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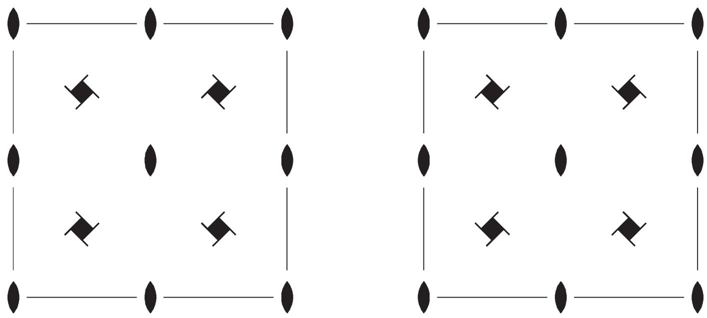

Figure 1.3.4.2
Space-group diagram of $I4_1$ (left) and its reflection in the plane $z = 0$ (right).

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

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

Different choices of a basis for a point group in general result in different matrix groups, and it is natural to consider two point groups as equivalent if they are transformed into each other by a basis transformation. This is entirely analogous to the situation of space groups, where space groups that only differ by the choice of coordinate system are regarded as equivalent. This notion of equivalence is applied at both the level of space groups and point groups.

Definition

Two space groups $\mathcal{G}$ and $\mathcal{G}'$ with point groups $\mathcal{P}$ and $\mathcal{P}'$, respectively, are said to belong to the same *geometric crystal class* if $\mathcal{P}$ and $\mathcal{P}'$ become the same matrix group once suitable bases for the three-dimensional space are chosen.

Equivalently, $\mathcal{G}$ and $\mathcal{G}'$ belong to the same geometric crystal class if the point group $\mathcal{P}'$ can be obtained from $\mathcal{P}$ by a basis transformation of the underlying vector space $\mathbb{V}^3$, *i.e.* if there is an invertible 3×3 matrix $\boldsymbol{P}$ such that

$$\mathcal{P}' = \{\boldsymbol{P}^{-1}\boldsymbol{W}\boldsymbol{P} \mid \boldsymbol{W} \in \mathcal{P}\}.$$

Also, two matrix groups $\mathcal{P}$ and $\mathcal{P}'$ are said to belong to the same geometric crystal class if they are conjugate by an invertible 3×3 matrix $\boldsymbol{P}$.

Historically, the geometric crystal classes in dimension 3 were determined much earlier than the space groups. They were obtained as the symmetry groups for the set of normal vectors of crystal faces which describe the morphological symmetry of crystals.

Note that for the geometric crystal classes in dimension 3 (and in all other odd dimensions) the distinction between orientation-preserving and orientation-reversing transformations is irrelevant, since any conjugation by an arbitrary transformation can already be realized by an orientation-preserving transformation. This is due to the fact that the inversion $-\boldsymbol{I}$ on the one hand commutes with every matrix $\boldsymbol{W}$, *i.e.* $(-\boldsymbol{I})\boldsymbol{W} = \boldsymbol{W}(-\boldsymbol{I})$, and on the other hand $\det(-\boldsymbol{I}) = -1$. If $\boldsymbol{P}$ is orientation reversing, one has $\det \boldsymbol{P} < 0$ and then $(-\boldsymbol{I})\boldsymbol{P} = -\boldsymbol{P}$ is orientation preserving because $\det(-\boldsymbol{P}) = -\det \boldsymbol{P} > 0$. But $(-\boldsymbol{P})^{-1}\boldsymbol{W}(-\boldsymbol{P}) = \boldsymbol{P}^{-1}\boldsymbol{W}\boldsymbol{P}$, hence the transformations by $\boldsymbol{P}$ and $-\boldsymbol{P}$ give the same result and one of $\boldsymbol{P}$ and $-\boldsymbol{P}$ is orientation preserving.

Remark: One often speaks of the geometric crystal classes as the *types of point groups*. This emphasizes the point of view in which a point group is regarded as the group of linear parts of a space group, written with respect to an *arbitrary basis* of $\mathbb{R}^n$ (not necessarily a lattice basis).

It is also common to state that *there are 32 point groups in three-dimensional space*. This is just as imprecise as saying that *there are 230 space groups*, since there are in fact infinitely many point groups and space groups.

What is meant when we say that two space groups have *the same point group* is usually that their point groups are of the same type (*i.e.* lie in the same geometric crystal class) and can thus be *made to coincide* by a suitable basis transformation.

Example

In the space group $P3$ the threefold rotation generating the point group is given by the matrix

$$\boldsymbol{W} = \begin{pmatrix} 0 & -1 & 0 \\ 1 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix},$$

whereas in the space group $R3$ (in the rhombohedral setting) the threefold rotation is given by the matrix

$$\boldsymbol{W}' = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}.$$

These two matrices are conjugate by the basis transformation

$$\boldsymbol{P} = \frac{1}{3}\begin{pmatrix} 1 & 0 & -1 \\ 0 & 1 & -1 \\ 1 & 1 & 1 \end{pmatrix},$$

which transforms the basis of the hexagonal setting into that of the rhombohedral setting. This shows that the space groups $P3$ and $R3$ belong to the same geometric crystal class.

The example is typical in the sense that different groups in the same geometric crystal class usually describe the same group of linear parts acting on different lattices, *e.g.* primitive and centred. Writing the action of the linear parts with respect to primitive bases of different lattices gives rise to different matrix groups.

1.3.4.3. Bravais types of lattices and Bravais classes

In the classification of space groups into geometric crystal classes, only the point-group part is considered and the translation lattice is ignored. It is natural that the converse point of view is also adopted, where space groups are grouped together according to their translation lattices, irrespective of what the point groups are.

We have already seen that a lattice can be characterized by its metric tensor, containing the scalar products of a primitive basis. If a point group $\mathcal{P}$ acts on a lattice $\mathbf{L}$, it fixes the metric tensor $\boldsymbol{G}$ of $\mathbf{L}$, *i.e.* $\boldsymbol{W}^{\mathrm{T}} \cdot \boldsymbol{G} \cdot \boldsymbol{W} = \boldsymbol{G}$ for all $\boldsymbol{W}$ in $\mathcal{P}$ and is thus a subgroup of the Bravais group $Aut(\mathbf{L})$ of $\mathbf{L}$. Also, a matrix group $\mathcal{B}$ is called a *Bravais group* if it is the Bravais group $Aut(\mathbf{L})$ for some lattice $\mathbf{L}$. The Bravais groups govern the classification of lattices.

Definition

Two lattices $\mathbf{L}$ and $\mathbf{L}'$ belong to the same *Bravais type of lattices* if their Bravais groups $Aut(\mathbf{L})$ and $Aut(\mathbf{L}')$ are the same matrix group when written with respect to suitable primitive bases of $\mathbf{L}$ and $\mathbf{L}'$.

Note that in order to have the same Bravais group, the metric tensors of the two lattices $\mathbf{L}$ and $\mathbf{L}'$ do not have to be the same or scalings of each other.

Example

The mineral rutile (TiO_2) has a space group of type $P4_2/mnm$ (136) with a primitive tetragonal cell with cell parameters $a = b = 4.594$ Å and $c = 2.959$ Å. The metric tensor of the translation lattice $\mathbf{L}$ is therefore

$$\boldsymbol{G} = \begin{pmatrix} 4.594^2 & 0 & 0 \\ 0 & 4.594^2 & 0 \\ 0 & 0 & 2.959^2 \end{pmatrix}$$

and the Bravais group of the lattice is generated by the fourfold rotation

$$\begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$