International Tables for Crystallography (2006). Vol. B, Section 1.5.2, p. 162.

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

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1.5.1. List of symbols

$\mathcal{G}$; $\mathcal{S}$	Group, especially space group; site-symmetry group
G	Element of group $\mathcal{G}$
$\mathcal{G}_0$	Symmorphic space group
$\mathcal{P}$ or $\bar{\mathcal{G}}$	Point group of space group $\mathcal{G}$
$\mathcal{T}$	Translation subgroup of space group $\mathcal{G}$
$\boldsymbol{R}, \boldsymbol{S}$; $\boldsymbol{W}$	Matrix; matrix part of a symmetry operation
$\boldsymbol{w}$	Column part of a symmetry operation
X	Point of point space
x, y, z; x_i	Coordinates of a point or coefficients of a vector
$\boldsymbol{x}$	Column of point coordinates or of vector coefficients
$\mathbf{L}$	Vector lattice of the space group $\mathcal{G}$
$\mathbf{a}, \mathbf{b}, \mathbf{c}$ or $(\mathbf{a}_k)^T$	Basis vectors or row of basis vectors of the lattice $\mathbf{L}$ of $\mathcal{G}$
$\mathbf{t}$	Vector of the lattice $\mathbf{L}$ of $\mathcal{G}$
$\mathbf{L}^*$	Reciprocal lattice of the space group $\mathcal{G}$
$\mathbf{a}^*, \mathbf{b}^*, \mathbf{c}^*$ or $(\mathbf{a}_k^*)$	Basis vectors or column of basis vectors of the reciprocal lattice $\mathbf{L}^*$
$\mathbf{K}$	Vector of the reciprocal lattice $\mathbf{L}^*$
$\mathbf{k}$	Vector of reciprocal space
$\mathcal{G}^*$	Reciprocal-space group
$\bar{\mathcal{G}}^{\mathbf{k}}$	Little co-group of $\mathbf{k}$
$\mathcal{L}^{\mathbf{k}}$	Little group of $\mathbf{k}$
$\Gamma(\mathcal{G})$	(Matrix) representation of $\mathcal{G}$

1.5.2. Introduction

This new 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 different numbers of types and 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 symmetry types 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) (1995) 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 50 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 $Pm\bar{3}m$. Similarly, Jan (1972) compared Wyckoff positions with points of the Brillouin zone when describing the symmetry $Pm\bar{3}$ 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 the 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 types of $\mathbf{k}$ vectors and symbols for them are introduced.

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

In this chapter we consider in more detail the reciprocal-space-group approach and show that widely used crystallographic conventions can be adopted for the classification of space-group representations. Some basic concepts are developed in Section 1.5.3. Possible conventions are discussed in Section 1.5.4. The consequences and advantages of this approach are demonstrated and discussed using examples in Section 1.5.5.

1.5.3. Basic concepts

The aim of this section is to give a brief overview of some of the basic concepts related to groups and their representations. Its content should be of some help to readers who wish to refresh their knowledge of space groups and representations, and to familiarize themselves with the kind of description in this chapter. However, it can not serve as an introductory text for these subjects. The interested reader is referred to books dealing with space-group theory, representations of space groups and their applications in solid-state physics: see Bradley & Cracknell (1972) or the forthcoming Chapter 1.2 of *IT* D (*Physical properties of crystals*) by Janssen (2001).

1.5.3.1. *Representations of finite groups*

Group theory is the proper tool for studying symmetry in science. The elements of the crystallographic groups are rigid motions (isometries) with regard to performing one after another. The set of all isometries that map an object onto itself always fulfils the group postulates and is called the symmetry or the symmetry group of that object; the isometry itself is called a symmetry operation. Symmetry groups of crystals are dealt with in this chapter. In addition, groups of matrices with regard to matrix multiplication (matrix groups) are considered frequently. Such groups will sometimes be called realizations or representations of abstract groups.

Many applications of group theory to physical problems are closely related to representation theory, *cf.* Rosen (1981) and

references