and PDB files. They are divided into 7 *lattice systems* based on the point group of the lattice. Within a single lattice system, Bravais lattices differ in their *centering type.* Note that there are situations where, for example in fluorine crystal, the unit cell is orthorhombic, but the arrangement of atoms within it has the symmetry of a monoclinic crystal system. In this case, the Bravais lattice is considered to be monoclinic with $\beta = \pi/2$.

The primitive cell can always be chosen so that it has the point symmetry of its Bravais lattice. Such cell centered at a lattice point is called *Wigner–Seitz cell.* It is unique and is the locus of space points that are closer to that lattice point than to any of the other lattice points. Often, the Wigner–Seitz cell has a complex shape, while parallelepiped-shaped primitive cell do not possess the point symmetry of the Bravais lattice. Therefore, it would be convenient to use a parallelepiped-shaped unit cell of minimal volume that possesses point symmetry of its Bravais lattice. However, for the hP lattice, there is no such parallelepiped, only a hexagonal prism. In this case, symmetry is usually sacrificed in favor of the simple form of a parallelepiped. The cells selected in this way are called *conventionally cells* (or Bravais cells).

Let $\boldsymbol{a}_i$ be the translation vectors of some lattice. A triple of numbers (ξ, η, ζ) is called *lattice coordinates* if the Cartesian coordinates are given by $\boldsymbol{r} = \sum_j \boldsymbol{a}_j \xi_j$. Lattice coordinates are found using the formula $\xi_i = \boldsymbol{\alpha}_i \boldsymbol{r}$, where $\boldsymbol{\alpha}_i$ are the basis vectors of the reciprocal lattice (inverse matrix). The basis is changed using the formula $\xi'_i = \sum_j (\boldsymbol{\alpha}'_i \boldsymbol{a}_j)\, \xi_j$. By default, lattice coordinates refer to the conventional cell. The standard choice of primitive vectors for lattices with non-trivial centering is as follows (in lattice coordinates; the inverse matrix is given below):

oC	oF,cF	oI,tI	cI	hR
$\frac{1}{2}\begin{pmatrix} 1 & 1 & 0 \\ -1 & 1 & 0 \\ 0 & 0 & 2 \end{pmatrix}$	$\frac{1}{2}\begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}$	$\frac{1}{2}\begin{pmatrix} 2 & 0 & 1 \\ 0 & 2 & 1 \\ 0 & 0 & 1 \end{pmatrix}$	$\frac{1}{2}\begin{pmatrix} -1 & 1 & 1 \\ 1 & -1 & 1 \\ 1 & 1 & -1 \end{pmatrix}$	$\frac{1}{3}\begin{pmatrix} -1 & 2 & -1 \\ -2 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix}$
$\begin{pmatrix} 1 & -1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} -1 & 1 & 1 \\ 1 & -1 & 1 \\ 1 & 1 & -1 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 & -1 \\ 0 & 1 & -1 \\ 0 & 0 & 2 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & -1 & 1 \\ 1 & 0 & 1 \\ -1 & 1 & 1 \end{pmatrix}$

The rhombohedral lattice needs special attention. Its orientation is chosen such that the main diagonal of the lattice coincides with the main diagonal of the Cartesian coordinate system, and the primitive vectors lie in the plane formed by the main diagonal $(1, 1, 1)$ and the corresponding Cartesian unit vector $\boldsymbol{e}_i$ such that

$\boldsymbol{a}_i = d\boldsymbol{e}_i + d\delta(1,1,1)$. The parameters (d,δ) are related to the standard parameters of the rhombohedral lattice $(a_{\rm rh},\alpha)$ by the relations $a_{\rm rh} = d\sqrt{1+2\delta+3\delta^2}$, $1-\cos\alpha = (1+2\delta+3\delta^2)^{-1}$. However, in most cases it is more convenient to represent it as a hexagonal lattice with two nodes at the points $(2/3,1/3,1/3)$ and $(1/3,2/3,2/3)$ such that the main diagonal of the original rhombohedral lattice coincides with the z-axis of the hexagonal lattice. The parameters of the hexagonal lattice are expressed in terms of the pair (d,δ) in a simple way: $3a = \sqrt{2}d$, $c = \sqrt{3}(1+3\delta)d$.

