normalizer, because it precisely interchanges the twofold rotations around axes parallel to the *a* and to the *b* axes. The translation $t(0, \frac{1}{2}, 0)$ maps X_1 to X_2, and hence X_1 and X_2 have site-symmetry groups which are conjugate under the affine normalizer of $\mathcal{G}$ and thus belong to the same Wyckoff set. Analogously, Y_1 and Y_2 belong to the same Wyckoff set, because $t(\frac{1}{2}, 0, 0)$ maps Y_1 to Y_2. Finally, the operation $\{m_{1\bar{1}0}|0, 0, \frac{1}{4}\}$ found in the affine normalizer maps X_1 to Y_1. This shows that the points of all four Wyckoff positions actually belong to the same Wyckoff set.

Geometrically, the positions in this Wyckoff set can be described as those points that lie on a twofold rotation axis.

The assignments of Wyckoff positions of plane and space groups to Wyckoff sets are discussed and tabulated in Chapter 3.4.

Remark: The previous example deserves some further discussion. The group $\mathcal{G}$ of type $P222_1$ belongs to the orthorhombic crystal family, and the conventional unit cell is spanned by three basis vectors **a**, **b**, **c** with lengths *a*, *b*, *c* and right angles between each pair of basis vectors. Unless the parameters *a* and *b* are equal because of some metric specialization, the operation $\{m_{1\bar{1}0}|0, 0, \frac{1}{4}\}$ of the affine normalizer is not an isometry but changes lengths. If it is desired that the metric properties are preserved, the full affine normalizer cannot be taken into account, but only the subgroup that consists of isometries. This subgroup is called the *Euclidean normalizer* of $\mathcal{G}$. (A detailed discussion of Euclidean normalizers of space groups and their tabulation are given in Chapter 3.5.)

Taking conjugacy of the site-symmetry groups under the Euclidean normalizer as a condition results in a notion of equivalence which lies between that of Wyckoff positions and Wyckoff sets. In the above example, the four Wyckoff positions would be merged into two classes represented by X_1 and Y_1, but X_1 and Y_1 would not be regarded as equivalent, since they are not related by an operation of the Euclidean normalizer.

It turns out, however, that in many cases this intermediate classification coincides with the Wyckoff sets, because points belonging to different Wyckoff positions are often related to each other by a translation contained in the affine normalizer. Since translations are always isometries, the translations contained in the affine normalizer always belong to the Euclidean normalizer as well.

1.4.4.4. Eigensymmetry groups and non-characteristic orbits

A crystallographic orbit $\mathcal{O}$ has been defined as the set of points $g(X)$ obtained by applying all operations of some space group $\mathcal{G}$ to a point $X \in \mathbb{E}^3$. From that it is clear that the set $\mathcal{O}$ is invariant as a whole under the action of operations in $\mathcal{G}$, since for some point $Y = g(X)$ in the orbit and $h \in \mathcal{G}$ one has $h(Y) = (hg)(X)$, which is again contained in $\mathcal{O}$ because hg belongs to $\mathcal{G}$. However, it is possible that the orbit $\mathcal{O}$ is also invariant under some isometries of $\mathbb{E}^3$ that are not contained in $\mathcal{G}$. Since the composition of two such isometries still keeps the orbit invariant, the set of all isometries leaving $\mathcal{O}$ invariant forms a group which contains $\mathcal{G}$ as a subgroup.

Definition

Let $\mathcal{O} = \{g(X)|g \in \mathcal{G}\}$ be the orbit of a point $X \in \mathbb{E}^3$ under a space group $\mathcal{G}$. Then the group $\mathscr{E}$ of isometries of $\mathbb{E}^3$ which leave $\mathcal{O}$ invariant as a whole is called the *eigensymmetry group* of $\mathcal{O}$.

Since the orbit is a discrete set, the eigensymmetry group has to be a space group itself. One distinguishes the following cases:

(i) The eigensymmetry group $\mathscr{E}$ equals the group $\mathcal{G}$ by which the orbit was generated. In this case the orbit is called a *characteristic orbit* of $\mathcal{G}$.

