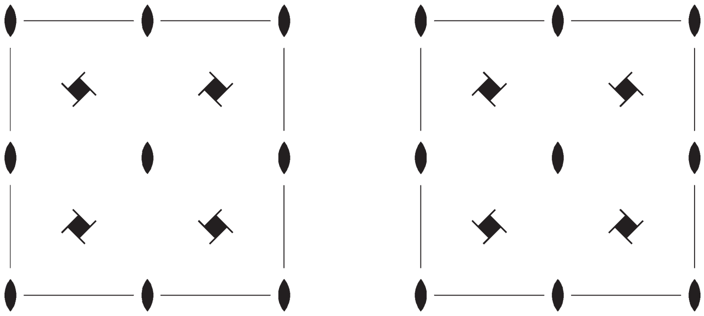

Figure 1.3.4.2
Space-group diagram of $I4_1$ (left) and its reflection in the plane $z = 0$ (right).

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