A diagram of the subordination (mutual transformations) of Bravais lattices is shown in Fig. 2.

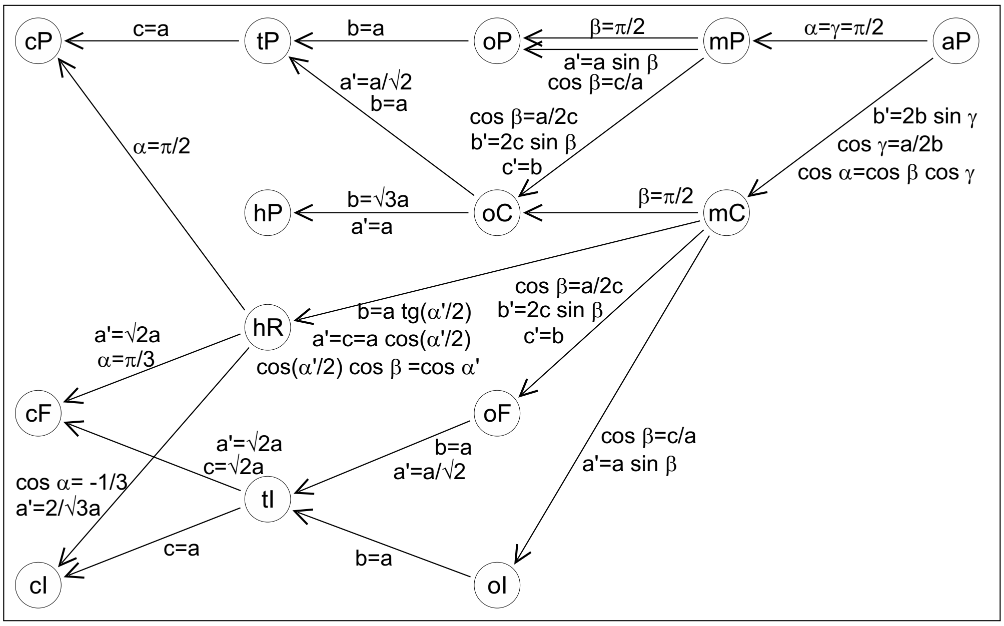


Figure 2: Bravais lattice transformations (lattices sorted by the number of independent parameters).

§3. Reciprocal lattice

The concept of a reciprocal lattice naturally arises when expanding a periodic function on a lattice into a trigonometric Fourier series (or vice versa). Consider the sum

$$\hat{f}(\boldsymbol{k}) = \sum_{\boldsymbol{r}} f(\boldsymbol{r}) \mathrm{e}^{\mathrm{i}\boldsymbol{k}\boldsymbol{r}},$$

where $\boldsymbol{r}$ runs through all lattice nodes. The functions $\mathrm{e}^{\mathrm{i}\boldsymbol{k}\boldsymbol{r}}$ and $\hat{f}(\boldsymbol{k})$ are periodic in the reciprocal lattice, defined by its primitive vectors

$$\boldsymbol{\alpha}_i = e_{ijk}\frac{2\pi}{v}\left(\boldsymbol{a}_j\times\boldsymbol{a}_k\right),$$

where $v = \boldsymbol{a}_1\cdot(\boldsymbol{a}_2\times\boldsymbol{a}_3)$ is the volume of the primitive cell. They satisfy the condition

$$\boldsymbol{a}_i\boldsymbol{\alpha}_j = 2\pi\delta_{ij}.$$

The inverse Fourier transform is given by the formula

$$f(\boldsymbol{r}) = \frac{1}{(2\pi)^3}\int \hat{f}(\boldsymbol{k})\mathrm{e}^{-\mathrm{i}\boldsymbol{k}\boldsymbol{r}}\,\mathrm{d}^3k,$$

where the integral is taken over the primitive cell of the reciprocal lattice. Note the formula

$$\sum_{\boldsymbol{r}} \mathrm{e}^{\mathrm{i}\boldsymbol{k}\boldsymbol{r}} = (2\pi)^3\delta(\boldsymbol{k}),$$

where the symbol $\delta(\boldsymbol{k})$ is considered a periodic function on the reciprocal lattice.

