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Example

Laue class: $12/m1$

Reflection conditions:

$$hkl : h + k = 2n;$$
$$h0l : h, l = 2n; \quad 0kl : k = 2n; \quad hk0 : h + k = 2n;$$
$$h00 : h = 2n; \quad 0k0 : k = 2n; \quad 00l : l = 2n.$$

As there are both c and n glide planes perpendicular to b, the diffraction symbol may be given as $1\,2/m\,1C1c1$ or as $1\,2/m\,1C1n1$. In analogy to the symbols of the possible space groups, $C1c1$ (9) and $C1\,2/c\,1$ (15), the diffraction symbol is called $1\,2/m\,1C1c1$.

For another cell choice, the reflection conditions are:

$$hkl : k + l = 2n;$$
$$h0l : h, l = 2n; \quad 0kl : k + l = 2n; \quad hk0 : k = 2n;$$
$$h00 : h = 2n; \quad 0k0 : k = 2n; \quad 00l : l = 2n.$$

For this second cell choice, the glide planes perpendicular to b are n and a. The diffraction symbol is given as $1\,2/m\,1A1n1$, in analogy to the symbols $A1n1$ (9) and $A1\,2/n\,1$ (15) adopted for the possible space groups.

3.1.4. Deduction of possible space groups

Reflection conditions, diffraction symbols, and possible space groups are listed in Table 3.1.4.1. For each crystal system, a different table is provided. The monoclinic system contains different entries for the settings with b, c and a unique. For monoclinic and orthorhombic crystals, all possible settings and cell choices are treated. In contradistinction to Table 4.3.2.1, which lists the space-group symbols for different settings and cell choices in a systematic way, the present table is designed with the aim to make space-group determination as easy as possible.

The left-hand side of the table contains the *Reflection conditions*. Conditions of the type $h = 2n$ or $h + k = 2n$ are abbreviated as h or $h + k$. Conditions like $h = 2n, k = 2n, h + k = 2n$ are quoted as h, k; in this case, the condition $h + k = 2n$ is not listed as it follows directly from $h = 2n, k = 2n$. Conditions with $l = 3n$, $l = 4n$, $l = 6n$ or more complicated expressions are listed explicitly.

From *left* to *right*, the table contains the integral, zonal and serial conditions. From *top* to *bottom*, the entries are ordered such that left columns are kept empty as long as possible. The leftmost column that contains an entry is considered as the 'leading column'. In this column, entries are listed according to increasing complexity. This also holds for the subsequent columns within the restrictions imposed by previous columns on the left. The make-up of the table is such that observed reflection conditions should be matched against the table by considering, within each crystal system, the columns from left to right.

The centre column contains the *Extinction symbol*. To obtain the complete diffraction symbol, the Laue-class symbol has to be added in front of it. Be sure that the correct Laue-class symbol is used if the crystal system contains two Laue classes. Particular care is needed for Laue class $\bar{3}m$ in the trigonal system, because there are two possible orientations of this Laue symmetry with respect to the crystal lattice, $\bar{3}m1$ and $\bar{3}1m$. The correct orientation can be obtained directly from the diffraction record.

The right-hand side of the table gives the *Possible space groups* which obey the reflection conditions. For crystal systems with two Laue classes, a subdivision is made according to the Laue symmetry. The entries in each Laue class are ordered according to their point groups. All space groups that match both the reflection conditions and the Laue symmetry, found in a diffraction experiment, are possible space groups of the crystal.

The space groups are given by their short Hermann–Mauguin symbols, followed by their number between parentheses, except for the monoclinic system, where full symbols are given (*cf.* Section 2.2.4). In the monoclinic and orthorhombic sections of Table 3.1.4.1, which contain entries for the different settings and cell choices, the 'standard' space-group symbols (*cf.* Table 4.3.2.1) are printed in bold face. Only these standard representations are treated in full in the space-group tables.

