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Effects of merohedric twinning on the diffraction pattern[1]

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In merohedric twinning, the lattices of the individuals are perfectly overlapped and the presence of twinning is not easily detected from the diffraction pattern, especially in the case of inversion twinning (class I). In general, the investigator has to consider three possible structural models: a crystal with space-group type H and point group P, either untwinned (**H model**) or twinned through an operation t in vector space (***t*-H model**), and an untwinned crystal with space group G whose point group P' is obtained as an extension of P through the twin operation t (**G model**). In 71 cases, consideration of the reflection conditions may directly rule out the **G** model; in seven other cases the reflection conditions suggest a space group which does not correspond to the extension of **H** by the twin operation and the structure solution or at least the refinement will fail. When the twin operation belongs to a different crystal family (class II*B* twinning: the crystal has a specialized metric), the *presence* of twinning can often be recognized by the peculiar effect it has on the reflection conditions.

1. Introduction

Twinning by merohedry (also known as merohedric[2] twinning) occurs when the twin operation t (the operation mapping the orientations of the individuals in a twin) is a symmetry operation for the lattice but not for the structure. The twin index is 1, meaning that the whole lattice is restored by the twin operation (for recent reviews, see Hahn & Klapper, 2003; Grimmer & Nespolo, 2006). This article presents a systematic derivation of the effects of twinning by merohedry on the diffraction pattern, in terms of the reflection conditions and diffraction symmetry.

Twinning is a point-group phenomenon, in the sense that t is an operation of a point group (in vector space) that produces a heterogeneous crystalline edifice not possessing a space group, but this edifice is built from homogeneous domains or individuals having the same chemical composition and the same structure but differing in their orientation in space (for details, see Nespolo *et al.*, 2004; Ferraris *et al.*, 2008). If the point groups of the individual are of type[3] P, and if P^* is the intersection group of the point groups of the individuals in their respective orientations, the twin operation t extends P^* (in the mathematical sense) to a chromatic point group $P_c' = \langle P^*,t\rangle$, where the chromatic nature comes precisely from t: P_c' contains both achromatic operations (symmetry operations for the individuals) and chromatic operations (operations mapping the orientations of the individuals) (for details, see Nespolo, 2004). In the case of twinning by merohedry, the lattices of the individuals are exactly overlapped and P_c' is an extension of P. The twin (chromatic) operations are obtained by forming the left coset tP; all these are equivalent under P. Alternatively, a right coset could be used as well. These operations constitute one twin law and any of them can be taken as the twin operation (coset representative). Let us take P' as the achromatic point group isomorphic to P_c': in the case of twinning by merohedry, it is always a supergroup of P. Hereafter, P' defined in this way is meant when the term 'symmetry of the twin' is used.

Twinning by merohedry has been classified into three classes (Nespolo & Ferraris, 2000).

Class I: the individual belongs to a non-centrosymmetric geometric crystal class and the twin operation belongs to the corresponding Laue class. In other words, the twin law (coset) contains the inversion and this can always be taken as the twin operation (coset representative).

Class II*A*: P' stays in the same crystal family as P but the twin operation does not belong to the Laue class of the indi-

[1] This article forms part of a special issue dedicated to mathematical crystallography, which will be published as a virtual special issue of the journal in 2014.
[2] Note that the expression 'merohedral twinning' which appears often in the literature is inappropriate: 'merohedral' indicates the symmetry of an individual, not that of a twin (see Catti & Ferraris, 1976).
[3] For details about the difference between point groups and point-group types, see Nespolo & Souvignier (2009).

vidual and thus the twin law does not contain the inversion. On inspection, the individual is seen to belong to one of the following 22 arithmetic crystal classes: $4P$, $4I$, $\bar{4}P$, $\bar{4}I$, $4/mP$, $4/mI$, $3R$, $3P$, $\bar{3}R$, $\bar{3}P$, $32P$, $3mP$, $\bar{3}mP$, $6P$, $\bar{6}P$, $6/mP$, $23P$, $23I$, $23F$, $m\bar{3}P$, $m\bar{3}I$, $m\bar{3}F$.

Class II*B*: the individual may belong to any crystal class but has a specialized metric and the twin operation belongs to a higher holohedry; P' belongs to a different crystal family than P. Quite obviously, the twin law does not contain the inversion but as for class II*A* the individual may or may not belong to a centrosymmetric crystal class.

The index of P in P', $[P':P]$, gives the maximum number of possible individuals of the twin. Class I and class II*A* twinning are collectively called 'syngonic merohedry' and include only twofold twin operations: a higher-degree rotation would in fact belong to a higher holohedry and would bring the symmetry of the twin to a different crystal family, *i.e.* corresponds to class II*B*, which is also known as 'metric merohedry' (Nespolo & Ferraris, 2000).

Let r be the number of independent twin laws; twins are divided into first-degree ($r = 1$) and higher-degree ($r > 1$) twins. Furthermore, twins are divided into manifold and twofold twins depending on whether at least one twin element[4] has order higher than 2 (Nespolo, 2004). For first-degree twofold twins (also called *binary twins*), the number of individuals is always $N = 2 = [P':P]$, whereas in the case of higher-degree or manifold twins the number N of individuals may be lower than $[P':P]$ (individuals not developed or lost by physical action). When $N < [P':P]$, some of the twin operations can be considered as 'inactive' operations because the individual they would generate is missing. Depending on whether $N = [P':P]$ or $N < [P':P]$, one speaks of a *complete twin* or an *incomplete twin* (Nespolo, 2004). The complete or incomplete character of the twin has profound effects on the symmetry of the diffraction pattern, as discussed later.

2. The diffraction symmetry of merohedric twins

The investigation of the possible presence of merohedric twinning based on the diffraction pattern may exploit two criteria: the reflection conditions and, for complete twins, the symmetry of the diffraction pattern.

Twinning by syngonic merohedry, with one single exception detailed below, does not affect the reflection conditions. Different is the case of class II*B* twinning, when non-space-group absences may arise, which are a distinct sign of twinning.[5] In this class the twin operation superimposes crystallographically independent reflections, so that the measured intensities are actually the sum of the intensities from each individual, scaled by their volume fraction (Catti & Ferraris, 1976). This effect is maximal in twinning by merohedry, where *all* the measured intensities are the unphased sum of intensities from the individuals. In other words, if a twin operation t relates the reflections $h_1k_1l_1$ of the first individual and $h_2k_2l_2$ of the second individual (in the axial setting of the first, taken also as axial setting of the twin), and if I_0 is the measured intensity, then

$$I_0(h_1k_1l_1) = vI(h_1k_1l_1) + (1 - v)I(h_2k_2l_2), \qquad (1)$$

where v is the fraction of the volume corresponding to the first individual. In the case of class I twins, where two individuals are related by an inversion, equation (1) becomes

$$I_0(hkl) = vI(hkl) + (1 - v)I(\overline{hkl}). \qquad (2)$$

Under Friedel's law (*i.e.* unless resonant scattering is substantial) $I(hkl) = I(\overline{hkl})$, thus the intensity I_0 is exactly the same when measured from a twinned sample or from an untwinned sample, centrosymmetric or not, having the same volume as the twinned edifice.

When instead the twin belongs to class II*A* or II*B*, the twin operation overlaps reflections that are non-equivalent even under Friedel's law: the presence of twinning may then hinder a correct derivation of the space group from the diffraction pattern. For class II*B*, the twin law may contain an operation of degree higher than 2, *i.e.* a crystallographic n-fold rotation with $n > 2$. Let this operation be $n_{[uvw]}$ (rotoinversions are of course allowed as well); then $[uvw]$ may also be the direction of a symmetry element for the individual, of order $m \geq 1$ (1 being the trivial case of the identity operation). The ratio n/m can be equal to 2 (a fourfold twin rotation about a twofold axis for the individual as in the case of a tetragonal metric specialization of an orthorhombic individual or of a cubic specialization of a tetragonal individual; a sixfold twin rotation about a threefold axis for the individual as in the case of a trigonal crystal twinned by twofold rotation about the unique axis) or higher (any case corresponding to $n > 2$ and $m = 1$ as well as a sixfold twin rotation about a twofold axis for the individual). The following five cases of class II*A* and class II*B* twinning have to be distinguished.

(*a*) First-degree class II*A* twins (*i.e.* binary twins): only a single twofold twin element occurs ($r = 1$); $[P':P] = 2$, the twin is composed of two individuals and is always complete.

(*b*) Higher-degree class II*A* twins: $r > 1$ independent twofold twin elements occur; $[P':P] = 2^r$, the complete twin is composed of 2^r individuals, an incomplete twin occurs when $N < 2^r$.

(*c*) First-degree class II*B* twins: only a single twin element occurs ($r = 1$), whose order is $n \geq 2$;

(i) n/m (as defined above) = 2: $[P':P] = 2$ and, exactly as in the case of binary twins, an incomplete twin is not possible; the only difference with respect to binary twins is that here the twin operation belongs to a different crystal family;

(ii) $n/m > 2$: $[P':P] = n/m$, the complete twin is composed of n/m individuals, an incomplete twin occurs when $N < n/m$.

(*d*) Higher-degree class II*B* twins: $r > 1$ twin elements occur, of which at least one has $n > 2$; $[P':P] = \Pi_i n_i/m_i$; the complete

[4] A twin element is the geometric element (plane, axis, centre) about which a twin operation is performed combined with the twin operation performed about it.

[5] Non-space-group absences are not an exclusive feature of twins, occurring also in modular structures, in particular polytypes and OD structures, where these absences come from the existence of local symmetry operations (Dornberger-Schiff, 1956). The non-space-group absences derived in this article are, however, typical of twinning, where they originate in the overlap of two or more orientations of the same diffraction pattern.

twin is composed of $\Pi_i n_i/m_i$ individuals, an incomplete twin occurs when $N < \Pi_i n_i/m_i$.