§4. Classification of crystallographic groups

There are a total of 230 space (crystallographic, Fedorov) groups listed in Table 2. Their notation consists of the Bravais lattice type and symmetry elements, as for point groups. Detailed terminology is given at IUCr Online Dictionary of Crystallography.

Geometric crystal class or simply *crystal class* is a group of rotational parts of the elements of a space group (they form a group). It is one of the 32 crystallographic point groups. Unlike the translation group, the point group of a crystal is not always the symmetry of the crystal, but only for *symmorphic* space groups (this is their definition). *Arithmetic crystal class* is a group of rotational parts and proper translations of the elements of a space group (they form a group). It is one of the 73 symmorphic groups. *Holohedry* is the point group of the Bravais lattice of the space group. Based on their holohedries, space groups are divided into 7 *crystal systems*: anorthic (a) or triclinic, monoclinic (m), orthorhombic (o), trigonal (tri), tetragonal (t), hexagonal (h), cubic (c). Crystallographic point groups classified by symmetry type and crystal system are listed in the table below:

	a	m	o	tri	t	h	c
Minimal	1			3	4	6	23
Pure rotoinversion					-4	-6	
Minimal centrosymmetric	-1			-3	4/m	6/m	m-3
Maximal enantiomorphic		2	222	32	422	622	432
Maximal polar		m	mm2	3m	4mm	6mm	-43m
Mixed rotoinversion					-42m	-6m2	
Maximal		2/m	mmm	-3m	4/mmm	6/mmm	m-3m

Crystallographic groups can be classified either by their linear components (crystal system – geometric class), or by their translational components (lattice system – Bravais lattice), or by both (arithmetic class). These classifications are not entirely compatible, since the trigonal symmetry class contains groups of the rhombohedral and hexagonal lattice systems, and the hexagonal lattice system contains groups of the trigonal and hexagonal crystal systems. Therefore, for classification, instead of crystal and lattice systems, so-called *crystal families* are used. There are 6 of them: anorthic (a), monoclinic (m), orthorhombic (o), tetragonal (t), hexagonal (h), cubic (c). In this case, the rhombohedral lattice is considered to be a specially centered hexagonal one. Then the classification hierarchy is consistent and includes: 1) crystal system, 2) crystal class, 3) lattice centering, 4) arithmetic class, 5) space group.

The maximal groups are P6/mmm, Pm-3m, Fm-3m, and Im-3m. Moreover, the sequence (Fm-3m, Pm-3m, Im-3m) is a chain of mutually minimal supergroups, and the group P6/mmm is connected to the cubic groups by the maximal subgroup R-3m.

§5. Structure of crystallographic groups

Symmorphic groups are formed by a simple combination of elements of point and translation groups (semi-direct product). In this case, for point groups with horizontal axes or parallel planes, there is sometimes ambiguity regarding their orientation relative to the lattice. These are the following symmorphic groups:

Cmm2	P321	P3m1	P-3m1	P-42m	I-42m	P-6m2
Amm2	P312	P31m	P-31m	P-4m2	I-4m2	P-62m

The order of a symmorphic group is equal to the product of the order of the point group and the number of vertices per conventional cell. Non-symmorphic groups are characterized by the presence of screw axes or glide planes. Examples of elements of non-symmorphic groups in two- and three-dimensional spaces are shown in Figs. 3 and 4. In particular, Fig. 4 shows the element

$$G_{124} = \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1/4 \\ 0 & 0 & 1 & 1/4 \end{pmatrix} = d(0, 1/4, 1/4)\ 0, y, z$$

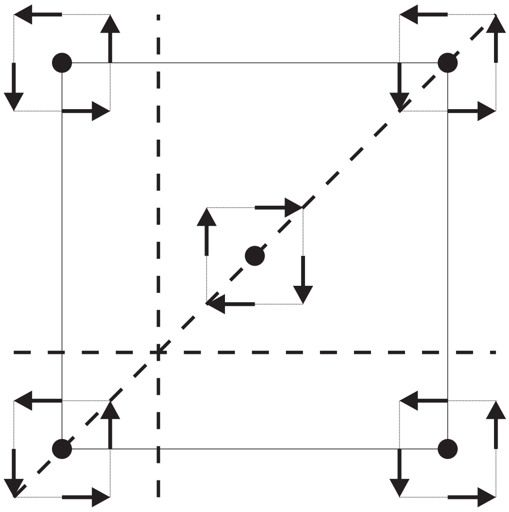


Figure 3: The non-symmorphic two-dimensional space group P4bm.

