

1. INTRODUCTION TO SPACE-GROUP SYMMETRY

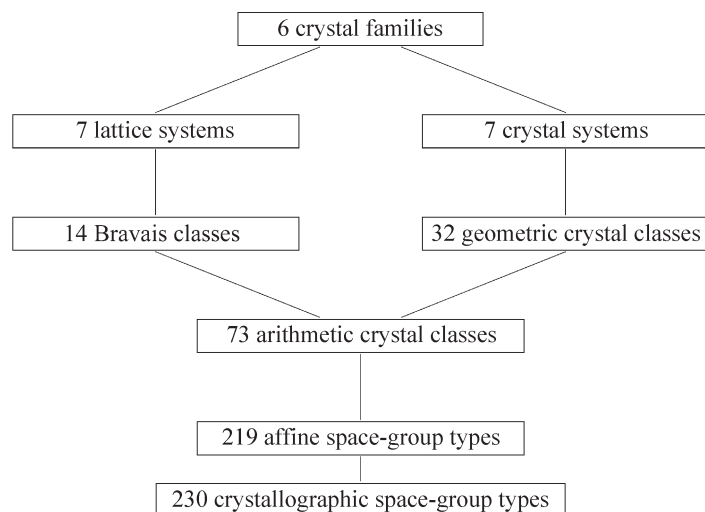


Figure 1.3.4.1
Classification levels for three-dimensional space groups.

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 (\mathbf{P}, \mathbf{p}) such that

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

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 $Pb2n$, which is a non-conventional setting for $Pnc2$ (30). In the conventional setting, the coset representatives of $Pnc2$ 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: $a_C = 3.5668 \text{ \AA}$ for carbon, $a_{Si} = 5.4310 \text{ \AA}$ for silicon and $a_{Ge} = 5.6579 \text{ \AA}$ 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

$$a_{Si}/a_C \cdot \mathbf{I}_3 \approx \begin{pmatrix} 1.523 & 0 & 0 \\ 0 & 1.523 & 0 \\ 0 & 0 & 1.523 \end{pmatrix}.$$

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 $P2$, 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 (\mathbf{P}, \mathbf{p}) with $\det \mathbf{P} > 0$. 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