The latter expression, $[P':P] = \Pi_i n_i/m_i$, includes all the others as subcases. P' is obtained by an extension of P by the independent twin operations $n_{[uvw]}$, and the index $[P':P]$ corresponds to the number of cosets (and thus to the number of twin laws plus one) and to $\Pi_i n_i/m_i$:

$$P' = \cup_i t_i P \quad (3)$$

where t_i is the ith coset representative ($t_1 = 1$). When the twin is complete, the symmetry of the diffraction pattern of the twinned edifice corresponds to *at least* P.[6] It may, however, be increased to a supergroup of P by the presence of twin elements, leading thus to a *diffraction enhancement of symmetry*, as was recognized earlier by Buerger (1954). The symmetry of the twin in the reciprocal space depends on the volume of the individuals, while the volume plays no role in the direct space, where only the orientations of the individuals, not their size, define the symmetry of the twin (exactly like the morphological symmetry of a crystal does not depend on the development of the individual faces). Only when the individuals related by the twin operations have the same volume is the diffraction enhancement of symmetry realized; equation (1) (two individuals) becomes

$$I_0(h_1k_1l_1) = I_0(h_2k_2l_2) = 0.5[I(h_1k_1l_1) + I(h_2k_2l_2)]. \quad (4)$$

However, this enhancement is *accidental* and differs radically from the homonymous phenomenon (see, for example, Sadanaga & Takeda, 1968; Iwasaki, 1972; Marumo & Saito, 1972; Perez-Mato & Iglesias, 1977; Sadanaga & Ohsumi, 1979) that is observed when a structure is composed of substructures (polytypes, cell-twins, homologous structures: see Nespolo *et al.*, 2004). There, a phase relation is introduced, while here a simple weighted sum of the intensities is obtained. The diffraction enhancement of symmetry in twins may lead to choosing a wrong space group; in this case, even when a solution of the structure is apparently obtained, the refinement does not converge satisfactorily and the presence of twinning should be suspected.

When $[P':P] > 2$, equation (2) is immediately generalized to

$$I_0(h_jk_jl_j) = \sum_i v_i I(h_ik_il_i), \text{ where } \sum_i v_i = 1 \quad (5)$$

and i runs from 1 to N, where N is the number of individuals. If the twin is complete and each individual takes one Nth of the volume of the twinned edifice, a diffraction enhancement of symmetry is observed and equation (5) becomes

$$I_0(h_jk_jl_j) = \sum_i I(h_ik_il_i)/N \quad (6)$$

where j is any of the indices covered by the running index i.

If the twin is incomplete, the diffraction enhancement of symmetry cannot be realized. In fact, the index i in equation (5) runs over a *subset* of the twin laws obtained by the coset decomposition of P' with respect to P. The result is *not* a group but a subset of elements of P' not forming a group (called a *complex* in group theory: Ledermann, 1964). The diffraction symmetry of an incomplete twin by syngonic merohedry is therefore the same as that of the untwinned crystal, independently from the volume of the individuals. For metric merohedry (class IIB) instead, incomplete twinning may even break the symmetry of the reflection conditions to that of a *lower* crystal family, as we are going to see in §6.2.

[6] For a twin by reticular merohedry this is no longer true in general; but here we deal with merohedric twins.

3. Point- and space-group extensions

Despite the point-group nature of twinning, consideration of the space group of the individuals may give some important information, in particular about the reflection conditions in the twinned and untwinned sample. Let H be the space-group type of the individual, whose point group is of type P, and let t be an operation in the vector space extending P to P': the extension is written as $P' = \langle P,t\rangle$. In general, one may find up to three models having the same reflection conditions: (i) an untwinned model (**H model** below); (ii) a twinned model in which the twin operation is t (***t*-H model** below); and (iii) an untwinned model in a space group of type G with point group $P' = \langle P,t\rangle$ (**G model** below). Fortunately, the three models do not always have the same reflection conditions and the purpose of the following sections is to give a general approach to differentiate the three models when this is possible.

As shown in §§5 and 6, in syngonic merohedry – with a single exception in class IIA discussed below – the twin operation t, which belongs to the crystal family of the individual, *does not alter* the reflection conditions of the individual. The reflection conditions in the ***t*-H** model are therefore the same as those in the **H** model. This is no longer the general case for class IIB twinning, because the twin operation belongs to a different crystal family and the diffraction pattern in many cases does not match the reflection conditions of any space-group type; in other words, non-space-group absences occur.

On the other hand, when a group G having $P' = \langle P,t\rangle$ shows the same reflection conditions as H, these cannot be used as a criterion to discriminate between the **H** and the **G** models. Hereafter, a group G having the same reflection conditions as H is indicated by $G^\#$. The relation between $G^\#$ and H can be of two types, but in both cases $G^\#$ and H have the translation subgroup (*i.e.* the lattice) in common because in twinning by merohedry the twin index is 1.

(i) $G^\# = \langle H,s\rangle$: $G^\#$ is a supergroup of H, obtained as an extension by a point space operation s corresponding to (having the same linear part as) the twin operation t; this occurs in the vast majority of cases. The operation s relates the same reflections $h_1k_1l_1$ and $h_2k_2l_2$ as t but, being a space-group operation, introduces a phase relation between them: when $t \neq \bar{1}$, the two models ***t*-H** and **G** can therefore be distinguished at the refinement stage, unless the diffraction enhancement of symmetry is present.

(ii) $G^\#$ is a group of higher order than H but not a supergroup of it. The two models ***t*-H** and **G** can then be easily distinguished at the structure solution stage even in the presence of diffraction enhancement of symmetry.

When instead no $G^{\#}$ groups exist, it is possible to differentiate the ***t*-H** and the **G** models already on the basis of the observed reflection conditions.

Giacovazzo (2011; Table 4.3) and Koch (2004; Table 1.3.4.2) present a list of the space-group types that may be simulated by the effects of twinning, without however analysing the criteria to differentiate between the **H** model and the ***t*-H** model on the one hand, and the **G** model on the other. Araki (1991), extending the work of Le Page *et al.* (1984), gives, for the case $[P':P] = 2$ and equi-volume individuals, a list of 'twin extinction' reflections for a subset of the possible twin laws: the presence of these reflections corresponds to the absence of a $G^{\#}$ group in our approach. Here we present a comprehensive analysis which deals with class II*B* twinning as well. The extensive list of reflection conditions given in the tables can be obtained from Table 3.1.4.1 in Volume *A* of *International Tables for Crystallography*, at least for class I and class II*A*, by considering the effect of the twin operations; for class II*B* one also has to consider the Euclidean and affine normalizers, as we are going to show.

4. Class I twinning

Because a lattice in E^3 (the Euclidean three-dimensional space) is always centrosymmetric, the reflection conditions are always the same for **H** and ***t*-H**. All symmorphic space groups have a centrosymmetric $G^{\#}$ supergroup: in fact, a symmorphic space group has either no reflection conditions, if the conventional unit cell is primitive, or integral reflection conditions only, if it is centred. For non-symmorphic space groups, when $G^{\#}$ exists, it is always a supergroup of H ($G = \langle H,\bar{1}\rangle$) with the exception of $H = I2_12_12_1$, which has no centrosymmetric supergroup but, having only integral reflection conditions, behaves like the symmorphic space group $I222$ and therefore has $G^{\#} = Immm$. On the basis of the observed reflection conditions, the following situations may occur.

(i) The reflection conditions are compatible with a non-centrosymmetric group H as well as with a centrosymmetric group $G^{\#}$: the three models **H, *t*-H** and **G** have to be tested, because no direct evidence of twinning can be obtained from the diffraction pattern, unless resonant scattering is significant. However, when the refinement leaves some unexplained features (like unusual thermal displacements or correlations between parameters suggesting strong pseudosymmetry), the presence of inversion twinning can reasonably be suspected. Structure refinement programs normally recognize this ambiguity *via* an intermediate value of the Flack parameter (Flack, 1983).

(ii) The reflection conditions are compatible with a non-centrosymmetric group H but there is no centrosymmetric group $G^{\#}$ with the same reflection conditions: the two models **H** and ***t*-H** are left, while the model **G** is ruled out. Exactly as in the previous case, the presence of twinning can be suggested by unexplained features.

(iii) The reflection conditions are compatible with a centrosymmetric group G but not with a non-centrosymmetric group H. In this case, both models **H** and ***t*-H** are excluded *a priori* and the presence of inversion twinning is ruled out.

Table 1
The 33 centrosymmetric space-group types having no non-centrosymmetric subgroup with the same reflection conditions.

Entries are ordered according to the diffraction symbol, as given in Looijenga-Vos & Buerger (2006), in the following indicated as LVB for the sake of brevity.

Crystal family	Diffraction symbol	G	No.
M	$P2_1/c$	$P2_1/c$	14
O	*Pban*	*Pban*	50
	Pbca	*Pbca*	61
	Pbcn	*Pbcn*	60
	Pcca	*Pcca*	54
	Pccn	*Pccn*	56
	Pnna	*Pnna*	52
	Pnnn	*Pnnn*	48
	Ccc(ab)	*Ccce*	68
	Ibca	*Ibca*	73
	Fddd	*Fddd*	70
T	*Pn--*	$P4/n$	85
		$P4/nmm$	129
	Pn-c	$P4_2/nmc$	137
	$P4_2/n$--	$P4_2/n$	86
	Pnb-	$P4/nbm$	125
	Pnc-	$P4_2/ncm$	138
	Pnn-	$P4_2/nnm$	134
	Pnbc	$P4_2/nbc$	133
	Pncc	$P4/ncc$	130
	Pnnc	$P4/nnc$	126
	$I4_1/a$--	$I4_1/a$	88
	Ia-d	$I4_1/amd$	141
	Iacd	$I4_1/acd$	142
C	*Pa--*	$Pa\bar{3}$	205
	Pn--	$Pn\bar{3}$	201
		$Pn\bar{3}m$	224
	Pn-n	$Pn\bar{3}n$	222
	Ia--	$Ia\bar{3}$	206
	Ia-d	$Ia\bar{3}d$	230
	Fd--	$Fd\bar{3}$	203
		$Fd\bar{3}m$	227
	Fd-c	$Fd\bar{3}c$	228

Table 1 gives the 33 centrosymmetric types of space groups corresponding to case (iii) above (among these, 30 are identified unequivocally from the reflection conditions only, the other three giving rise to pairs of hemihedral and holohedral centrosymmetric types with the same reflection conditions). If the observed reflection conditions correspond to one of these 33 cases, class I twinning can be excluded *a priori*.

