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$a = b$, then the eigensymmetry group of an orbit can belong to the tetragonal family.

Note: A space group $\mathcal{G}$ is equal to the intersection of the eigensymmetry groups of the orbits of all its positions. If none of the positions of a space group $\mathcal{G}$ gives rise to a characteristic orbit, this means that each single orbit under $\mathcal{G}$ does not have $\mathcal{G}$ as its symmetry group, but a larger group that contains $\mathcal{G}$ as a proper subgroup. It may thus be necessary to have the union of at least two orbits under $\mathcal{G}$ to obtain a structure that has precisely $\mathcal{G}$ as its group of symmetry operations.

Examples

(1) For the group $\mathcal{G}$ of type *Pmmm* (47) all Wyckoff positions with no further special values of the coordinates give rise to characteristic orbits, because the point group of $\mathcal{G}$ is a holohedry and the general coordinates allow no further translations. However, there are various 'specializations' of the positions that give rise to extraordinary orbits. For example, setting x to the special value $\frac{1}{4}$ for the general position introduces the additional translation $t(\frac{1}{2}, 0, 0)$. In fact, for all positions in which the first coordinate has no specified value (positions 2*i*–2*l*, 4*w*–4*z*, 8α), setting $x = \frac{1}{4}$ introduces the translation $t(\frac{1}{2}, 0, 0)$ and thus gives rise to an extraordinary orbit. In all these cases, the resulting eigensymmetry group is of type *Pmmm* with primitive lattice basis $\frac{1}{2}\mathbf{a}, \mathbf{b}, \mathbf{c}$.

(2) For the group $\mathcal{G}$ of type *Pmm*2 (25) no Wyckoff position gives rise to a characteristic orbit, because this is a polar group (with respect to the c axis). Any orbit of a point with third coordinate z allows an additional mirror plane normal to the c axis and located at $0, 0, z$. For example, the general position gives rise to a non-characteristic orbit with eigensymmetry group *Pmmm* (47). Since the general coordinates allow no additional translation, this is not an extraordinary orbit. However, setting $x = \frac{1}{4}$ for the general position introduces the translation $t(\frac{1}{2}, 0, 0)$ (as in the above example) and thus gives rise to an extraordinary orbit. The eigensymmetry group is *Pmmm* with primitive lattice basis $\frac{1}{2}\mathbf{a}, \mathbf{b}, \mathbf{c}$.
On the other hand, the special positions $x, 0, z$ (Wyckoff position 2*e*) and $x, \frac{1}{2}, z$ (Wyckoff position 2*f*) both have the same eigensymmetry group as the general position and setting $x = \frac{1}{4}$ for each, giving $\frac{1}{4}, 0, z$ and $\frac{1}{4}, \frac{1}{2}, z$, results in these positions having the same eigensymmetry group as the $\frac{1}{4}, y, z$ case of the general position.

(3) For a group $\mathcal{G}$ of type $P\bar{4}c2$ (116) the general-position coordinates are

(1) x, y, z	(2) $\bar{x}, \bar{y}, z$	(3) $y, \bar{x}, \bar{z}$	(4) $\bar{y}, x, \bar{z}$
(5) $x, \bar{y}, z + \frac{1}{2}$	(6) $\bar{x}, y, z + \frac{1}{2}$	(7) $y, x, \bar{z} + \frac{1}{2}$	(8) $\bar{y}, \bar{x}, \bar{z} + \frac{1}{2}$

A point x, y, z in a general position does not give rise to an extraordinary orbit because, owing to the general coordinates, there can not be any additional translation. Furthermore, the point group $\bar{4}m2$ of $\mathcal{G}$ has index 2 in the holohedry $4/mmm$. Thus, in order to have a non-characteristic orbit one would require an inversion in some point as an additional operation. But an inversion in p_1, p_2, p_3 would map x, y, z to $\bar{x} + 2p_1, \bar{y} + 2p_2, \bar{z} + 2p_3$ and no such point is contained in the orbit for generic x, y, z. The point x, y, z therefore gives rise to a characteristic orbit.
However, if the point in a general position is chosen with $x = y$, one indeed obtains an additional inversion at $0, 0, \frac{1}{4}$ which maps x, x, z to the orbit point $\bar{x}, \bar{x}, \bar{z} + \frac{1}{2}$ (general position point No. 8). This orbit thus is non-characteristic, but it is not extraordinary, since no additional translation is introduced. The eigensymmetry group obtained is $P4_2/mcm$ (132).
On the other hand, if the general position is chosen with $y = 0$, no additional inversion is obtained, but the translation by $\frac{1}{2}\mathbf{c}$ maps $x, 0, z$ to $x, 0, z + \frac{1}{2}$ (general-position point No. 5). The position $x, 0, z$ therefore gives rise to an extraordinary orbit with eigensymmetry group $P\bar{4}m2$ (115).