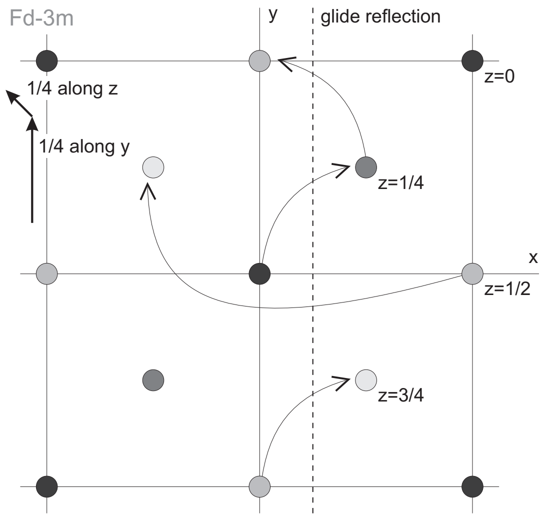


Figure 4: The non-symmorphic group Fd-3m.

A separate class consists of enantiomorphic groups, which differ from one another by left/right-handed orientation of the screw axis. There are 11 such pairs:

C_4	D_4	D_4	C_3	D_3	D_3	C_6	C_6	D_6	D_6	O
$P4_1$	$P4_122$	$P4_12_12$	$P3_1$	$P3_112$	$P3_121$	$P6_1$	$P6_2$	$P6_122$	$P6_222$	$P4_132$
$P4_3$	$P4_322$	$P4_32_12$	$P3_2$	$P3_212$	$P3_221$	$P6_5$	$P6_4$	$P6_522$	$P6_422$	$P4_332$

In crystallography, the orbits of a space group are known as *regular point systems*. The stabilizer of a point is its *site symmetry*. Points with the identity as their stabilizer are in *general positions*; all others are in special positions. The order of a space group is the number of general positions in the conventional cell (multiplicity of the general position). A space group is uniquely determined by any of its regular point systems, provided that the stabilizer of that system is known. Orbits grouped by symmetry equivalence are called *Wyckoff positions* of the space group. The orbits (Wyckoff positions) of maximal cubic groups are listed in Table 3.

§6. Other discrete groups of spatial symmetries

In addition to point and space groups, there are rod groups (a total of 75) and layer groups (80), which describe the symmetry of uniaxial (polymers) and biaxial structures (layered crystals such as silicates, smectics, and monomolecular layers), respectively. Two-dimensional space groups (there are 17 of them) are shown in Fig. 5. In two-dimensional space, border groups (7) are also defined. See classification of subperiodic groups in p. 6 of vol. E of International Tables for Crystallography.