Example

The diffraction pattern of a compound has Laue class mmm. The crystal system is thus orthorhombic. The diffraction spots are indexed such that the reflection conditions are $0kl : l = 2n$; $h0l : h + l = 2n$; $h00 : h = 2n$; $00l : l = 2n$. Table 3.1.4.1 shows that the diffraction symbol is $mmmPcn$–. Possible space groups are $Pcn2$ (30) and $Pcnm$ (53). For neither space group does the axial choice correspond to that of the standard setting. For No. 30, the standard symbol is $Pnc2$, for No. 53 it is $Pmna$. The transformation from the basis vectors $\mathbf{a}_e, \mathbf{b}_e, \mathbf{c}_e$, used in the experiment, to the basis vectors $\mathbf{a}_s, \mathbf{b}_s, \mathbf{c}_s$ of the standard setting is given by $\mathbf{a}_s = \mathbf{b}_e, \mathbf{b}_s = -\mathbf{a}_e$ for No. 30 and by $\mathbf{a}_s = \mathbf{c}_e, \mathbf{c}_s = -\mathbf{a}_e$ for No. 53.

Possible pitfalls

Errors in the space-group determination may occur because of several reasons.

(1) *Twinning of the crystal*

Difficulties that may be encountered are shown by the following example. Say that a monoclinic crystal (b unique) with the angle β fortuitously equal to $\sim 90°$ is twinned according to (100). As this causes overlap of the reflections hkl and $\bar{h}kl$, the observed Laue symmetry is mmm rather than $2/m$. The same effect may occur within one crystal system. If, for instance, a crystal with Laue class $4/m$ is twinned according to (100) or (110), the Laue class $4/mmm$ is simulated (twinning by merohedry, *cf.* Catti & Ferraris, 1976, and Koch, 1999). Further examples are given by Buerger (1960). Errors due to twinning can often be detected from the fact that the observed reflection conditions do not match any of the diffraction symbols.

(2) *Incorrect determination of reflection conditions*

Either too many or too few conditions may be found. For serial reflections, the first case may arise if the structure is such that its projection on, say, the b direction shows pseudo-periodicity. If the pseudo-axis is b/p, with p an integer, the reflections $0k0$ with $k \neq p$ are very weak. If the exposure time is not long enough, they may be classified as unobserved which, incorrectly, would lead to the reflection condition $0k0 : k = p$. A similar situation may arise for zonal conditions, although in this case there is less danger of errors. Many more reflections are involved and the occurrence of pseudo-periodicity is less likely for two-dimensional than for one-dimensional projections.

For 'structural' or non-space-group absences, see Section 2.2.13.

The second case, too many observed reflections, may be due to multiple diffraction or to radiation impurity. A textbook description of multiple diffraction has been given by Lipson & Cochran (1966). A well known case of radiation impurity in X-ray diffraction is the contamination of a copper target with iron. On a photograph taken with the radiation from such a target, the iron radiation with $\lambda(\mathrm{Fe}) \sim 5/4\lambda(\mathrm{Cu})$ gives a reflection spot $4h_l4k_l4l$ at the position $5h_l5k_l5l$ for copper $[\lambda(\mathrm{Cu}\ K\bar{\alpha}) = 1.5418\ \text{Å}, \lambda(\mathrm{Fe}\ K\bar{\alpha}) = 1.9373\ \text{Å}]$. For reflections $0k0$, for instance, this may give rise to reflected intensity at the copper 050 position so that, incorrectly, the condition $0k0 : k = 2n$ may be excluded.

Table 3.1.4.1. *Reflection conditions, diffraction symbols and possible space groups*

TRICLINIC. Laue class $\bar{1}$

Reflection conditions	Extinction symbol	Point group	
		1	$\bar{1}$
None	P–	$P1(1)$	$P\bar{1}$ (2)