To identify the space-group types corresponding to case (ii), one has to consider the effect of the extension of H by $s = \bar{1}$, which gives zero to six different types G. Zero means that no extension by inversion is possible: this is the case for 22 of the 24 space-group types containing a screw axis n_τ where $\tau \neq n/2$; the two exceptions are $F4_132$ and $I4_132$. The largest number of extensions (namely six) occurs for $P2_12_12$. Among the space-group types G obtained as $\langle H,\bar{1}\rangle$, there exists at most one having the same reflection conditions as H: it is hereafter indicated as $G^{\#}$. When no $G^{\#}$ exists, or when no centrosymmetric extension is possible, and the reflection conditions correspond to the **H** model, the **G** model is automatically ruled

Table 2
The 26 biaxial non-centrosymmetric non-symmorphic types of space groups H, classified by their corresponding diffraction symbol, and the corresponding centrosymmetric group $G^{\#}$ showing the same reflection conditions (in all but one case $G^{\#}$ is the centrosymmetric supergroup of H).

In five cases (shown in bold in the H column and by dashes in the $G^{\#}$ column) no $G^{\#}$ exists and an inversion twin cannot be mistaken for a centrosymmetric untwinned crystal: in other words, the **G** model is ruled out on the basis of the observed reflection conditions. The superscript * means that $G^{\#}$ is not a supergroup of H. Entries are ordered according to the diffraction symbol, as given in LVB. For monoclinic groups, a shortened (unoriented) diffraction symbol is given.

Diffraction symbol	H	No.	$G^{\#}$ (class I)	No.
$P2_1$	$P2_1$	4	$P2_1/m$	11
P--2_1	**$P222_1$**	**17**	---	---
P-2_12_1	**$P2_12_12$**	**18**	---	---
$P2_12_12_1$	**$P2_12_12_1$**	**19**	---	---
P-a-	$Pma2$	28	$Pmam$ ($Pmma$)	51
Pc	Pc	7	$P2/c$	13
P-c-	$Pmc2_1$	26	$Pmcm$ ($Pmma$)	51
P-n-	$Pmn2_1$	31	$Pmmn$	59
Pba-	$Pba2$	32	$Pbam$	55
Pca-	$Pca2_1$	29	$Pcam$ ($Pbcm$)	57
Pcc-	$Pcc2$	27	$Pccm$	49
Pna-	$Pna2_1$	33	$Pnam$ ($Pnma$)	62
Pnc-	$Pnc2$	30	$Pncm$ ($Pmna$)	53
Pnn-	$Pnn2$	34	$Pnnm$	58
C--2_1	**$C222_1$**	**20**	---	---
Cc	Cc	9	$C2/c$	15
C-c-	$Cmc2_1$	36	$Cmcm$	63
Ccc-	$Ccc2$	37	$Cccm$	66
A---	$Amm2$	38	$Ammm$ ($Cmmm$)	65
A-a-	$Ama2$	40	$Amam$ ($Cmcm$)	63
$A(bc)$--	$Aem2$	39	$Aemm$ ($Cmme$)	67
$A(bc)a$-	$Aea2$	41	$Aeam$ ($Cmce$)	64
I---	$I2_12_12_1$	24	$Immm$*	71
Iba-	$Iba2$	45	$Ibam$	72
I-(ac)-	$Ima2$	46	$Imam$ ($Imma$)	74
Fdd-	**$Fdd2$**	**43**	---	---

out, but the possible presence of inversion twinning has to be checked.

Tables 2 to 5 list the 101 merohedral non-symmorphic types of space groups H that can give rise to 148 twin laws (class I and class IIA), indicated by a coset representative; three twin laws in the tetragonal crystal family (indicated by the symbol { in Table 3) have been split into two, because two different coset representatives give different results in terms of G (in one case, $G^{\#}$ exists for one coset representative but not for the others; in the other two cases, no extension $G^{\#}$ is possible for one coset representative while an extension exists for the other but with additional reflection conditions), leading to a total of 150 cases to be considered. A $G^{\#}$ group exists only in 78 cases ($G^{\#}$ is a supergroup of H in 71 cases): for the other 72 cases, the **G** model can be excluded on simple inspection of the reflection conditions.

For the 78 space-group types H for which the $G^{\#}$ group exists, the three models, **H**, ***t*-H** and **G**, are indistinguishable; using **G** when the sample is to some extent pseudo-centrosymmetric does not necessarily hinder the structure solution, unless resonant scattering is substantial, likely resulting only in apparent disorder or abnormal displacement parameters. The intensity distribution is more centric in disordered crystals than in twins (Rees, 1980), and the statistical analysis of the intensities can help distinguish the **G** model from the ***t*-H** model.

Table 3
Classification of the 34 merohedral non-symmorphic space-group types H in the tetragonal crystal family, which can give rise to 42 twin laws.

Three twin laws (indicated by the symbol {) have been split into two, because two different coset representatives give different results in terms of G, leading to a total of 45 cases. Among these, ten cannot be extended by a twofold operation s corresponding to the twin operation t ('no extension' in the table), and 16 more do have such an extension but none of the corresponding supergroups G has the same reflection conditions as H ('---' in the table). For these 26 cases (16 for class I and ten for class IIA) the **G** model is ruled out on the basis of the observed reflection conditions: H in the corresponding row is shown in bold, accompanied by dashes in the last column. For the other 19 cases, the group $G^{\#}$ having the same reflection conditions as H is given; in the tetragonal crystal family, $G^{\#}$ is always a supergroup of H. Entries are ordered according to the diffraction symbol, as given in LVB.

Diffraction symbol	H	No.	t	$G^{\#}$	No.
Non-centrosymmetric hemihedral (only class I twinning possible)					
P-2_1-	**$P42_12$**	**90**	$\bar{1}$	---	---
	$P\bar{4}2_1m$	**113**		---	---
$P4_2$--	**$P4_222$**	**93**		---	---
$P4_22_1$-	**$P4_22_12$**	**94**		---	---
$P4_1$--	**$P4_122$**	**91**		**no extension**	---
	$P4_322$	**95**		**no extension**	---
$P4_12_1$--	**$P4_12_12$**	**92**		**no extension**	---
	$P4_32_12$	**96**		**no extension**	---
P--c	$P4_2mc$	105		$P4_2/mmc$	131
	$P\bar{4}2c$	112			
P-2_1c	**$P\bar{4}2_1c$**	**114**		---	---
P-b-	$P4bm$	100		$P4/mbm$	127
	$P\bar{4}b2$	117			
P-bc	$P4_2bc$	106		$P4_2/mbc$	135
P-c-	$P4_2cm$	101		$P4_2/mcm$	132
	$P\bar{4}c2$	116			
P-cc	$P4cc$	103		$P4/mcc$	124
P-n-	$P4_2nm$	102		$P4_2/mnm$	136
	$P\bar{4}n2$	118			
P-nc	$P4nc$	104		$P4/mnc$	128
$I4_1$--	**$I4_122$**	**98**		---	---
I--d	**$I4_1md$**	**109**		---	---
	$I\bar{4}2d$	**122**		---	---
I-c-	$I4cm$	108		$I4/mcm$	140
	$I\bar{4}c2$	120			
I-cd	**$I4_1cd$**	**110**		---	---
Centrosymmetric hemihedral (only class IIA twinning possible)					
$P4_2$--	**$P4_2/m$**	**84**	{ **$2_{[100]}$**	---	---
			{ **$2_{[110]}$**	**no extension**	---
Pn--	**$P4/n$**	**85**	{ **$2_{[100]}$**	---	---
			{ $2_{[110]}$	$P4/nmm$	129
$P4_2/n$--	**$P4_2/n$**	**86**	**$2_{[100]}$**	---	---
Tetartohedral (both class I and class IIA twinning possible)					
$P4_2$--	**$P4_2$**	**77**	$\bar{1}$	$P4_2/m$	84
			$2_{[100]}$	$P4_222$	93
			$m_{[100]}$	---	---
$P4_1$--	**$P4_1$**	**76**	**$\bar{1}$**	**no extension**	---
			$2_{[100]}$	$P4_122$	91
			$m_{[100]}$	**no extension**	---
	$P4_3$	**78**	**$\bar{1}$**	**no extension**	---
			$2_{[100]}$	$P4_322$	95
			$m_{[100]}$	**no extension**	---
$I4_1$--	**$I4_1$**	**80**	**$\bar{1}$**	---	---
			$2_{[100]}$	$I4_122$	98
			{ **$m_{[100]}$**	---	---
			{ **$m_{[110]}$**	**no extension**	---
$I4_1/a$--	**$I4_1/a$**	**88**	**$2_{[100]}$**	---	---

Table 4
Classification of the 27 merohedral non-symmorphic space-group types H in the hexagonal crystal family, which can give rise to 61 twin laws.