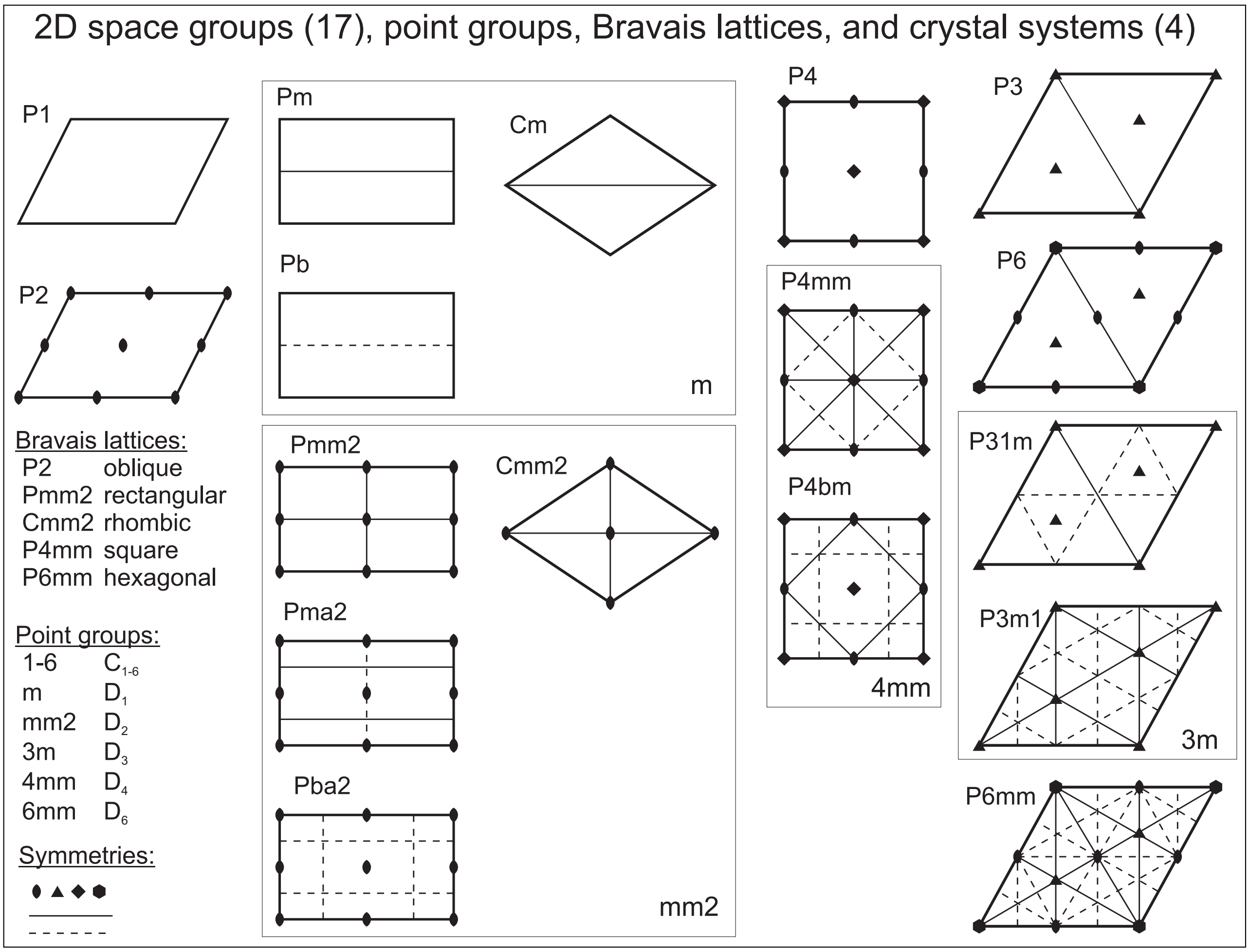


Figure 5: Two-dimensional space groups.

§7. Elements of the mathematical theory of crystal symmetry

Let E_n be an Euclidean space. Recall that the following groups are defined in it: the groups of linear $GL(n,\mathbb{R})$ and proper linear $SL(n,\mathbb{R})$ transformations, the groups of orthogonal transformations $O(n)$ and proper rotations $SO(n)$, groups of translations $T(n,\mathbb{R})$ and lattice translations $T(n,\mathbb{Z}) = L$, the group of motions of Euclidean space (isometry group) $E(n) = O(n) \ltimes T(n,\mathbb{R})$, the affine group $Aff(\mathbb{R}^n) = GL(n,\mathbb{R}) \ltimes T(n,\mathbb{R})$.