MONOCLINIC, Laue class $2/m$

Unique axis b				Laue class $1\ 2/m\ 1$		
Reflection conditions				Point group		
hkl $0kl$ $hk0$	$h0l$ $h00$ $00l$	$0k0$	Extinction symbol	2	m	$2/m$
			$P1{-}1$	**$P121$** (3)	**$P1m1$** (6)	**$P1\ 2/m\ 1$** (10)
		k	$P12_11$	**$P12_11$** (4)		**$P1\ 2_1/m\ 1$** (11)
	h		$P1a1$		$P1a1$ (7)	$P1\ 2/a\ 1$ (13)
	h	k	$P1\ 2_1/a\ 1$			$P1\ 2_1/a\ 1$ (14)
	l		$P1c1$		**$P1c1$** (7)	**$P1\ 2/c\ 1$** (13)
	l	k	$P1\ 2_1/c\ 1$			**$P1\ 2_1/c\ 1$** (14)
	$h+l$		$P1n1$		$P1n1$ (7)	$P1\ 2/n\ 1$ (13)
	$h+l$	k	$P1\ 2_1/n\ 1$			$P1\ 2_1/n\ 1$ (14)
$h+k$	h	k	$C1{-}1$	**$C121$** (5)	**$C1m1$** (8)	**$C1\ 2/m\ 1$** (12)
$h+k$	h, l	k	$C1c1$		**$C1c1$** (9)	**$C1\ 2/c\ 1$** (15)
$k+l$	l	k	$A1{-}1$	$A121$ (5)	$A1m1$ (8)	$A1\ 2/m\ 1$ (12)
$k+l$	h, l	k	$A1n1$		$A1n1$ (9)	$A1\ 2/n\ 1$ (15)
$h+k+l$	$h+l$	k	$I1{-}1$	$I121$ (5)	$I1m1$ (8)	$I1\ 2/m\ 1$ (12)
$h+k+l$	h, l	k	$I1a1$		$I1a1$ (9)	$I1\ 2/a\ 1$ (15)
Unique axis c				**Laue class $1\ 1\ 2/m$**		
Reflection conditions				Point group		
hkl $0kl$ $h0l$	$hk0$ $h00$ $0k0$	$00l$	Extinction symbol	2	m	$2/m$
			$P11{-}$	$P112$ (3)	$P11m$ (6)	$P11\ 2/m$ (10)
		l	$P112_1$	$P112_1$ (4)		$P11\ 2_1/m$ (11)
	h		$P11a$		$P11a$ (7)	$P11\ 2/a$ (13)
	h	l	$P11\ 2_1/a$			$P11\ 2_1/a$ (14)
	k		$P11b$		$P11b$ (7)	$P11\ 2/b$ (13)
	k	l	$P11\ 2_1/b$			$P11\ 2_1/b$ (14)
	$h+k$		$P11n$		$P11n$ (7)	$P11\ 2/n$ (13)
	$h+k$	l	$P11\ 2_1/n$			$P11\ 2_1/n$ (14)
$h+l$	h	l	$B11{-}$	$B112$ (5)	$B11m$ (8)	$B11\ 2/m$ (12)
$h+l$	h, k	l	$B11n$		$B11n$ (9)	$B11\ 2/n$ (15)
$k+l$	k	l	$A11{-}$	$A112$ (5)	$A11m$ (8)	$A11\ 2/m$ (12)
$k+l$	h, k	l	$A11a$		$A11a$ (9)	$A11\ 2/a$ (15)
$h+k+l$	$h+k$	l	$I11{-}$	$I112$ (5)	$I11m$ (8)	$I11\ 2/m$ (12)
$h+k+l$	h, k	l	$I11b$		$I11b$ (9)	$I11\ 2/b$ (15)

(3) *Incorrect assignment of the Laue symmetry*

This may be caused by pseudo-symmetry or by 'diffraction enhancement'. A crystal with pseudo-symmetry shows small deviations from a certain symmetry, and careful inspection of the diffraction pattern is necessary to determine the correct Laue class. In the case of diffraction enhancement, the symmetry of the diffraction pattern is higher than the Laue symmetry of the crystal. Structure types showing this phenomenon are rare and have to fulfil specified conditions. For further discussions and references, see Perez-Mato & Iglesias (1977).

3.1.5. Diffraction symbols and possible space groups

Table 3.1.4.1 contains 219 extinction symbols which, when combined with the Laue classes, lead to 242 different diffraction symbols. If, however, for the monoclinic and orthorhombic systems

references