Among these, 29 cannot be extended by a twofold operation s corresponding to the twin operation t ('no extension' in the table), and two more have such an extension but none of the corresponding supergroups G has the same reflection conditions as H ('---' in the table): for these 31 cases (15 for class I and 16 for class IIA) the **G** model is ruled out on the basis of the observed reflection conditions: H in the corresponding row is shown in bold, accompanied by dashes in the last column. For the other 30 cases, the group $G^{\#}$ having the same reflection conditions as H is given; for two cases, $G^{\#}$ is not a supergroup of H (indicated by superscript *). Entries are ordered according to the diffraction symbol, as given in LVB.

Diffraction symbol	H	No.	t	$G^{\#}$	No.
Non-centrosymmetric hemihedral (only class I twinning possible)					
P--c	$P6_3mc$	186	$\bar{1}$	$P6_3/mmc$	194
	$P\bar{6}2c$	190			
P-c-	$P6_3cm$	185		$P6_3/mcm$	193
	$P\bar{6}c2$	188			
R-c	$R3c$	161		$R\bar{3}c$	167
$P6_3$--	**$P6_322$**	**182**		**---**	**---**
$P6_2$--	**$P6_222$**	**180**		**no extension**	**---**
	$P6_422$	**181**		**no extension**	**---**
$P6_1$--	**$P6_122$**	**178**		**no extension**	**---**
	$P6_522$	**179**		**no extension**	**---**
P-cc	$P6cc$	184		$P6/mcc$	192
Centrosymmetric hemihedral (only class IIA twinning possible)					
$P6_3$--	**$P6_3/m$**	**176**	**$m_{[100]}$**	**---**	**---**
P--c	$P\bar{3}1c$	163	$m_{[001]}$	$P6_3/mmc$	194
P-c-	$P\bar{3}c1$	165	$m_{[001]}$	$P6_3/mcm$	193
Tetartohedral or ogdohedral (both class I and class IIA twinning possible)					
$P3_1$--	**$P3_1$**	**144**	**$\bar{1}$**	**no extension**	**---**
			$2_{[210]}$	$P3_112$	151
			$2_{[100]}$	$P3_121$	152
			$2_{[001]}$	$P6_4$	172
			$m_{[001]}$	**no extension**	**---**
			$m_{[100]}$	**no extension**	**---**
			$m_{[210]}$	**no extension**	**---**
	$P3_112$	**151**	**$\bar{1}$**	**no extension**	**---**
			$2_{[001]}$	$P6_422$	181
			$m_{[001]}$	**no extension**	**---**
	$P3_121$	**152**	**$\bar{1}$**	**no extension**	**---**
			$2_{[001]}$	$P6_422$	181
			$m_{[001]}$	**no extension**	**---**
	$P3_2$	**145**	**$\bar{1}$**	**no extension**	**---**
			$2_{[210]}$	$P3_212$	153
			$2_{[100]}$	$P3_221$	154
			$2_{[001]}$	$P6_2$	171
			$m_{[001]}$	**no extension**	**---**
			$m_{[100]}$	**no extension**	**---**
			$m_{[210]}$	**no extension**	**---**
	$P3_212$	**153**	**$\bar{1}$**	**no extension**	**---**
			$2_{[001]}$	$P6_222$	180
			$m_{[001]}$	**no extension**	**---**
	$P3_221$	**154**	**$\bar{1}$**	**no extension**	**---**
			$2_{[001]}$	$P6_222$	180
			$m_{[001]}$	**no extension**	**---**
P--c	$P31c$	159	$\bar{1}$	$P\bar{3}1c$	163
			$m_{[001]}$	$P\bar{6}2c$	190
			$2_{[001]}$	$P6_3mc$*	186
P-c-	$P3c1$	158	$\bar{1}$	$P\bar{3}c1$	165
			$m_{[001]}$	$P\bar{6}c2$	188
			$2_{[001]}$	$P6_3cm$*	185
$P6_3$--	**$P6_3$**	**173**	$\bar{1}$	$P6_3/m$	176
			$2_{[100]}$	$P6_322$	182
			$m_{[100]}$	**no extension**	**---**
$P6_2$--	**$P6_2$**	**171**	**$\bar{1}$**	**no extension**	**---**
			$2_{[100]}$	$P6_222$	180
			$m_{[100]}$	**no extension**	**---**

Table 4 (continued)

Diffraction symbol	H	No.	t	$G^{\#}$	No.
	$P6_4$	**172**	**$\bar{1}$**	**no extension**	**---**
			$2_{[100]}$	$P6_422$	181
			$m_{[100]}$	**no extension**	**---**
$P6_1$--	**$P6_1$**	**169**	**$\bar{1}$**	**no extension**	**---**
			$2_{[100]}$	$P6_122$	178
			$m_{[100]}$	**no extension**	**---**
	$P6_5$	**170**	**$\bar{1}$**	**no extension**	**---**
			$2_{[100]}$	$P6_522$	179
			$m_{[100]}$	**no extension**	**---**

5. Class IIA twinning

In class IIA twinning, the twin operation does not belong to the Laue class of the individual and the twin law (coset) does not contain the inversion. The twin operation is therefore either a twofold rotation or a mirror reflection (a higher-degree rotation would bring the symmetry of the twin to a different crystal family and corresponds to class IIB). Triclinic, monoclinic and orthorhombic space groups do not need to be considered here, because any group–subgroup relation in these three crystal families gives rise to class I twinning. The analysis is shown in Tables 3 to 5.

As in class I twinning, the models **H** and ***t*-H** are not distinguishable on the basis of the observed reflection conditions, with one exception, which is easily understood by analysing the effect of the operations of the Euclidean normalizer of H on the diffraction pattern. The Euclidean normalizer $N_E(H)$ (also known as the Cheshire group) is the subgroup of the Euclidean group (*i.e.* the group of all isometries of the Euclidean space) containing all the operations that map H onto itself by conjugation, *i.e.* all the operations e of E such that $ehe^{-1} \in H$ for all h in H (Koch *et al.*, 2006; Koch & Fischer, 2006). As a consequence, the Euclidean normalizer $N_E(H)$ also maps the symmetry elements of H onto themselves: it represents the *symmetry of the symmetry pattern*.

Because the elements of $N_E(H)$ map H onto itself, they also map the weighted reciprocal lattice[7] of H onto itself, *i.e.* they do not affect the reflection conditions of H. Furthermore, the inversion never directly affects the reflection conditions; therefore, to judge whether or not a class IIA twin operation t affects the reflection conditions of the individual, one simply needs to see whether the symmetry operation s that corresponds to t belongs to the Laue class $L[N_E(H)]$ of the Euclidean normalizer of H or not.

As pointed out by Koch (2004), $L[N_E(H)]$ corresponds to the holohedry for all H but $Pa\bar{3}$. For the latter case, $N_E(H)$ is $Ia\bar{3}$ and thus $L[N_E(H)] = m\bar{3}$, whereas the holohedry of $Pa\bar{3}$ is of course $m\bar{3}m$. This means that the operations in $m\bar{3}m$ not contained in $m\bar{3}$ *do* affect the reflection conditions of $Pa\bar{3}$: but these are precisely the operations in the non-trivial coset of $m\bar{3}m$ with respect to $m\bar{3}$, *i.e.* the operations in a class IIA twin law of an $m\bar{3}$ individual. In fact, the reflection conditions of

[7] The weighted reciprocal lattice is obtained by assigning to each node of the reciprocal lattice a 'weight' that corresponds to $|F(hkl)|$ (Shmueli, 2008).

Table 5
Classification of the 14 merohedral non-symmorphic space-group types H in the cubic crystal family, which can give rise to 18 twin laws.

Among these, eight cannot be extended by a twofold operation s corresponding to the twin operation t (four indicated as 'no extension', four with a * meaning that they do have a $G^{\#}$ with the same reflection conditions as H but this is not a supergroup of H) and six more (indicated by dashes) have such an extension but none of the corresponding supergroups G has the same reflection conditions as H. For four of the eight non-existing extensions $\langle H,s\rangle$, a $G^{\#}$ with the same reflection conditions as H does exist but it is not a supergroup of H. For the ten cases for which no $G^{\#}$ exists (seven for class I and three for class IIA), the **G** model is ruled out on the basis of the observed reflection conditions: H in the corresponding row is shown in bold, accompanied by dashes in the last column. For the other eight cases, the group $G^{\#}$ having the same reflection conditions as H is given; of these, four are supergroups of H, the other four, indicated by the superscript *, are not. Entries are ordered according to the diffraction symbol, as given in LVB.

Diffraction symbol	H	No.	t	$G^{\#}$	No.
Non-centrosymmetric hemihedral (only class I twinning possible)					
$P2_1$--, $P4_2$--	$\mathbf{P4_232}$	**208**	$\bar{1}$	---	---
$P4_1$--	$\mathbf{P4_132}$	**213**		**no extension**	---
	$\mathbf{P4_332}$	**212**		**no extension**	---
P--n	$P\bar{4}3n$	218		$Pm\bar{3}n$	223
$I4_1$--	$\mathbf{I4_132}$	**214**		---	---
I--d	$\mathbf{I\bar{4}3d}$	**220**		---	---
$F4_1$--	$\mathbf{F4_132}$	**210**		---	---
F--c	$F\bar{4}3c$	219		$Fm\bar{3}c$	226
Centrosymmetric hemihedral (only class IIA twinning possible)					
Pa--	$\mathbf{Pa\bar{3}}$	**205**	$m_{[110]}$	**no extension**	---
Pn--	$Pn\bar{3}$	201	$m_{[110]}$	$Pn\bar{3}m$	224
Ia--	$\mathbf{Ia\bar{3}}$	**206**	$\mathbf{m_{[110]}}$	---	---
Fd--	$Fd\bar{3}$	203	$m_{[110]}$	$Fd\bar{3}m$	227
Tetartohedral (both class I and class IIA twinning possible)					
$P2_1$--, $P4_2$--	$\mathbf{P2_13}$	**198**	$\bar{\mathbf{1}}$	---	---
			$2_{[110]}$	$P4_232$*	208
			$m_{[110]}$	**no extension**	---
I---	$I2_13$	199	$\bar{1}$	$Im\bar{3}$*	204
			$2_{[110]}$	$I432$*	211
			$m_{[110]}$	$I\bar{4}3m$*	217

$Pa\bar{3}$ are $0kl$: $k = 2n$, $h00$: $h = 2n$ (with cyclic permutation of h, k, l). Any operation in the twin law (up to cyclic permutation of h, k, l) brings to overlap $0eu$ (e = *e*ven, u = *u*neven) reflections (present) of the first individual with $0ue$ reflections (absent) of the second individual so that the observed reflection conditions become $0kl$: $k = 2n$ or $l = 2n$, $h00$: $h = 2n$ (with cyclic permutation of h, k, l), which do not occur in any group whose conventional cell is primitive, allowing thus the identification of the presence of class IIA twinning for this particular case.