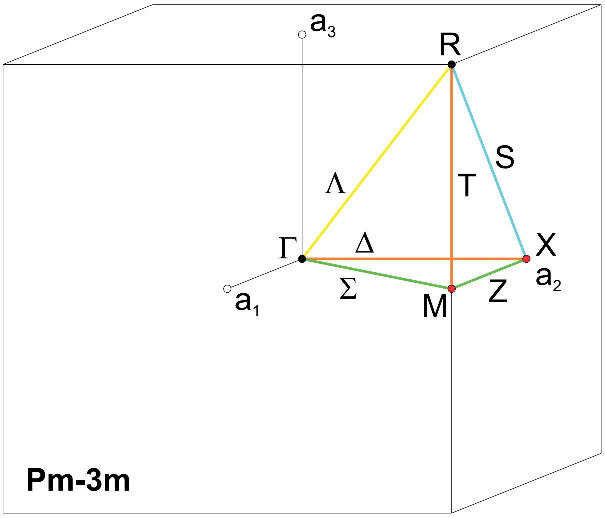
Crystal C is a periodic structure in E_n, *lattice* $L \simeq \mathbb{Z}^n$ is the set of points $\sum_{i=1}^n l_i a_i$, where $a_i \in E_n$ are the lattice constants. *Crystallographic group* Γ is a discrete subgroup of $E(n)$ with a finite fundamental domain. Two groups are equivalent if they are conjugate in the affine group $Aff(n)$. If conjugacy is restricted to orientation-preserving transformations, there are 230 groups in $n = 3$; otherwise, there are 219. *Point group* F is a subgroup of $O(n)$ that leaves invariant a certain crystal C. Each crystallographic group Γ is uniquely determined by the triple $\{F, L, \alpha\}$, where $\alpha : F \to E_n/L$ represents non-primitive translations, so that the symmetry transformations is $(f,l)x = fx + \alpha(f) + l$. The triple $\{F, L, \alpha\}$ defines an extension of the group F by the group L (an invariant subgroup of the extension), where the automorphism of the group L is defined as $\psi_f(l) = fl$, and the cocycle is $\chi(f_1, f_2) = \alpha(f_1) + f_1\alpha(f_2) - \alpha(f_1 f_2)$. The function α must satisfy the following conditions: 1) the normalization $\alpha(1) = 0$, 2) the condition that the group Γ is closed under multiplication $\chi(f_1, f_2) \in L$, 3) the associativity of the product $(1 - f_1)\chi(f_2, f_3) = (f_3^{-1} - 1)\chi(f_1, f_2)$. If $\alpha \equiv 0$, the extension splits, and $\Gamma = F \ltimes L$ is *symmorphic. The class* of a crystallographic group is determined by the point group that generates it. Groups whose linear subgroups are conjugate in $GL(n,\mathbb{R})$ belong to the same class. Groups whose rotational parts are conjugate in $GL(n,\mathbb{Z})$ belong to the same *arithmetic class* (arithmetic classes correspond to symmorphic groups). In the basis of lattice translation vectors, the matrix of the linear part of the transformations is integer, so the point symmetries of the lattice itself are described by finite subgroups in $GL(n,\mathbb{Z})$ (up to conjugacy). The *geometric* (respectively, *arithmetic*) *holohedry* of the crystallographic group Γ is defined as the smallest subgroup of lattice symmetries containing the group of rotational parts of transformations from Γ up to conjugation in $GL(n,\mathbb{Z})$ (respectively, $GL(n,\mathbb{R})$). Note that finite subgroups in $GL(n,\mathbb{Z})$ correspond to symmorphic groups. Crystallographic groups belong to the same *crystal system* (respectively, to the same *Bravais lattice type*), if their geometric (respectively, arithmetic) holohedries coincide. Number of different groups and holohedries in low-dimensional spaces are listed below:

Dimension of space, n	1	2	3	4
Number of crystallographic groups	2	17	230	4783
Number of arithmetic classes (symmorphic groups)	2	13	73	710
Number of geometric classes (point groups)	2	10	32	227
Number of arithmetic holohedries (Bravais lattices)	1	5	14	64
Number of geometric holohedries (crystal systems)	1	4	7	33
Number of maximal finite subgroups in $GL(n,\mathbb{Z})$	1	2	4	9

