International Tables for Crystallography (2016). Vol. A, Section 1.3.4.1, pp. 31–33.

excluding 1. In particular, if the translation part of a coset representative is a lattice vector, it is usually chosen as the zero vector $\boldsymbol{o}$.

Note that due to the fact that $\mathcal{T}$ is a normal subgroup of $\mathcal{G}$, a system of coset representatives for the right cosets is at the same time a system of coset representatives for the left cosets.

1.3.3.3. Symmorphic and non-symmorphic space groups

If a coset with respect to the translation subgroup contains an operation of the form $(\boldsymbol{W}, \boldsymbol{w})$ with $\boldsymbol{w}$ a vector in the translation lattice, it is clear that the same coset also contains the operation $(\boldsymbol{W}, \boldsymbol{o})$ with trivial translation part. On the other hand, if a coset does not contain an operation of the form $(\boldsymbol{W}, \boldsymbol{o})$, this may be caused by an inappropriate choice of origin. For example, the operation $(-\boldsymbol{I}, (1/2, 1/2, 1/2))$ is turned into the inversion $(-\boldsymbol{I}, (0, 0, 0))$ by moving the origin to 1/4, 1/4, 1/4 (*cf.* Section 1.5.1.1 for a detailed treatment of origin-shift transformations).

Depending on the actual space group $\mathcal{G}$, it may or may not be possible to choose the origin such that every coset with respect to $\mathcal{T}$ contains an operation of the form $(\boldsymbol{W}, \boldsymbol{o})$.

Definition

Let $\mathcal{G}$ be a space group with translation subgroup $\mathcal{T}$. If it is possible to choose the coordinate system such that every coset of $\mathcal{G}$ with respect to $\mathcal{T}$ contains an operation $(\boldsymbol{W}, \boldsymbol{o})$ with trivial translation part, $\mathcal{G}$ is called a *symmorphic* space group, otherwise $\mathcal{G}$ is called a *non-symmorphic* space group.

One sees that the operations with trivial translation part form a subgroup of $\mathcal{G}$ which is isomorphic to a subgroup of the point group $\mathcal{P}$. This subgroup is the group of operations in $\mathcal{G}$ that fix the origin and is called the *site-symmetry group* of the origin (site-symmetry groups are discussed in detail in Section 1.4.4). It is the distinctive property of symmorphic space groups that they contain a subgroup which is isomorphic to the full point group. This may in fact be seen as an alternative definition for symmorphic space groups.

Proposition. A space group $\mathcal{G}$ with point group $\mathcal{P}$ is symmorphic if and only if it contains a subgroup isomorphic to $\mathcal{P}$. For a non-symmorphic space group $\mathcal{G}$, every finite subgroup of $\mathcal{G}$ is isomorphic to a proper subgroup of the point group.

Note that every finite subgroup of a space group is a subgroup of the site-symmetry group for some point, because finite groups cannot contain translations. Therefore, a symmorphic space group is characterized by the fact that it contains a site-symmetry group isomorphic to its point group, whereas in non-symmorphic space groups all site-symmetry groups have orders strictly smaller than the order of the point group.

Symmorphic space groups can easily be constructed by choosing a lattice $\mathbf{L}$ and a point group $\mathcal{P}$ which acts on $\mathbf{L}$. Then $\mathcal{G} = \{(\boldsymbol{W}, \boldsymbol{w}) \mid \boldsymbol{W} \in \mathcal{P}, \boldsymbol{w} \in \mathbf{L}\}$ is a space group in which the coset representatives can be chosen as $(\boldsymbol{W}, \boldsymbol{o})$.

Non-symmorphic space groups can also be constructed from a lattice $\mathbf{L}$ and a point group $\mathcal{P}$. What is required is a system of coset representatives with respect to $\mathcal{T}$ and these are obtained by choosing for each operation $\boldsymbol{W} \in \mathcal{P}$ a translation part $\boldsymbol{w}$. Owing to the translations, it is sufficient to consider vectors $\boldsymbol{w}$ with components between 0 and 1. However, the translation parts cannot be chosen arbitrarily, because for a point-group operation of order k, the operation $(\boldsymbol{W}, \boldsymbol{w})^k$ has to be a translation $(\boldsymbol{I}, \boldsymbol{t})$ with $\boldsymbol{t} \in \mathbf{L}$. Working this out, this imposes the restriction that

$$(\boldsymbol{W}^{k-1} + \ldots + \boldsymbol{W} + \boldsymbol{I})\boldsymbol{w} \in \mathbf{L}.$$