The distinction between the ***t*-H** and **G** models is analogous with the case of class I twinning. In class IIA, there are 29 types of space groups H for which no $G^{\#}$ exists for the given t. If the reflection conditions corresponding to one of these groups are observed, the **G** model can be immediately ruled out. If the refinement is not satisfactory, the presence of twinning should be reasonably suspected (Tables 3–5).

For the other cases where class IIA twinning is possible, the diffraction patterns of ***t*-H** and **G** cannot be differentiated from the reflection conditions, and the measured intensities obey equation (1). In the presence of diffraction enhancement of symmetry, a wrong space group might be chosen, but even if a solution of the structure is apparently obtained, the structure refinement would not reasonably converge; the presence of twinning should therefore be suspected. Otherwise, the distribution of the intensities does not match any of the space-group types suggested by the reflection conditions, a clear indication of the presence of twinning. Finally, if $G^{\#}$ is not a supergroup of H (this is the case for $H = P31c$, $P3c1$, $P2_13$ and $I2_13$, whose $G^{\#}$ are, respectively, $P6_3mc$, $P6_3cm$, $P4_232$, $I432$ and $I\bar{4}3m$), the structure simply cannot be solved in $G^{\#}$.

6. Class II*B* twinning

In the case of class IIB twinning, the symmetry of the twin belongs to a different crystal family than the individual. This is realized in the presence of a specialized metric, which is not an intrinsic feature of the crystal but rather an 'accident' that occurs only in a certain range of chemical–physical conditions. This 'accident' seems, however, much more frequent than one would suspect (Janner, 2004*a*,*b*); consequently, class IIB twinning has to be seriously taken into account. If this type of twinning is suspected, collecting the diffraction pattern sufficiently far from the conditions giving rise to the metric specialization should resolve the ambiguity because reflections that were overlapped appear split. However, because the presence of twinning is normally not suspected *a priori*, and because it is not always possible to run the experiment in different conditions, a detailed analysis of the effects of class IIB twinning on the diffraction pattern is certainly of interest for the experimental crystallographer. As we are going to show, non-space-group absences are of great help in a large number of cases. It is also to be emphasized that the discrepancy between the metric symmetry and the symmetry of the intensity distribution is an indication of the possible presence of class IIB twinning. However, when diffraction enhancement of symmetry is realized, the discrepancy may no longer occur.

The three models, **H**, ***t*-H** and **G**, can very often be distinguished for class IIB twinning, because only in a limited number of cases a group $G^{\#}$ having point group $P' = \langle P,t\rangle$ and the same reflection conditions as H exists, and because class IIB twinning does affect the reflection conditions in a large

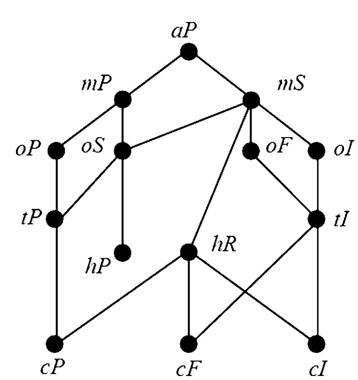

Figure 1
Graph showing the path through Bravais types of lattices obtained by metric specialization. Each node represents a Bravais type of lattice, each edge a possible metric specialization. Modified after Fig. 3 in Grimmer & Nespolo (2006).

Table 6
Non-symmorphic space-group types with the corresponding $G^{\#}$ (if any) in the crystal family corresponding to the metric specialization given in the first column by the corresponding standard symbol.

$G^{\#}$ has the same reflection conditions as H when expressed in a common setting (* indicates that $G^{\#}$ is not a supergroup of H). In bold are the space-group types for which either an extension in the different crystal family is not possible, or no $G^{\#}$ group exists in that crystal family: these are the cases where the **G** model can be excluded on the basis of the observed reflection conditions. The 'incompatible' entry in the diffraction symbol means that the observed reflection conditions are incompatible with the different crystal family suggested by the metric: this indication alone is sufficient to rule out the **G** model. The diffraction symbols for the $m \rightarrow hR$ specialization are only apparently different; the change of setting is responsible for this apparent difference. Entries are ordered according to the diffraction symbol in the different crystal family (crystal family of the twin), as given in LVB.

Metric specialization	Diffraction symbol in the lower family	Diffraction symbol in the higher family	H	No.	$G^{\#}$	No.
$m \rightarrow o$	$P2_1$	P--2_1	$P2_1$ ($\beta = 90°$)	4	$P22_12$ ($P222_1$)	17
			$P2_1/m$ ($\beta = 90°$)	**11**	**---**	**---**
		C--2_1	$P2_1$ ($a = c$)	4	$C222_1$	20
			$P2_1/m$ ($a = c$)	11	$C222_1$*	20
	Pc	P-c-	Pc ($\beta = 90°$)	7	$Pmc2_1$	26
			$P2/c$ ($\beta = 90°$)	13	$Pmcm$ ($Pmma$)	51
		C--(ab)	Pc ($a = c$)	7	$Cmme$	67
			$P2/c$ ($a = c$)	13	$Cmme$	67
	Cc	C-c-	Cc ($\beta = 90°$)	9	$Cmc2_1$	36
			$C2/c$ ($\beta = 90°$)	15	$Cmcm$	63
		I-(ac)-	Cc ($\cos\beta = -c/a$)	9	$Imam$ ($Imma$)	74
			$C2/c$ ($\cos\beta = -c/a$)	15	$Imam$ ($Imma$)	74
		incompatible	**Cc** ($\cos\beta = a/2c$)	**9**	**---**	**---**
			$C2/c$ ($\cos\beta = a/2c$)	**15**	**---**	**---**
	$P2_1/c$	incompatible	**$P2_1/c$** (both)	**14**	**---**	**---**
$m \rightarrow t$	$P2_1$	$P4_2$--	$P2_1$	4	$P4_2$*	77
			$P2_1/m$	11	$P4_2/m$*	84
	Pc	Pn--	$P2/c$	13	$P4/n$	85
	Cc	incompatible	**$C2/c$**	**15**	**---**	**---**
$m \rightarrow h$	$P2_1$	$P6_3$--	$P2_1$	4	$P6_3$	173
			$P2_1/m$	11	$P6_3/m$	176
	Cc	R-c	Cc	9	$R3c$	161
			$C2/c$	15	$R\bar{3}c$	167
$o \rightarrow t$	$P2_12_1$-	P-2_1-	$P2_12_12$	18	$P42_12$, $P\bar{4}2_1m$	90, 113
	P--2_1	$P4_2$--	$P222_1$	17	$P4_222$*	93
	C--2_1		$C222_1$	20	$P4_222$*	93
	$P2_12_12_1$	$P4_22_1$-	$P2_12_12_1$	19	$P4_22_12$*	94
	Ccc-	P--c	$Ccc2$	37	$P4_2mc$, $P\bar{4}2c$	105, 112
			$Cccm$	66	$P4_2/mmc$	131
	Pba-	P-b-	$Pba2$	32	$P4bm$, $P\bar{4}b2$	100, 117
			$Pbam$	55	$P4/mbm$	127
	Pcc-	P-c-	$Pcc2$	27	$P4_2cm$, $P\bar{4}c2$	101, 116
			$Pccm$	49	$P4_2/mcm$	132
	Pnn-	P-n-	$Pnn2$	34	$P4_2nm$, $P\bar{4}n2$	102, 118
			$Pnnm$	58	$P4_2/mnm$	136
	P--n	Pn--	$Pmmn$	59	$P4/nmm$	129
	C--(ab)		$Cmme$	67	$P4/nmm$	129
	$Ccce$	Pn-c	$Ccce$	68	$P4_2/nmc$	137
	$Pban$	Pnb-	$Pban$	50	$P4/nbm$	125
	$Pccn$	Pnc-	$Pccn$	56	$P4_2/ncm$	138
	$Pnnn$	Pnn-	$Pnnn$	48	$P4_2/nnm$	134
	I---	I---	$I2_12_12_1$	24	$I422$*	97
	Fdd-	I--d	$Fdd2$	43	$I4_1md$, $I\bar{4}2d$	109, 122
	Iba-	I-c-	$Iba2$	45	$I4cm$, $I\bar{4}c2$	108, 120
			$Ibam$	72	$I4/mcm$	140
	$Fddd$	Ia-d	$Fddd$	70	$I4_1/amd$	141
	P--a	incompatible	**$Pmma$**	**51**	**no extension**	**---**
	P-a-		**$Pma2$**	**28**	**no extension**	**---**
	P-c-		**$Pmc2_1$**	**26**	**no extension**	**---**
	P-n-		**$Pmn2_1$**	**31**	**no extension**	**---**
	P-na		**$Pmna$**	**53**	**no extension**	**---**
	Pn-a		**$Pnma$**	**62**	**no extension**	**---**
	Pca-		**$Pca2_1$**	**29**	**no extension**	**---**
	Pnc-		**$Pnc2$**	**30**	**no extension**	**---**
	Pna-		**$Pna2_1$**	**33**	**no extension**	**---**
	Pbc-		**$Pbcm$**	**57**	**no extension**	**---**
	$Pbca$		**$Pbca$**	**61**	**no extension**	**---**
	$Pbcn$		**$Pbcn$**	**60**	**no extension**	**---**
	$Pcca$		**$Pcca$**	**54**	**no extension**	**---**
	$Pnna$		**$Pnna$**	**52**	**no extension**	**---**