a	1	C_1	1	**P1**
	-1	C_i	2	**P-1**
m	2	C_2	3	**P2** P2_1 **C2**
	m	C_s	6	**Pm** Pc **Cm** Cc
	2/m	C_{2h}	10	**P2/m** P2_1/m **C2/m** P2/c P2_1/c C2/c
o	222	D_2	16	**P222** P22$2_1$ P$2_1 2_1$2 P$2_1 2_1 2_1$ C22$2_1$ **C222** **F222** **I222** I$2_1 2_1 2_1$
	mm2	C_{2v}	25	**Pmm2** Pmc2_1 Pcc2 Pma2 Pca2_1 Pnc2 Pmn2_1 Pba2 Pna2_1 Pnn2 **Cmm2** Cmc2_1 Ccc2 **Amm2** Abm2 Ama2 Aba2 **Fmm2** Fdd2 **Imm2** Iba2 Ima2
	mmm	D_{2h}	47	**Pmmm** Pnnn Pccm Pban Pmma Pnna Pmna Pcca Pbam Pccn Pbcm Pnnm Pmmn Pbcn Pbca Pnma Cmcm Cmca **Cmmm** Cccm Cmma Ccca **Fmmm** Fddd **Immm** Ibam Ibca Imma
t	4	C_4	75	**P4** P4_1 P4_2 P4_3 **I4** I4_1
	-4	S_4	81	**P-4** **I-4**
	4/m	C_{4h}	83	**P4/m** P4_2/m P4/n P4_2/n **I4/m** I4_1/a
	422	D_4	89	**P422** P4$2_1$2 P$4_1$22 P$4_1 2_1$2 P$4_2$22 P$4_2 2_1$2 P$4_3$22 P$4_3 2_1$2 **I422** I$4_1$22
	4mm	C_{4v}	99	**P4mm** P4bm P4_2cm P4_2nm P4cc P4nc P4_2mc P4_2bc **I4mm** I4cm I4_1md I4_1cd
	-42m	D_{2d}	111	**P-42m** P-42c P-4$2_1$m P-4$2_1$c **P-4m2** P-4c2 P-4b2 P-4n2 **I-4m2** I-4c2 **I-42m** I-42d
	4/mmm	D_{4h}	123	**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
h	3	C_3	143	**P3** P3_1 P3_2 **R3**
	-3	C_{3i}	147	**P-3** **R-3**
	32	D_3	149	**P312** **P321** P$3_1$12 P$3_1$21 P$3_2$12 P3$1_2$21 **R32**
	3m	C_{3v}	156	**P3m1** **P31m** P3c1 P31c **R3m** R3c
	-3m	D_{3d}	162	**P-31m** P-31c **P-3m1** P-3c1 **R-3m** R-3c
	6	C_6	168	**P6** P6_1 P6_5 P6_2 P6_4 P6_3
	-6	C_{3h}	174	**P-6**
	6/m	C_{6h}	175	**P6/m** P6_3/m
	622	D_6	177	**P622** P$6_1$22 P$6_5$22 P$6_2$22 P$6_4$22 P$6_3$22
	6mm	C_{6v}	183	**P6mm** P6cc P6_3cm P6_3mc
	-6m2	D_{3h}	187	**P-6m2** P-6c2 **P-62m** P-62c
	6/mmm	D_{6h}	191	**P6/mmm** P6/mcc P6_3/mcm P6_3/mmc
c	23	T	195	**P23** **F23** **I23** P$2_1$3 I$2_1$3
	m-3	T_h	200	**Pm-3** Pn-3 **Fm-3** Fd-3 **Im-3** Pa-3 Ia-3
	432	O	207	**P432** P$4_2$32 **F432** F$4_1$32 **I432** P$4_3$32 P$4_1$32 I$4_1$32
	-43m	T_d	215	**P-43m** **F-43m** **I-43m** P-43n F-43c I-43d
	m-3m	O_h	221	**Pm-3m** Pn-3n Pm-3n Pn-3m **Fm-3m** Fm-3c Fd-3m Fd-3c **Im-3m** Ia-3d

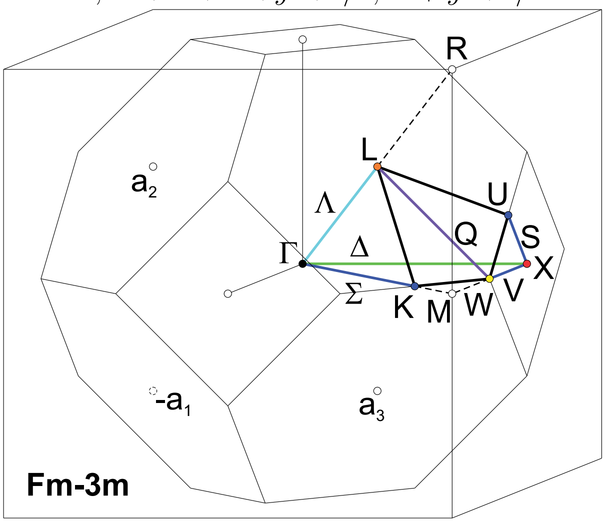
Table 2: Space Groups. Shown are crystal family, crystal class, and the number of the first group in the class. Symmorphic groups are highlighted.