Once translation parts $\boldsymbol{w}$ are found that fulfil all these restrictions, one finally has to check whether the space group obtained this way is (by accident) symmorphic, but written with respect to an inappropriate origin. A change of origin by $\boldsymbol{p}$ is realized by conjugating the matrix–column pair $(\boldsymbol{W}, \boldsymbol{w})$ by the translation $(\boldsymbol{I}, -\boldsymbol{p})$ (*cf.* Section 1.5.1 on transformations of the coordinate system) which gives

$$(\boldsymbol{I}, -\boldsymbol{p})(\boldsymbol{W}, \boldsymbol{w})(\boldsymbol{I}, \boldsymbol{p}) = (\boldsymbol{W}, \boldsymbol{W}\boldsymbol{p} + \boldsymbol{w} - \boldsymbol{p}) = (\boldsymbol{W}, \boldsymbol{w} + (\boldsymbol{W} - \boldsymbol{I})\boldsymbol{p}).$$

Thus, the space group just constructed is symmorphic if there is a vector $\boldsymbol{p}$ such that $(\boldsymbol{W} - \boldsymbol{I})\boldsymbol{p} + \boldsymbol{w} \in \mathbf{L}$ for each of the coset representatives $(\boldsymbol{W}, \boldsymbol{w})$.

The above considerations also show how every space group can be assigned to a symmorphic space group in a canonical way, namely by setting the translation parts of coset representatives with respect to $\mathcal{T}$ to $\boldsymbol{o}$. This has the effect that screw rotations are turned into rotations and glide reflections into reflections. The Hermann–Mauguin symbol (see Section 1.4.1 for a detailed discussion of Hermann–Mauguin symbols) of the symmorphic space group to which an arbitrary space group is assigned is simply obtained by replacing any screw rotation symbol N_m by the corresponding rotation symbol N and every glide reflection symbol a, b, c, d, e, n by the symbol m for a reflection. A space group is found to be symmorphic if no such replacement is required, *i.e.* if the Hermann–Mauguin symbol only contains the symbols 1, 2, 3, 4, 6 for rotations, $\bar{1}$, $\bar{3}$, $\bar{4}$, $\bar{6}$ for rotoinversions and m for reflections.

Example

The space groups with Hermann-Mauguin symbols $P4mm$, $P4bm$, $P4_2cm$, $P4_2nm$, $P4cc$, $P4nc$, $P4_2mc$, $P4_2bc$ are all assigned to the symmorphic space group with Hermann–Mauguin symbol $P4mm$.

1.3.4. Classification of space groups

In this section we will consider various ways in which space groups may be grouped together. For the space groups themselves, the natural notion of equivalence is the classification into *space-group types*, but the point groups and lattices from which the space groups are built also have their own classification schemes into *geometric crystal classes* and *Bravais types of lattices*, respectively.

Some other types of classifications are relevant for certain applications, and these will also be considered. The hierarchy of the different classification levels and the numbers of classes on the different levels in dimension 3 are displayed in Fig. 1.3.4.1.

1.3.4.1. Space-group types

The main motivation behind studying space groups is that they allow the classification of crystal structures according to their symmetry properties. Since many properties of a structure can be derived from its group of symmetries alone, this allows the investigation of the properties of many structures simultaneously.

On the other hand, even for the same crystal structure the corresponding space group may look different, depending on the chosen coordinate system (see Chapter 1.5 for a detailed discussion of transformations to different coordinate systems). Because it is natural to regard two realizations of a group of symmetry operations with respect to two different coordinate systems as equivalent, the following notion of equivalence between space groups is natural.

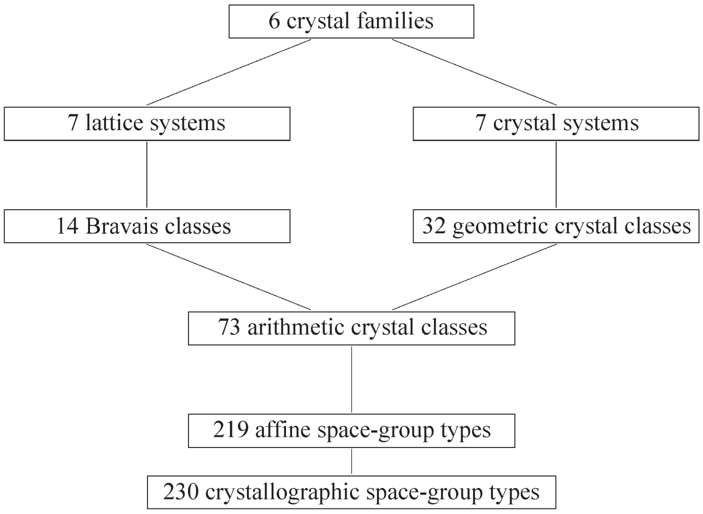

Figure 1.3.4.1
Classification levels for three-dimensional space groups.