Table 6 (continued)

Metric specialization	Diffraction symbol in the lower family	Diffraction symbol in the higher family	*H*	No.	$G^{\#}$	No.
	C-c-		***Cmc*2₁**	**36**	**no extension**	**---**
			Cmcm	**63**	**no extension**	**---**
	C-c(*ab*)		***Cmce***	**64**	**no extension**	**---**
	A-a-		***Ama*2**	**40**	**no extension**	**---**
	A(*bc*)--		***Aem*2**	**39**	**no extension**	**---**
	A(*bc*)*a*-		***Aea*2**	**41**	**no extension**	**---**
	I--a		***Imma***	**74**	**---**	**---**
	I-a-		***Ima*2**	**46**	**no extension**	**---**
	Ibca		***Ibca***	**73**	**---**	**---**
$o \rightarrow h$	C--2_1	$P6_3$--	$C222_1$	20	$P6_322$	182
	C-c-	incompatible	***Cmc*2₁**	**36**	**---**	**---**
	Ccc-		***Ccc*2**	**37**	**---**	**---**
	A-a-		***Ama*2**	**40**	**---**	**---**
	C-c-		***Cmcm***	**63**	**---**	**---**
	Ccc-		***Cccm***	**66**	**---**	**---**
$o \rightarrow c$	$P2_12_12_1$	$P2_1$--, $P4_2$	$P2_12_12_1$	19	$P2_13$	198
	Pbca	*Pa--*	*Pbca*	61	$Pa\bar{3}$	205
	Pnnn	*Pn--*	*Pnnn*	48	$Pn\bar{3}$	201
	I---	*I---*	$I2_12_12_1$	24	$I2_13$	199
	Ibca	*Ia--*	*Ibca*	73	$Ia\bar{3}$	206
	Fddd	*Fd--*	*Fddd*	70	$Fd\bar{3}$	203
$t \rightarrow c$	$P4_22_1$-	$P2_1$--, $P4_2$	$P4_22_12$	94	$P4_232$*	208
	Pnn-	*Pn--*	$P4_2/nnm$	134	$Pn\bar{3}m$	224
$h \rightarrow c$	*R-c*	*F--c*	$R3c$	161	$F\bar{4}3c$	219
			$R\bar{3}c$	167	$Fm\bar{3}c$	226

number of cases, thus making **H** and ***t*-H** often distinguishable on the basis of the observed reflection conditions. The metric specializations leading to a different crystal family are shown in Fig. 1.

6.1. Differentiating H and G models in class II*B* twinning

For a symmorphic space group *H*, there always exists a symmorphic supergroup $G^{\#} = \langle H,s \rangle$ in the higher crystal family corresponding to the specialized metric that has the same reflection conditions as *H*. Therefore, for a symmorphic space group the reflection conditions never allow one to discriminate between the **H** and the **G** models. Furthermore, the search for $G^{\#}$ in the case of class II*B* twinning is limited to cases when P' is a minimal supergroup of *P*: further steps do not need to be considered explicitly because they either correspond to class II*A* twinning possibly accompanying class II*B* twinning (when the supergroup stays in the same crystal family) or to a further ascent in the crystal families, which is considered independently (for example, a cubic specialization of a monoclinic metric can be considered as a two-step process, the first one being an orthorhombic or a tetragonal specialization, the second step the cubic specialization of the latter). The analysis of non-symmorphic space groups is given in Table 6 and the results can be summarized in the following remarks.

(i) Non-symmorphic space groups with a specialized metric that can have a $G^{\#}$ supergroup in a different crystal family belong to the monoclinic, orthorhombic, tetragonal and hexagonal (rhombohedral lattice) crystal families.

(ii) Some space groups have more than one possible metric specialization leading to a $G^{\#}$ supergroup (Fig. 1). This is the case for monoclinic *H* with specialized orthorhombic, tetragonal, hexagonal (*via oS*), rhombohedral (if the conventional unit cell is *C*-centred) or cubic metric, and for orthorhombic *H* with specialized tetragonal, cubic or hexagonal (if the conventional unit cell is *S*-centred) metric.

(iii) Orthorhombic space groups with a tetragonal metric but with different types of glides on [100] and [010] have no tetragonal extensions; furthermore, if the diffraction pattern is indexed with respect to tetragonal axes, inconsistent reflection conditions are observed on reciprocal planes that should be equivalent, a clear sign of the lower structural symmetry with respect to the lattice symmetry. In particular, a diffraction symbol cannot be written in the tetragonal setting: this is the meaning of the entries ‘incompatible’ in Table 6. The same occurs for non-holoaxial orthorhombic groups or *C*-centred monoclinic groups with a hexagonal metric (where it is impossible to have three sets of equivalent planes). If such a contradiction between the observed reflection conditions and the metric of the unit cell is observed, the **G** model can be excluded *a priori*.

(iv) Because only two cases of cubic $G^{\#}$ for a tetragonal *H* occur, Table 6 gives these two examples only, without listing all the others as having no $G^{\#}$.

The procedure to derive the conditions expressed in Table 6 can be illustrated with the example of an *oS* specialization of an *mP* crystal obtained when $a = c$, which is particularly instructive. Five types of monoclinic non-symmorphic groups have an *mP* type of lattice: $P2_1$, $P2_1/m$, Pc, $P2/c$ and $P2_1/c$. They can be gathered in three sets having the same reflection conditions (Fig. 2). A *b*-unique *mP* crystal can always be described with an *mB* cell, *mP* and *mB* corresponding just to a change of axes. The space-group symbols and the reflection conditions for this non-standard setting change accordingly as shown in Fig. 2. The result can equally be described in a *c*-unique *mC* setting. If one now assumes a metric specialization $a = c$ for the original *mP* setting, the centred cells become orthorhombic, which means that the crystal is described in an *oB* (*b*-unique setting) or *oC* (*c*-unique setting) cell. The diffraction symbol corresponding to the reflection conditions in the *oC* setting is given in the last column of Fig. 2. There we see that the metric specialization leads to $G^{\#} = C222_1$ (only possible type of space group for the diffraction symbol C--2_1) for $P2_1$, and to *Cmme* (only possible type of space group for the diffraction symbol *C*--*e*) for *Pc* and *P*2/*c*. On the other hand, the reflection conditions of $P2_1/m$ with an *oC* metric specialization correspond again to $C222_1$, which is not a supergroup of $P2_1/m$, and those of $P2_1/c$ do not correspond to any orthorhombic group. In fact, the diffraction symbol one would obtain by reading off the $P2_1/c$ reflection conditions in the *oC* setting would be C--$2_1/(ab)$, which does not correspond to any type of space group. This should be a clear indication of the presence of twinning.

With analogous arguments it is easy to show that an *oI* metric specialization of a non-symmorphic *mC* crystal (space group of type *Cc* or *C*2/*c*), obtained if $\cos\beta = -c/a$, leads to reflection conditions *I*-*a*- which correspond to $G^{\#} = Imam$ (*Imma* in the standard setting). On the other hand, an *oF* metric specialization of the same *mC* crystal, obtained if $\cos\beta = 2a/c$, leads to reflection conditions *Fd*--, which do not correspond to any orthorhombic type of space group: Table 6 shows the entry 'incompatible' in such a case.

Table 6 shows that for 33 types of space groups with specialized metric, the reflection conditions are not compatible with a group in the higher crystal family: the **G** model can then be ruled out on simple inspection of the reflection conditions. Furthermore, in eight cases $G^{\#}$ is not a supergroup of *H*; in seven of these, a structure solution cannot be obtained in $G^{\#}$, a clear indication of the presence of twinning. The eighth case corresponds to the *oC* ($a = c$) specialization of $P2_1/m$, for which $G^{\#} = C222_1$ is a supergroup of the $P2_1$ non-centrosymmetric maximal subgroup of *H*: in the absence of resonant scattering, a structure solution can be obtained but the lack of inversion centre in the adopted model would leave anomalies, for example in the description of the thermal motion of the atoms, which should prompt the investigator to check a centrosymmetric group. However, the centrosymmetric supergroup of $C222_1$ (*Cmcm*) has additional reflection conditions which are violated in the diffraction pattern of a $P2_1/m$ crystal with *oC* metric specialization.