Pm-3m, $0 < z < x < y < 1/2$



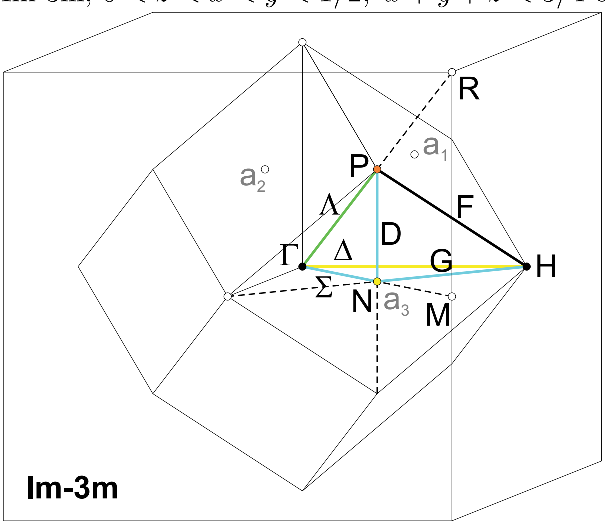
a	Γ	m-3m	O_h	1	0	0	0	
b	R	m-3m	O_h	1	1/2	1/2	1/2	
c	M	4/mmm	D_{4h}	3	1/2	1/2	0	
d	X	4/mmm	D_{4h}	3	0	1/2	0	
e	Δ	4mm	C_{4v}	6	0	y	0	
f	T	4mm	C_{4v}	6	1/2	1/2	z	
g	Λ	3m	C_{2v}	8	x	x	x	
h	Z	mm2	D_{1h}	12	x	1/2	0	
i	Σ	mm2	C_{2v}	12	x	x	0	
j	S	mm2	D_{1h}	12	x	1/2	x	
k	ΓXM	m	C_{1v}	24	x	y	0	
l	RXM	m	C_{1h}	24	x	1/2	z	
m	ΓRX	m	C_{1v}	24	x	y	x	ΓRM
n		1		48				

Fm-3m, $0 < z < x < y < 1/2,\ x + y < 1/2$



a	Γ	m-3m	O_h	1	0	0	0	M
b	H	m-3m	O_h	1	0	1/2	0	R
c	P	-43m	T_d	2	1/4	1/4	1/4	
d	N	mmm	D_{2h}	6	1/4	1/4	0	
e	Δ	4mm	C_{4v}	6	0	y	0	
f	$\Lambda + F'$	3m	C_{3v}	8	x	x	x	F
g	D	mm2	C_{2v}	12	1/4	1/4	z	
h	Σ	mm2	C_{2v}	12	x	x	0	
i	G	mm2	C_{2v}	12	x	$1/2 - x$	0	
j	ΓHN	m	C_{1v}	24	x	y	0	
k	$\Gamma H'PN$	m	C_{1v}	24	x	x	z	$HPN, \Gamma HP$
l		1		48				

Im-3m, $0 < z < x < y < 1/2,\ x + y + z < 3/4$ or $0 < z < x < y,\ y + z < 1/2$



a	Γ	m-3m	O_h	1	0	0	0	R
b	X	4/mmm	D_{4h}	3	0	1/2	0	M
c	L	-3m	D_{3d}	4	1/4	1/4	1/4	
d	W	-42m	D_{2d}	6	3/4	0	1/2	
e	Δ	4mm	C_{4v}	6	0	y	0	
f	Λ	3m	C_{3v}	8	x	x	x	
g	V	mm2	C_{2v}	12	x	1/2	0	
h	$\Sigma + S'$	mm2	C_{2v}	12	x	x	0	S, K, U
i	Q	2	C_2	24	1/4	y	$1/2 - y$	
j	ΓXM	m	C_{1v}	24	x	y	0	XWU
k	$\Gamma X'M$	m	C_{1v}	24	x	x	z	
l		1		48				XML

Table 3: Wigner–Seitz cell and orbits of maximal cubic groups. Shown are position as Wyckoff symbol and in reciprocal lattice notations, stabilizer, multiplicity, lattice coordinates, and equivalent points or paths.