Definition

Two space groups $\mathcal{G}$ and $\mathcal{G}'$ are called *affinely equivalent* if $\mathcal{G}'$ can be obtained from $\mathcal{G}$ by a change of the coordinate system. In terms of matrix–column pairs this means that there must exist a matrix–column pair $(\boldsymbol{P}, \boldsymbol{p})$ such that

$$\mathcal{G}' = \{(\boldsymbol{P}, \boldsymbol{p})^{-1}(\boldsymbol{W}, \boldsymbol{w})(\boldsymbol{P}, \boldsymbol{p}) \mid (\boldsymbol{W}, \boldsymbol{w}) \in \mathcal{G}\}.$$

The collection of space groups that are affinely equivalent with $\mathcal{G}$ forms the *affine type* of $\mathcal{G}$.

In dimension 2 there are 17 affine types of plane groups and in dimension 3 there are 219 affine space-group types. Note that in order to avoid misunderstandings we refrain from calling the space-group types *affine classes*, since the term classes is usually associated with *geometric crystal classes* (see below).

Grouping together space groups according to their space-group type serves different purposes. On the one hand, it is sometimes convenient to consider the same crystal structure and thus also its space group with respect to different coordinate systems, *e.g.* when the origin can be chosen in different natural ways or when a phase transition to a higher- or lower-symmetry phase with a different conventional cell is described. On the other hand, different crystal structures may give rise to the same space group once suitable coordinate systems have been chosen for both. We illustrate both of these perspectives by an example.

Examples

(i) The space group $\mathcal{G}$ of type *Pban* (50) has a subgroup $\mathcal{H}$ of index 2 for which the coset representatives relative to the translation subgroup are the identity e: x, y, z, the twofold rotation g: $-x, y, -z$, the n glide h: $x + \frac{1}{2}, y + \frac{1}{2}, -z$ and the b glide k: $-x + \frac{1}{2}, y + \frac{1}{2}, z$. This subgroup is of type *Pb*2*n*, which is a non-conventional setting for *Pnc*2 (30). In the conventional setting, the coset representatives of *Pnc*2 are given by g': $-x, -y, z$, h': $-x, y + \frac{1}{2}, z + \frac{1}{2}$ and k': $x, -y + \frac{1}{2}, z + \frac{1}{2}$, *i.e.* with the z axis as rotation axis for the twofold rotation. The subgroup $\mathcal{H}$ can be transformed to its conventional setting by the basis transformation $(\mathbf{a}', \mathbf{b}', \mathbf{c}') = (\mathbf{c}, \mathbf{a}, \mathbf{b})$. Depending on whether the perspective of the full group $\mathcal{G}$ or the subgroup $\mathcal{H}$ is more important for a crystal structure, the groups $\mathcal{G}$ and $\mathcal{H}$ will be considered either with respect to the basis $\mathbf{a}, \mathbf{b}, \mathbf{c}$ (conventional for $\mathcal{G}$) or to the basis $\mathbf{a}', \mathbf{b}', \mathbf{c}'$ (conventional for $\mathcal{H}$).

(ii) The elements carbon, silicon and germanium all crystallize in the *diamond structure*, which has a face-centred cubic unit cell with two atoms shifted by 1/4 along the space diagonal of the conventional cubic cell. The space group is in all cases of type $Fd\bar{3}m$ (227), but the cell parameters differ: $a_{\rm C}$ = 3.5668 Å for carbon, $a_{\rm Si}$ = 5.4310 Å for silicon and $a_{\rm Ge}$ = 5.6579 Å for germanium (measured at 298 K). In order to scale the conventional cell of carbon to that of silicon, the coordinate system has to be transformed by the diagonal matrix

$$a_{\rm Si}/a_{\rm C} \cdot \boldsymbol{I}_3 \approx \begin{pmatrix} 1.523 & 0 & 0 \\ 0 & 1.523 & 0 \\ 0 & 0 & 1.523 \end{pmatrix}.$$

By a famous theorem of Bieberbach (see Bieberbach, 1911, 1912), affine equivalence of space groups actually coincides with the notion of abstract group isomorphism as discussed in Section 1.1.6.

Bieberbach theorem

Two space groups in n-dimensional space are isomorphic if and only if they are conjugate by an affine mapping.