	$\xrightarrow{\textit{B-centred cell}}$	$\xrightarrow{\textit{c-unique setting}}$	$\xrightarrow{\textit{oC metric}}$
$P2_1$, $P2_1/m$ $0k0{:}k = 2n$	$B2_1$, $B2_1/m$ $hkl{:}h+l = 2n$ $h0l{:}h+l = 2n$ $hk0{:}\ h = 2n$ $0kl{:}\ l = 2n$ $h00{:}h = 2n$ $00l{:}l = 2n$ $0k0{:}k = 2n$	$C112_1$, $C112_1/m$ $hkl{:}h+k = 2n$ $hk0{:}h+k = 2n$ $h0l{:}h = 2n$ $0kl{:}k = 2n$ $h00{:}h = 2n$ $00l{:}l = 2n$ $0k0{:}k = 2n$	C--2_1
Pc, $P2/c$ $h0l{:}l = 2n$ $00l{:}l = 2n$	Be, $B2/e$ $hkl{:}h+l = 2n$ $h0l{:}h,l = 2n$ $hk0{:}\ h = 2n$ $0kl{:}\ l = 2n$ $h00{:}h = 2n$ $00l{:}l = 2n$	$C11e$, $C112/e$ $hkl{:}h+k = 2n$ $hk0{:}h,k = 2n$ $h0l{:}h = 2n$ $0kl{:}k = 2n$ $h00{:}h = 2n$ $00k{:}k = 2n$	C--(ab)
$P2_1/c$ $h0l{:}l = 2n$ $00l{:}l = 2n$ $0k0{:}k = 2n$	$B2_1/e$ $hkl{:}h+l = 2n$ $h0l{:}h,l = 2n$ $hk0{:}h = 2n$ $0kl{:}l = 2n$ $h00{:}h = 2n$ $00l{:}l = 2n$ $0k0{:}k = 2n$	$C112_1/e$ $hkl{:}h+k = 2n$ $hk0{:}h,k = 2n$ $h0l{:}\ h = 2n$ $0kl{:}\ k = 2n$ $h00{:}h = 2n$ $00l{:}l = 2n$ $0k0{:}k = 2n$	$(C$--$2_1/(ab))$

Figure 2
Scheme showing how the reflection conditions of non-symmorphic space groups with *mP* lattice and metric specialization $a = c$ are transformed by the choice of a *B*-centred cell, then transformed to a *C*-centred *c*-unique setting. The last column shows the corresponding orthorhombic diffraction symbol. For $P2_1/c$, the diffraction symbol is in parentheses because it does not correspond to any orthorhombic space group: a distinction is therefore possible, provided the investigator does not miss the fact that the condition $h0l$: $l = 2n$, which would correspond to *C*-*c*(*ab*), is missing.

6.2. Differentiating H and *t*-H models in class II*B* twinning

In metric merohedry one has to compare the reflection conditions of *H* modified by *t* with those of any group belonging to a different crystal family: when they coincide, an ambiguity may in principle exist, but in many cases the result is actually unambiguous, as we are going to see.

The number of twin laws potentially modifying the reflection conditions of *H* is rather large, but one can significantly reduce the number of cases to be considered by the aid of the normalizers. In class II*B* twinning, this analysis is no longer limited to the Euclidean normalizers but has to make use of the affine normalizers, *i.e.* the normalizers of *H* with respect to the group of all affine mappings, which are no longer restricted to isometries but include also deformations – those deformations necessary to specialize the metric of *H* to that of *G*. The affine normalizer does not depend on the metrical properties of the space group, while the Euclidean normalizer does. Therefore, in general a space group may have more than one Euclidean normalizer, depending on the metric specialization. Space groups are classified, in terms of their normalizers, as follows (Koch *et al.*, 2006):

(i) Cubic, hexagonal, trigonal and tetragonal space groups, as well as 21 types of orthorhombic space groups in which the symmetry elements along the crystallographic axes are of the same type, have only one type of Euclidean normalizer, which also coincides with the affine normalizer.

(ii) The other 38 types of orthorhombic space groups have more than one Euclidean normalizer, as a function of the metric specialization; the affine normalizer coincides with the highest-symmetry Euclidean normalizer.

Table 7
Effect of class II*B* twinning on the reflection conditions of tetragonal crystals with a cubic metric.

Space-group types with the same reflection conditions are listed in a single entry, ordered according to the diffraction symbol in the lower crystal family, as in LVB. When the action of a twin operation modifies the reflection conditions in such a way that they become equivalent to those of one or more cubic groups, the corresponding cubic diffraction symbol is given, otherwise the entry 'incompatible' occurs. The structure of the table follows that used by LVB, *e.g.* l is used as a shorthand notation for $l = 2n$, but equivalent reflection conditions on $0kl$ and $h0l$ are given explicitly because they may be differently affected by incomplete twinning. Reflection conditions *modified* by the twin operations are shown in bold; when the twin operation annihilates a set of reflection conditions, the entry '***ann***' is shown. A comma stands for the Boolean *and* (as in LVB), a forward slash stands for the Boolean *or* (never occurring for untwinned crystals). Twin operations producing non-space-group absences are shown in bold. Monoclinic space groups with a tetragonal normalizer whose fourfold axis is along the monoclinic twofold axis are listed here because their diffraction symbol, when expressed in the tetragonal setting of the normalizer, corresponds to a tetragonal group (see §6.2).

Diffraction symbol in the lower crystal family	*H*	No.	Twin operation (coset representative)	Diffraction symbol in the different crystal family	*hkl*	*hk*0	0*kl*	*h*0*l*	*hhl*	*hh*±*h*	*hh*0	00*l*	0*k*0	*h*00
P-2_1-	$P42_12$	90											*k*	*h*
	$P\bar{4}2_1m$	113												
			$\mathbf{4}_{[100]}$	incompatible									***ann***	*h*
			$\mathbf{4}_{[010]}$	incompatible									*k*	***ann***
			both	*P*---									***ann***	***ann***
$P4_2$--	$P4_2$	77										*l*		
	$P4_2/m$	84												
	$P4_222$	93												
			any	*P*---								***ann***		
$P4_22_1$-	$P4_22_12$	94		$P2_1$--, $P4_2$--								*l*	*k*	*h*
			any	$P2_1$--, $P4_2$--								*l*	*k*	*h*
$P4_1$--	$P4_1$	76										$l = 4n$		
	$P4_3$	78												
	$P4_122$	91												
	$P4_322$	95												
			any	*P*---								***ann***		
$P4_12_1$-	$P4_12_12$	92										$l = 4n$	*k*	*h*
	$P4_32_12$	96												
			any	$P2_1$--, $P4_2$--								***l***	*k*	*h*
P--*c*	$P4_2mc$	105							*l*	*h*		*l*		
	$P\bar{4}2c$	112												
	$P4_2/mmc$	131												
			any	incompatible					***ann***	*h*		***ann***		
P-2_1c	$P\bar{4}2_1c$	114							*l*	*h*		*l*	*k*	*h*
			any	incompatible					***ann***	*h*		*l*	*k*	*h*
P-*b*-	*P*4*bm*	100					*k*	*h*					*k*	*h*
	$P\bar{4}b2$	117												
	*P*4/*mbm*	127												
			$\mathbf{4}_{[100]}$	incompatible			***k/l***	***ann***					***ann***	*h*
			$\mathbf{4}_{[010]}$	incompatible			***ann***	***h/l***					*k*	***ann***
			both	*P*---			***ann***	***ann***					***ann***	***ann***
P-*bc*	$P4_2bc$	106					*k*	*h*	*l*	*h*		*l*	*k*	*h*
	$P4_2/mbc$	135												
			$\mathbf{4}_{[100]}$	incompatible			***k/l***	***ann***	***ann***	*h*		*l*	*k*	*h*
			$\mathbf{4}_{[010]}$	incompatible			***ann***	***h/l***	***ann***	*h*		*l*	*k*	*h*
			both	incompatible			***ann***	***ann***	***ann***	*h*		*l*	*k*	*h*
P-*c*-	$P4_2cm$	101					*l*	*l*				*l*		
	$P\bar{4}c2$	116												
	$P4_2/mcm$	132												
			$\mathbf{4}_{[100]}$	incompatible			***k/l***	***ann***				***ann***		
			$\mathbf{4}_{[010]}$	incompatible			***ann***	***h/l***				***ann***		
			both	*P*---			***ann***	***ann***				***ann***		
P-*cc*	*P*4*cc*	103					*l*	*l*	*l*	*h*		*l*		
	*P*4/*mcc*	124												
			$\mathbf{4}_{[100]}$	incompatible			***k/l***	***ann***	***ann***	*h*		***ann***		
			$\mathbf{4}_{[010]}$	incompatible			***ann***	***h/l***	***ann***	*h*		***ann***		
			both	incompatible			***ann***	***ann***	***ann***	*h*		***ann***		
P-*n*-	$P4_2nm$	102					*k*+*l*	*h*+*l*				*l*	*k*	*h*
	$P\bar{4}n2$	118												
	$P4_2/mnm$	136												
			$\mathbf{4}_{[100]}$	incompatible			*k*+*l*	***ann***				*l*	*k*	*h*
			$\mathbf{4}_{[010]}$	incompatible			***ann***	*h*+*l*				*l*	*k*	*h*
			both	$P2_1$--, $P4_2$--			***ann***	***ann***				*l*	*k*	*h*
P-*nc*	*P*4*nc*	104					*k*+*l*	*h*+*l*	*l*	*h*		*l*	*k*	*h*
	*P*4/*mnc*	128												
			$\mathbf{4}_{[100]}$	incompatible			*k*+*l*	***ann***	***ann***	*h*		*l*	*k*	*h*
			$\mathbf{4}_{[010]}$	incompatible			***ann***	*h*+*l*	***ann***	*h*		*l*	*k*	*h*
			both	incompatible			***ann***	***ann***	***ann***	*h*		*l*	*k*	*h*

Table 7 (continued)

