

3. ADVANCED TOPICS ON SPACE-GROUP SYMMETRY

Engel *et al.* (1984) enumerated for all space-group types those non-characteristic orbits that refer to special coordinates, but they excluded all further ones that are based on specialized metrical parameters of the generating space groups or on the simultaneous specialization of metrical and coordinate parameters. A computer program which enables the determination of non-characteristic orbits is now available (*NONCHAR* on the Bilbao Crystallographic Server at <http://www.cryst.ehu.es>). Lawrenson & Wondratschek (1976) listed the extraordinary orbits of the plane groups, and Matsumoto & Wondratschek (1987) listed the non-characteristic orbits of the plane groups.

The special, but not exceptional, case in which a non-characteristic orbit is produced only if both the coordinates and metric are specialized deserves extra concern. The crystallographic orbits from $R\bar{3}6f$ x, y, z with $x = \frac{1}{4}, y = 0, z = \frac{1}{2}$ or $x = \frac{1}{4}, y = \frac{1}{2}, z = 0$ and with the rhombohedral angle $\alpha = 90^\circ$ may be used as an example. The eigensymmetry of the corresponding point configurations is $Pm\bar{3}n6c, d$ (corresponding to the position of the Cr atoms in the crystal structure of Cr_3Si). Accordingly, the lattice complex $R\bar{3}f$ comprises $Pm\bar{3}n c$ as limiting complex. $Pm\bar{3}n c$ shows special integral reflection conditions ($hkl: h + k + l = 2n$ or $h = 2n + 1, k = 4n, l = 4n + 2; h, k, l$ permutable), which of course hold for all orbits of that type, *i.e.* also for the special orbits from $R\bar{3}f$ described above. As geometrical structure factors are independent of metrical parameters, these reflection conditions are even valid for crystallographic orbits from $R\bar{3}f$ with $a \neq 90^\circ$ if the coordinates are restricted to $\frac{1}{4}, 0, \frac{1}{2}$ or to $\frac{1}{4}, \frac{1}{2}, 0$.

In general, the following statement holds: if a lattice complex causes special reflection conditions then exactly these conditions are also valid for any crystallographic orbit that refers to a comprehensive complex of that lattice complex if, in addition, this crystallographic orbit may be described by the same coordinate triplets as an orbit of the lattice complex under consideration.

3.4.3. Descriptive lattice-complex symbols and the assignment of Wyckoff positions to lattice complexes

3.4.3.1. Descriptive symbols

3.4.3.1.1. Introduction

For the study of relations between crystal structures, lattice-complex symbols are desirable that show as many relations between point configurations as possible. To this end, Hermann (1960) derived descriptive lattice-complex symbols that were further developed by Donnay *et al.* (1966) and completed by Fischer *et al.* (1973). These symbols describe the arrangements of the points in the point configurations and refer directly to the coordinate descriptions of the Wyckoff positions. Since a lattice complex, in general, contains Wyckoff positions with different coordinate descriptions, it may be represented by several different descriptive symbols. The symbols are further affected by the settings of the space group. The present section is restricted to the fundamental features of the descriptive symbols. Details have been described by Fischer *et al.* (1973). Tables 3.4.3.2 and 3.4.3.3 give for each Wyckoff position of a plane group or a space group, respectively, the multiplicity, the Wyckoff letter, the oriented site symmetry, the reference symbol of the corresponding lattice complex and the descriptive symbol.⁴ The comparatively short

⁴ Some of the descriptive symbols listed in Table 3.4.3.3 differ slightly from those derived by Fischer *et al.* (1973) and used in editions of *International Tables for Crystallography* Volume A before 2002.

Table 3.4.3.1

Descriptive symbols of invariant lattice complexes in their characteristic Wyckoff position

Descriptive symbol	Crystal family	Characteristic Wyckoff position
<i>C</i>	<i>o</i> <i>m</i>	$Cmmm a$ $C2/m a$
<i>D</i>	<i>c</i> <i>o</i>	$Fd\bar{3}m a$ $Fddd a$
vD	<i>t</i>	$I4_1/amd a$
<i>E</i>	<i>h</i>	$P6_3/mmc c$
<i>F</i>	<i>c</i> <i>o</i>	$Fm\bar{3}m a$ $Fmmm a$
<i>G</i>	<i>h</i>	$P6/mmm c$
<i>I</i>	<i>c</i> <i>t</i> <i>o</i>	$Im\bar{3}m a$ $I4/mmm a$ $Immm a$
<i>J</i>	<i>c</i>	$Pm\bar{3}m c$
<i>J*</i>	<i>c</i>	$Im\bar{3}m b$
<i>M</i>	<i>h</i>	$R\bar{3}m e$
<i>N</i>	<i>h</i>	$P6/mmm f$
<i>P</i>	<i>c</i> <i>h</i> <i>t</i> <i>o</i> <i>m</i> <i>a</i>	$Pm\bar{3}m a$ $P6/mmm a$ $P4/mmm a$ $Pmmm a$ $P2/m a$ $P\bar{1} a$
${}^+Q$	<i>h</i>	$P6_222 c$
<i>R</i>	<i>h</i>	$R\bar{3}m a$
<i>S</i>	<i>c</i>	$I\bar{4}3d a$
<i>S*</i>	<i>c</i>	$Ia\bar{3}d d$
<i>T</i>	<i>c</i> <i>o</i>	$Fd\bar{3}m c$ $Fddd c$
vT	<i>t</i>	$I4_1/amd c$
${}^+V$	<i>c</i>	$I4_132 c$
<i>V*</i>	<i>c</i>	$Ia\bar{3}d c$
<i>W</i>	<i>c</i>	$Pm\bar{3}n c$
<i>W*</i>	<i>c</i>	$Im\bar{3}m d$
${}^+Y$	<i>c</i>	$P4_332 a$
${}^+Y^*$	<i>c</i>	$I4_132 a$
<i>Y**</i>	<i>c</i>	$Ia\bar{3}d b$

descriptive symbols condense complicated verbal descriptions of the point configurations of lattice complexes.

3.4.3.1.2. Invariant lattice complexes

An invariant lattice complex in its characteristic Wyckoff position is represented by a capital letter (sometimes in combination with a superscript). The first column of Table 3.4.3.1 gives a complete list of these symbols in alphabetical order. The characteristic Wyckoff positions are shown in column 3. Lattice complexes from different crystal families but with the same coordinate description for their characteristic Wyckoff positions receive the same descriptive symbol. If necessary, the crystal family may be stated explicitly by a small letter (column 2) preceding the lattice-complex symbol: *c* cubic, *t* tetragonal, *h* hexagonal, *o* orthorhombic, *m* monoclinic, *a* anorthic (triclinic).