(ii) The eigensymmetry group $\mathscr{E}$ contains $\mathcal{G}$ as a proper subgroup. Then the orbit is called a *non-characteristic orbit*.

(iii) If the eigensymmetry group $\mathscr{E}$ contains translations that are not contained in $\mathcal{G}$, *i.e.* if $\mathcal{T}_\mathcal{G}$ is a proper subgroup of $\mathcal{T}_\mathscr{E}$, the orbit is called an *extraordinary orbit*. Of course, extraordinary orbits are a special kind of non-characteristic orbits.

Non-characteristic orbits are closely related to the concept of *lattice complexes*, which are discussed in Chapter 3.4. An extensive listing of non-characteristic orbits of space groups can be found in Engel *et al.* (1984).

The fact that an orbit of a space group has a larger eigensymmetry group is an important example of a pair of groups that are in a group–subgroup relation. Knowledge of subgroups and supergroups of a given space group play a crucial role in the analysis of phase transitions, for example, and are discussed in detail in Chapter 1.7.

The occurrence of non-characteristic orbits does not require the point *X* to be chosen at a special position. Even the general position of a space group $\mathcal{G}$ may give rise to a non-characteristic orbit. Moreover, special values of the coordinates of the general position may give rise to additional eigensymmetries without the position becoming a special position. Conversely, the orbit of a point at a special position need not be non-characteristic.

Example

We compare space groups of types $P4_1$ (76) and $P4_2$ (77). For a space group of type $P4_1$, the general position with generic coordinates x, y, z gives rise to a characteristic orbit, whereas the general-position orbit for a space group of type $P4_2$ consists of the points $X_1 = \begin{pmatrix} x \\ y \\ z \end{pmatrix}$, $X_2 = \begin{pmatrix} \overline{x} \\ \overline{y} \\ z \end{pmatrix}$, $X_3 = \begin{pmatrix} \overline{y} \\ x \\ z + \frac{1}{2} \end{pmatrix}$ and $X_4 = \begin{pmatrix} y \\ \overline{x} \\ z + \frac{1}{2} \end{pmatrix}$. An inversion $\{\overline{1}|0, 0, 2z\}$ in 0, 0, *z* interchanges X_1 and X_2, and maps X_3 to $y, \overline{x}, z - \frac{1}{2}$, which is clearly equivalent to X_4 under a translation. This shows that the general-position orbit for a space group of type $P4_2$ is a non-characteristic orbit, and the eigensymmetry group of this orbit is of type $P4_2/m$ (84), where the origin has to be shifted to the inversion point 0, 0, *z* to obtain the conventional setting. Since the unit cell and the orbit are unchanged, but the point group of $P4_2$ is a subgroup of index 2 in the point group of $P4_2/m$, the orbit points must belong to a special position for $P4_2/m$, namely the position labelled 4*j*. In the conventional setting of $P4_2/m$, a point belonging to this Wyckoff position is given by *x*, *y*, 0 and one finds that the orbit of this point in special position is characteristic, *i.e.* its eigensymmetry group is just $P4_2/m$.

If we assume that the metric of the space group is not special, the eigensymmetry group is restricted to the same crystal family (for the definition of 'specialized' metrics, *cf.* Section 1.3.4.3 and Chapter 3.5). Therefore, a space group $\mathcal{G}$ for which the point group is a holohedry can only have non-characteristic orbits by additional translations, *i.e.* extraordinary orbits. However, if we allow specialized metrics, the eigensymmetry group may belong to a higher crystal family. For example, if a space group belongs to the orthorhombic family, but the unit cell has equal parameters

$a = b$, 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 $2i$–$2l$, $4w$–$4z$, 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 $2e$) and $x, \frac{1}{2}, z$ (Wyckoff position $2f$) 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 $4p$) 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 $4p$ 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

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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:

references