This theorem is by no means obvious. Recall that for point groups the situation is very different, since for example the abstract cyclic group of order 2 is realized in the point groups of space groups of type *P*2, *Pm* and $P\bar{1}$, generated by a twofold rotation, reflection and inversion, respectively, which are clearly not equivalent in any geometric sense. The driving force behind the Bieberbach theorem is the special structure of space groups having an infinite normal translation subgroup on which the point group acts.

In crystallography, a notion of equivalence slightly stronger than affine equivalence is usually used. Since crystals occur in physical space and physical space can only be transformed by orientation-preserving mappings, space groups are only regarded as equivalent if they are conjugate by an *orientation-preserving* coordinate transformation, *i.e.* by an affine mapping that has a linear part with positive determinant.

Definition

Two space groups $\mathcal{G}$ and $\mathcal{G}'$ are said to belong to the same *space-group type* if $\mathcal{G}'$ can be obtained from $\mathcal{G}$ by an orientation-preserving coordinate transformation, *i.e.* by conjugation with a matrix–column pair $(\boldsymbol{P}, \boldsymbol{p})$ with $\det \boldsymbol{P} > 0$. In order to distinguish the space-group types explicitly from the affine space-group types (corresponding to the isomorphism classes), they are often called *crystallographic space-group types*.

The (crystallographic) space-group type collects together the infinitely many space groups that are obtained by expressing a single space group with respect to all possible right-handed coordinate systems for the point space.

Example

We consider the space group $\mathcal{G}$ of type $I4_1$ (80) which is generated by the right-handed fourfold screw rotation g: $-y, x + 1/2, z + 1/4$ (located at $-1/4, 1/4, z$), the centring translation t: $x + 1/2, y + 1/2, z + 1/2$ and the integral translations of a primitive tetragonal lattice. Conjugating the group $\mathcal{G}$ to $\mathcal{G}' = m\mathcal{G}m^{-1}$ by the reflection m in the plane $z = 0$ turns the right-handed screw rotation g into the left-handed screw

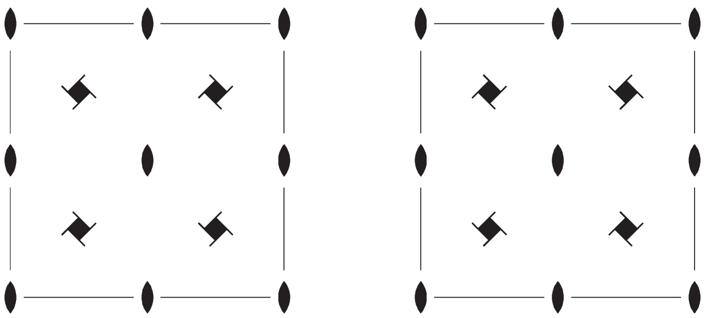

Figure 1.3.4.2
Space-group diagram of $I4_1$ (left) and its reflection in the plane $z = 0$ (right).

rotation g': $-y, x + 1/2, z - 1/4$, and one might suspect that $\mathcal{G}'$ is a space group of the same affine type but of a different crystallographic space-group type as $\mathcal{G}$. However, this is not the case because conjugating $\mathcal{G}$ by the translation $n = t(0, 1/2, 0)$ conjugates g to $g'' = ngn^{-1}$: $-y + 1/2, x + 1, z + 1/4$. One sees that g'' is the composition of g' with the centring translation t and hence g'' belongs to $\mathcal{G}'$. This shows that conjugating $\mathcal{G}$ by either the reflection m or the translation n both result in the same group $\mathcal{G}'$. This can also be concluded directly from the space-group diagrams in Fig. 1.3.4.2. Reflecting in the plane $z = 0$ turns the diagram on the left into the diagram on the right, but the same effect is obtained when the left diagram is shifted by $\frac{1}{2}$ along either **a** or **b**.

The groups $\mathcal{G}$ and $\mathcal{G}'$ thus belong to the same crystallographic space-group type because $\mathcal{G}$ is transformed to $\mathcal{G}'$ by a shift of the origin by $\frac{1}{2}\mathbf{b}$, which is clearly an orientation-preserving coordinate transformation.

Enantiomorphism

The 219 affine space-group types in dimension 3 result in 230 crystallographic space-group types. Since an affine type either forms a single space-group type (in the case where the group obtained by an orientation-reversing coordinate transformation can also be obtained by an orientation-preserving transformation) or splits into two space-group types, this means that there are 11 affine space-group types such that an orientation-reversing coordinate transformation cannot be compensated by an orientation-preserving transformation.

