1.5. Crystallographic viewpoints in the classification of space-group representations

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1.5.1. List of abbreviations and symbols

BC	Bradley & Cracknell (1972)
CDML	Cracknell, Davies, Miller & Love (1979)
IT A	*International Tables for Crystallography*, Volume A (2005)
irreps	Irreducible representations
$\mathbf{L}$; $\mathbf{L}^*$	Vector lattice of a space group $\mathcal{G}$; reciprocal lattice of $\mathcal{G}$
$\mathbf{t}$	Vector of the lattice $\mathbf{L}$ of $\mathcal{G}$
$\mathbf{k}$	Vector of the reciprocal space
$\mathbf{K}$	Vector of the reciprocal lattice $\mathbf{L}^*$ [see Note (1)]
$\mathbf{a}, \mathbf{b}, \mathbf{c}$; $\mathbf{a}^*, \mathbf{b}^*, \mathbf{c}^*$	Basis vectors of the crystal lattice; basis vectors of the reciprocal lattice
$(\mathbf{a})^T$	Row of basis vectors [see Note (2)]
$(\mathbf{a}^*)$	Column of basis vectors of the reciprocal lattice $\mathbf{L}^*$
X	Point of point space
x, y, z; k_x, k_y, k_z	Point coordinates; vector coefficients
$\boldsymbol{x}$; $\boldsymbol{r}$	Column of point coordinates; column of vector coefficients
$(\boldsymbol{k})^T$	Row of coefficients of a reciprocal-space vector [see Note (2)]
a, b, c	Lengths of the basis vectors of the lattice
α, β, γ	Parameters of $\mathbf{k}$-vector coefficients in CDML
a^*, b^*, c^*	Lengths of the basis vectors of the reciprocal lattice
$\boldsymbol{M}, \boldsymbol{R}, \boldsymbol{D}, \boldsymbol{S}$	Matrices
$\boldsymbol{W}$	Matrix part of a mapping
$\boldsymbol{w}$	Column part of a mapping
$(\boldsymbol{A}, \boldsymbol{a})$, $(\boldsymbol{W}, \boldsymbol{w})$	Matrix–column pairs
$\mathcal{G}$; $\mathcal{G}_0$; $(\mathcal{G})^*$	Group or space group; symmorphic space group; reciprocal-space group
$\mathcal{T}$	Translation subgroup of $\mathcal{G}$
$\mathcal{P}$ or $\overline{\mathcal{G}}$; $\mathcal{Q}$	Point group; holohedral point group
$\mathcal{S}$	Site-symmetry group
$\overline{\mathcal{G}}^{\mathbf{k}}$; $\mathcal{L}^{\mathbf{k}}$	Little co-group of $\mathbf{k}$; little group of $\mathbf{k}$
g, h, e	Group elements of $\mathcal{G}$
2, 3, m	Symmetry operations
$\Gamma(\mathcal{G})$	(Matrix) representation of the group $\mathcal{G}$

Notes: (1) In crystallography, vectors are designated by lower-case bold-face letters. With $\mathbf{K}$ we make an exception in order to follow the tradition of physics. A crystallographic alternative could be $\mathbf{t}^*$. (2) In crystallography, point coordinates or vector coefficients are written as columns. Therefore, columns are taken as 'normal'. In order to distinguish rows from columns (the coefficients k_i of vectors in reciprocal space, *i.e.* the Miller indices, and the basis of the crystal lattice are written as rows), rows are regarded as transposed columns and are thus marked by $(\ldots)^T$.

1.5.2. Introduction

This chapter on representations widens the scope of the general topics of reciprocal space treated in this volume.

Space-group representations play a growing role in physical applications of crystal symmetry. They are treated in a number of papers and books but comparison of the terms and the listed data is difficult. The main reason for this is the lack of standards in the classification and nomenclature of representations. As a result, the reader is confronted with barely comparable notations used by the different authors, see *e.g.* Stokes & Hatch (1988), Table 7.

The $\mathbf{k}$ vectors, which can be described as vectors in reciprocal space, play a decisive role in the description and classification of space-group representations. Their symmetry properties are determined by the so-called *reciprocal-space group* $(\mathcal{G})^*$ which is always isomorphic to a symmorphic space group $\mathcal{G}_0$. The different symmetries of $\mathbf{k}$ vectors correspond to the different kinds of point orbits in the symmorphic space groups $\mathcal{G}_0$. The classification of point orbits into Wyckoff positions in *International Tables for Crystallography* Volume A (*IT* A) (2005) can be used directly to classify the irreducible representations of a space group, abbreviated *irreps*; the Wyckoff positions of the symmorphic space groups $\mathcal{G}_0$ form a basis for a *natural* classification of the irreps. This was first discovered by Wintgen (1941). Similar results have been obtained independently by Raghavacharyulu (1961), who introduced the term reciprocal-space group. In this chapter a classification of irreps is provided which is based on Wintgen's idea.

Although this idea is now more than 60 years old, it has been utilized only rarely and has not yet found proper recognition in the literature and in the existing tables of space-group irreps. Slater (1962) described the correspondence between the special $\mathbf{k}$ vectors of the Brillouin zone and the Wyckoff positions of space group $Pm\overline{3}m$. Similarly, Jan (1972) compared Wyckoff positions with points of the Brillouin zone when describing the symmetry $Pm\overline{3}$ of the Fermi surface for the pyrite structure. However, the widespread tables of Miller & Love (1967), Zak *et al.* (1969), Bradley & Cracknell (1972) (abbreviated as BC), Cracknell *et al.* (1979) (abbreviated as CDML), and Kovalev (1986) have not made use of this kind of classification and its possibilities, and existing tables are unnecessarily complicated, *cf.* Boyle (1986).

In addition, historical reasons have obscured the classification of irreps and impeded their application. The first considerations of irreps dealt only with space groups of translation lattices (Bouckaert *et al.*, 1936). Later, other space groups were taken into consideration as well. Instead of treating these (lower) symmetries as such, their irreps were derived and classified by starting from the irreps of lattice space groups and proceeding to those of lower symmetry. This procedure has two consequences:

(1) those $\mathbf{k}$ vectors that are special in a lattice space group are also correspondingly listed in the low-symmetry space group even if they have lost their special properties due to the symmetry reduction;

(2) during the symmetry reduction unnecessary new symbols of $\mathbf{k}$ vectors are introduced.

The use of the reciprocal-space group $(\mathcal{G})^*$ avoids both these detours.

The relations between the special $\mathbf{k}$ vectors as listed by CDML and the Wyckoff positions of the space groups of *IT* A have been derived and displayed in figures and tables for a few space groups by Aroyo & Wondratschek (1995). The $\mathbf{k}$-vector classification scheme based on Wintgen's (1941) reciprocal-space group approach has been applied meanwhile to all space groups. The compilation of Brillouin-zone figures and $\mathbf{k}$-vector correlation tables for the 230 space groups constitutes the wavevector database of the Bilbao Crystallographic Server (1998), a website of crystallographic databases and programs that can be used free