Knowledge of the eigensymmetry groups of the different positions for a group is of utmost importance for the analysis of diffraction patterns. Atoms in positions that give rise to non-characteristic orbits, in particular extraordinary orbits, may cause systematic absences that are not explained by the space-group operations. These absences are specified as *special reflection conditions* in the space-group tables of this volume, but only as long as no specialization of the coordinates is involved. For the latter case, the possible existence of systematic absences has to be deduced from the tables of noncharacteristic orbits. Reflection conditions are discussed in detail in Chapter 1.6.

Example

For the group $\mathcal{G}$ of type *Pccm* (49) the special position $\frac{1}{2}, 0, z$ (Wyckoff position 4*p*) gives rise to an extraordinary orbit, since it allows the additional translation $\frac{1}{2}\mathbf{c}$. The special reflection condition corresponding to this additional translation is the integral reflection condition *hkl*: $l = 2n$. However, if the z coordinate in position 4*p* is set to $z = \frac{1}{8}$, the eigensymmetry group also contains the translation $\frac{1}{4}\mathbf{c}$. In this case, the special reflection condition becomes *hkl*: $l = 4n$.

1.4.5. Sections and projections of space groups

By B. Souvignier

In crystallography, two-dimensional sections and projections of crystal structures play an important role, *e.g.* in structure determination by Fourier and Patterson methods or in the treatment of twin boundaries and domain walls. Planar sections of three-dimensional scattering density functions are used for finding approximate locations of atoms in a crystal structure. They are indispensable for the location of Patterson peaks corresponding to vectors between equivalent atoms in different asymmetric units (the Harker vectors).

1.4.5.1. Introduction

A two-dimensional section of a crystal pattern takes out a slice of a crystal pattern. In the mathematical idealization, this slice is regarded as a two-dimensional plane, allowing one, however, to distinguish its upper and lower side. Depending on how the slice is oriented with respect to the crystal lattice, the slice will be invariant by translations of the crystal pattern along zero, one or two linearly independent directions. A section resulting in a slice with two-dimensional translational symmetry is called a *rational section* and is by far the most important case for crystallography.

Because the slice is regarded as a two-sided plane, the symmetries of the full crystal pattern that leave the slice invariant fall into two types:

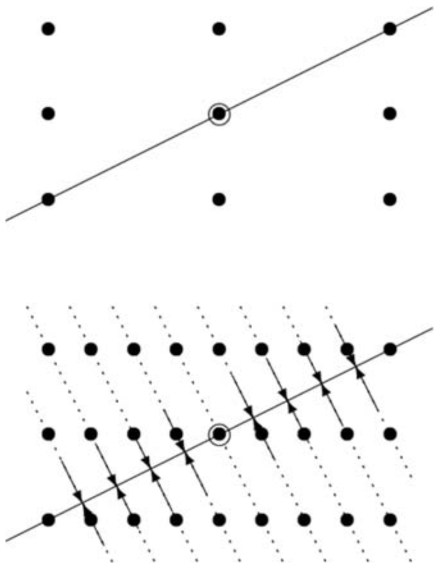

Figure 1.4.5.1
Duality between section and projection.

(i) If a symmetry operation of the slice maps its upper side to the upper side, a vector normal to the slice is fixed.
(ii) If a symmetry operation of the slice maps the upper side to the lower side, a vector normal to the slice is mapped to its opposite and the slice is turned upside down.

Therefore, the symmetries of two-dimensional rational sections are described by *layer groups*, *i.e.* subgroups of space groups with a two-dimensional translation lattice. Layer groups are *subperiodic groups* and for their elaborate discussion we refer to Chapter 1.7 and *IT* E (2010).