Groups that differ only by their handedness are closely related to each other and share many properties. One addresses this phenomenon by the concept of *enantiomorphism*.

Example

Let $\mathcal{G}$ be a space group of type $P4_1$ (76) generated by a fourfold right-handed screw rotation $(4^+_{001}, (0, 0, 1/4))$ and the translations of a primitive tetragonal lattice. Then transforming the coordinate system by a reflection in the plane $z = 0$ results in a space group $\mathcal{G}'$ with fourfold left-handed screw rotation $(4^-_{001}, (0, 0, 1/4)) = (4^+_{001}, (0, 0, -1/4))^{-1}$. The groups $\mathcal{G}$ and $\mathcal{G}'$ are isomorphic because they are conjugate by an affine mapping, but $\mathcal{G}'$ belongs to a different space-group type, namely $P4_3$ (78), because $\mathcal{G}$ does not contain a fourfold left-handed screw rotation with translation part $\frac{1}{4}\mathbf{c}$.

Definition

Two space groups $\mathcal{G}$ and $\mathcal{G}'$ are said to form an *enantiomorphic pair* if they are conjugate under an affine mapping, but not under an orientation-preserving affine mapping.

If $\mathcal{G}$ is the group of isometries of some crystal pattern, then its enantiomorphic counterpart $\mathcal{G}'$ is the group of isometries of the mirror image of this crystal pattern.

The splitting of affine space-group types of three-dimensional space groups into pairs of crystallographic space-group types gives rise to the following 11 enantiomorphic pairs of space-group types: $P4_1/P4_3$ (76/78), $P4_122/P4_322$ (91/95), $P4_12_12/P4_32_12$ (92/96), $P3_1/P3_2$ (144/145), $P3_112/P3_212$ (151/153), $P3_121/P3_221$ (152/154), $P6_1/P6_5$ (169/173), $P6_2/P6_4$ (170/172), $P6_122/P6_522$ (178/179), $P6_222/P6_422$ (180/181), $P4_332/P4_132$ (212/213). These groups are easily recognized by their Hermann–Mauguin symbols, because they are the primitive groups for which the Hermann–Mauguin symbol contains one of the screw rotations 3_1, 3_2, 4_1, 4_3, 6_1, 6_2, 6_4 or 6_5. The groups with fourfold screw rotations and body-centred lattices do not give rise to enantiomorphic pairs, because in these groups the orientation reversal can be compensated by an origin shift, as illustrated in the example above for the group of type $I4_1$.

Example

A well known example of a crystal that occurs in forms whose symmetry is described by enantiomorphic pairs of space groups is quartz. For low-temperature α-quartz there exists a left-handed and a right-handed form with space groups $P3_121$ (152) and $P3_221$ (154), respectively. The two individuals of opposite chirality occur together in the so-called Brazil twin of quartz. At higher temperatures, a phase transition leads to the higher-symmetry β-quartz forms, with space groups $P6_422$ (181) and $P6_222$ (180), which still form an enantiomorphic pair.

1.3.4.2. Geometric crystal classes

We recall that the point group of a space group is the group of linear parts occurring in the space group. Once a basis for the underlying vector space is chosen, such a point group is a group of 3×3 matrices. A point group is characterized by the relative positions between the rotation and rotoinversion axes and the reflection planes of the operations it contains, and in this sense a point group is independent of the chosen basis. However, a suitable choice of basis is useful to highlight the geometric properties of a point group.

Example

A point group of type $3m$ is generated by a threefold rotation and a reflection in a plane with normal vector perpendicular to the rotation axis. Choosing a basis **a**, **b**, **c** such that **c** is along the rotation axis, **a** is perpendicular to the reflection plane and **b** is the image of **a** under the threefold rotation (*i.e.* **b** lies in the plane perpendicular to the rotation axis and makes an angle of 120° with **a**), the matrices of the threefold rotation and the reflection with respect to this basis are

$$\begin{pmatrix} 0 & -1 & 0 \\ 1 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \text{ and } \begin{pmatrix} -1 & 1 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

A different useful basis is obtained by choosing a vector $\mathbf{a}'$ in the reflection plane but neither along the rotation axis nor perpendicular to it and taking $\mathbf{b}'$ and $\mathbf{c}'$ to be the images of $\mathbf{a}'$ under the threefold rotation and its square. Then the matrices of the threefold rotation and the reflection with respect to the basis $\mathbf{a}'$, $\mathbf{b}'$, $\mathbf{c}'$ are