Analogous to two-dimensional sections of a crystal pattern, one can also consider the penetration of crystal patterns by a straight line, which is the idealization of a one-dimensional section taking out a rod of the crystal pattern. If the penetration line is along the direction of a translational symmetry of the crystal pattern, the rod has one-dimensional translational symmetry and its group of symmetries is a *rod group*, *i.e.* a subgroup of a space group with a one-dimensional translation lattice. Rod groups are also subperiodic groups, *cf. IT* E for their detailed treatment and listing.

A projection along a direction **d** into a plane maps a point of a crystal pattern to the intersection of the plane with the line along **d** through the point. If the projection direction is not along a rational lattice direction, the projection of the crystal pattern will contain points with arbitrarily small distances and additional restrictions are required to obtain a discrete pattern (*e.g.* the cut-and-project method used in the context of quasicrystals). We avoid any such complication by assuming that **d** is along a rational lattice direction. Furthermore, one is usually only interested in *orthogonal* projections in which the projection direction is perpendicular to the projection plane. This has the effect that spheres in three-dimensional space are mapped to circles in the projection plane.

Although it is also possible to regard the projection plane as a two-sided plane by taking into account from which side of the plane a point is projected into it, this is usually not done. Therefore, the symmetries of projections are described by ordinary plane groups.

Sections and projections are related by the *projection–slice theorem* (Bracewell, 2003) of Fourier theory: A section in reciprocal space containing the origin (the so-called zero layer) corresponds to a projection in direct space and *vice versa*. The projection direction in the one space is normal to the slice in the other space. This correspondence is illustrated schematically in Fig. 1.4.5.1. The top part shows a rectangular lattice with $b/a = 2$ and a slice along the line defined by $2x + y = 0$. Normalizing $a = 1$, the distance between two neighbouring lattice points in the slice is $\sqrt{5}$. If the pattern is restricted to this slice, the points of the corresponding diffraction pattern in reciprocal space must have distance $1/\sqrt{5}$ and this is precisely obtained by projecting the lattice points of the reciprocal lattice onto the slice.

The different, but related, viewpoints of sections and projections can be stated in a simple way as follows: For a section perpendicular to the c axis, only those points of a crystal pattern are considered which have z coordinate equal to a fixed value z_0 or in a small interval around z_0. For a projection along the c axis, all points of the crystal pattern are considered, but their z coordinate is simply ignored. This means that all points of the crystal pattern that differ only by their z coordinate are regarded as the same point.

1.4.5.2. Sections

For a space group $\mathcal{G}$ and a point X in the three-dimensional point space $\mathbb{E}^3$, the site-symmetry group of X is the subgroup of operations of $\mathcal{G}$ that fix X. Analogously, one can also look at the subgroup of operations fixing a one-dimensional line or a two-dimensional plane. If the line is along a rational direction, it will be fixed at least by the translations of $\mathcal{G}$ along that direction. However, it may also be fixed by a symmetry operation that reverses the direction of the line. The resulting subgroup of $\mathcal{G}$ that fixes the line is a *rod group*.

Similarly, a plane having a normal vector along a rational direction is fixed by translations of $\mathcal{G}$ corresponding to a two-dimensional lattice. Again, the plane may also be fixed by additional symmetry operations, *e.g.* by a twofold rotation around an axis lying in the plane, by a rotation around an axis normal to the plane or by a reflection in the plane.

Definition

A *rational planar section* of a crystal pattern is the intersection of the crystal pattern with a plane containing two linearly independent translation vectors of the crystal pattern. The intersecting plane is called the *section plane*.

A *rational linear section* of a crystal pattern is the intersection of the crystal pattern with a line containing a translation vector of the crystal pattern. The intersecting line is called the *penetration line*.

A planar section is determined by a vector **d** which is perpendicular to the section plane and a continuous parameter s, called the *height*, which gives the position of the plane on the line along **d**.

A linear section is specified by a vector **d** parallel to the penetration line and a point in a plane perpendicular to **d** giving the intersection of the line with that plane.

Definition

(i) The symmetry group of a planar section of a crystal pattern is the subgroup of the space group $\mathcal{G}$ of the crystal pattern that leaves the section plane invariant as a whole.

If the section is a rational section, this symmetry group is a *layer group*, *i.e.* a subgroup of a space group which contains translations only in a two-dimensional plane.

references