Diffraction symbol in the lower crystal family	H	No.	Twin operation (coset representative)	Diffraction symbol in the different crystal family	hkl	hk0	0kl	h0l	hhl	hh±h	hh0	00l	0k0	h00
Pn--†	P4/n	85				h+k							k	h
	P4/nmm	129												
	P1c1	7												
	P12/c1	13												
	Cc	9												
	C2/c	15												
			$\mathbf{4}_{[100]}$	incompatible		***ann***							***ann***	h
			$\mathbf{4}_{[010]}$	incompatible		***ann***							k	***ann***
			both	P---		***ann***							***ann***	***ann***
$P4_2n$-‡	$P4_2/n$	86				h+k						l	k	h
	$P12_1/c1$	14												
			any	$P2_1$--, $P4_2$--		***ann***						l	k	h
Pn-c	$P4_2/nmc$	137				h+k			l	h		l	k	h
			any	incompatible		***ann***			***ann***	h		l	k	h
Pnb-	P4/nbm	125				h+k	k	h					k	h
			$\mathbf{4}_{[100]}$	incompatible		***h/h+k***	***k/l***	***h/h+l***					***ann***	h
			$\mathbf{4}_{[010]}$	incompatible		***k/h+k***	***k/k+l***	***h/l***					k	***ann***
			both	P---		***ann***	***ann***	***ann***					***ann***	***ann***
Pnbc	$P4_2/nbc$	133				h+k	k	h	l	h		l	k	h
			$\mathbf{4}_{[100]}$	incompatible		***h/h+k***	***k/l***	***h/h+l***	***ann***	h		l	k	h
			$\mathbf{4}_{[010]}$	incompatible		***k/h+k***	***k/k+l***	***h/l***	***ann***	h		l	k	h
			both	incompatible		***ann***	***ann***	***ann***	***ann***	h		l	k	h
Pnc-	$P4_2/ncm$	138				h+k	l	l				l	k	h
			$\mathbf{4}_{[100]}$	incompatible		***k/h+k***	***k/l***	***l/h+l***				l	k	h
			$\mathbf{4}_{[010]}$	incompatible		***h/h+k***	***l/k+l***	***h/l***				l	k	h
			both	$P2_1$--, $P4_2$--		***ann***	***ann***	***ann***				l	k	h
Pncc	P4/ncc	130				h+k	l	l	l	h		l	k	h
			$\mathbf{4}_{[100]}$	incompatible		***k/h+k***	***k/l***	***l/h+l***	***ann***	h		l	k	h
			$\mathbf{4}_{[010]}$	incompatible		***h/h+k***	***l/k+l***	***h/l***	***ann***	h		l	k	h
			both	incompatible		***ann***	***ann***	***ann***	***ann***	h		l	k	h
Pnn-	$P4_2/nnm$	134				h+k	k+l	h+l				l	k	h
			any	Pn--		h+k	k+l	h+l				l	k	h
Pnnc	P4/nnc	126				h+k	k+l	h+l	l	h		l	k	h
			any	incompatible		h+k	k+l	h+l	***ann***	h		l	k	h
$I4_1$--	$I4_1$	80			h+k+l	h+k	k+l	h+l	l	h		l = 4n	k	h
	$I4_122$	98												
			any	I---	h+k+l	h+k	k+l	h+l	l	h		***l***	k	h
I--d	$I4_1md$	109			h+k+l	h+k	k+l	h+l	§	h = 4n	h	l = 4n	k	h
	$I\bar{4}2d$	122												
			any	incompatible	h+k+l	h+k	k+l	h+l	***l***	h = 4n	***ann***	***l***	k	h
I-c-	I4cm	108			h+k+l	h+k	k,l	h,l	l	h		l	k	h
	$I\bar{4}c2$	120												
	I4/mcm	140												
			$\mathbf{4}_{[100]}$	incompatible	h+k+l	h+k	k,l	***h+l***	l	h		l	k	h
			$\mathbf{4}_{[010]}$	incompatible	h+k+l	h+k	***k+l***	h,l	l	h		l	k	h
			both	I---	h+k+l	h+k	***k+l***	***h+l***	l	h		l	k	h
I-cd	$I4_1cd$	110			h+k+l	h+k	k,l	h,l	§	h = 4n	h	l = 4n	k	h
			$\mathbf{4}_{[100]}$	incompatible	h+k+l	h+k	k,l	***h+l***	***l***	h = 4n	h	***l***	k	h
			$\mathbf{4}_{[010]}$	incompatible	h+k+l	h+k	***k+l***	h,l	***l***	h = 4n	h	***l***	k	h
			both	incompatible	h+k+l	h+k	***k+l***	***h+l***	***l***	h = 4n	h	***l***	k	h
$I4_1/a$--	$I4_1/a$	88			h+k+l	h,k	k+l	h+l	l	h	h	***l = 4n***	k	h
			any	I---	h+k+l	***h+k***	k+l	h+l	l	h	***ann***	***l***	k	h
Ia-d	$I4_1/amd$	141			h+k+l	h,k	k+l	h+l	§	h = 4n	h	l = 4n	k	h
			any	incompatible	h+k+l	***h+k***	k+l	h+l	***l***	h = 4n	***ann***	***l***	k	h
Iacd	$I4_1/acd$	142			h+k+l	h,k	k,l	h,l	§	h = 4n	h	l = 4n	k	h
			any	incompatible	h+k+l	h,k	k,l	h,l	***l***	h = 4n	h	***l***	k	h

† The monoclinic groups P1c1, P12/c1, Cc and C2/c with specialized metric $a = c^{1/2}$, $\beta = 135°$ have a tetragonal normalizer and their diffraction symbol is Pn– when expressed in the tetragonal setting. See §6.2. ‡ The monoclinic group $P12_1/c1$ with specialized metric $a = c^{1/2}$, $\beta = 135°$ has a tetragonal normalizer and its diffraction symbol is $P4_2/n$– when expressed in the tetragonal setting. See §6.2. § $2h + l = 4n$.

(iii) Affine normalizers of monoclinic and triclinic space groups are not isomorphic to any group of motions and cannot be characterized by a space-group symbol.

The above classification is based on the fact that a metric specialization does not necessarily increase the symmetry of the normalizer. This is the case, for example, for tetragonal space groups: in fact, the normalizer acts on the types of symmetry elements, but a tetragonal space group has only a single fourfold axis, even if $c = a$, and this axis is not fixed by a fourfold rotation about [100] or [010]. Similarly, *Pcca* (one of the 21 types of orthorhombic space-group types having only one Euclidean normalizer) is not self-conjugate by a fourfold rotation about [001] even if $a = b$, because it has twofold axes along [100] but twofold *screw* axes along [010]. Therefore, *Pcca* has only one Euclidean normalizer, *Pmmm* (basis vectors of the normalizer: **a**/2, **b**/2, **c**/2), which is also its affine normalizer. On the other hand, *Pbam* has the same type of symmetry elements (twofold screw axes) along [100] and [010] and perpendicular to them [a glide plane whose glide component is along the *other* axis in the (001) plane] so that for $a = b$ the two directions become equivalent. *Pbam* therefore has two Euclidean normalizers: *Pmmm* **a**/2, **b**/2, **c**/2, if $a \neq b$, and *P*4/*mmm* **a**/2, **b**/2, **c**/2, if $a = b$; the latter is also the affine normalizer. Since the *m* mirror perpendicular to [001] is of a different nature with respect to the glide planes *b* and *a*, this type of space group has no cubic normalizer even in the case of a cubic metric ($a = b = c$).

When dealing with twins, one has to consider the possibility of a higher-order rotation about an axis as a consequence of metric specialization, even if that rotation does not belong to the affine normalizer of the space group. In the case where the normalizer increases as a function of the metric specialization, the reflection conditions are not influenced by class II*B* twinning, whereas for the other cases the effect of class II*B* twinning on the reflection conditions has to be explicitly worked out. In other terms, space-group types have to be classified in terms of the effect of a metric specialization on both the symmetry of the lattice and the Euclidean normalizer.

Symmorphic types of space groups only possess integral reflection conditions, and this only if their conventional unit cell is not primitive. A twin operation *t* may affect the integral reflection conditions only if *t* is not compatible with the conventional unit cell of the individual: for example, a $4_{[010]}$ rotation when the conventional cell is *A*- or *B*-centred brings to overlap present reflections from an individual with absent reflections from another individual, whereas it has no influence if the conventional unit cell is *C*-, *I*- or *F*-centred. Therefore, in the following analysis only those symmorphic space-group types whose conventional unit cell is not compatible with *t* are considered, the others having their reflection conditions unaffected by *t*.

(*a*) The symmetry of the lattice of cubic, hexagonal and trigonal crystals with hexagonal lattices cannot be increased by a metric specialization; therefore, these crystal systems never give class II*B* twinning.

(*b*) The symmetry of the lattices of trigonal crystals with rhombohedral lattices is increased to cubic by metric specialization (to *cP*, *cF* and *cI* when α = 90°, 60° and 109.47°, respectively), but the affine normalizer is either rhombohedral or hexagonal.

(*c*) The lattice of tetragonal crystals becomes cubic in the presence of a metric specialization ($c = a$); however, tetragonal space groups have only one Euclidean (and thus also affine) normalizer, which is still tetragonal; class II*B* twinning does in general affect the reflection conditions of tetragonal crystals (Table 7).

(*d*) For the 21 types of orthorhombic space groups that have only one type of Euclidean normalizer, the same conclusion as for the tetragonal space groups holds.

(*e*) Among the 38 types of orthorhombic space groups with more than one Euclidean normalizer, two subtypes have to be distinguished (Table 8).

(i) Space groups for which metric specialization enhances the Euclidean normalizer up to cubic symmetry are not influenced in their reflection conditions by class II*B* twinning (see, however, the special case of *Pbca* described below).

(ii) Space groups for which metric specialization enhances the Euclidean normalizer only up to tetragonal symmetry do not show any effect on their reflection conditions when class II*B* twinning corresponds to a tetragonal metric with $a = b$, while class II*B* twinning according to a cubic metric or a tetragonal metric with $a = c$ or $b = c$ does affect the reflection conditions.

(*f*) Monoclinic space groups with an orthorhombic metric specialization may simulate the reflection conditions of an orthorhombic crystal, as shown in Fig. 2 and Table 6; class II*B* twinning does not influence the reflection conditions because the twin operations can only be twofold rotations about symmetry directions of an orthorhombic lattice and mirror reflections across planes normal to them. The same is true for the *hR* specialization of *mS* crystals (Table 6). All monoclinic groups have tetragonal normalizers, which however may correspond to three different metric specializations (see Koch *et al.*, 2006). The first, 'trivial', specialization is obtained for $a = c$ and β = 90°, for which the fourfold axis is along the monoclinic *c* axis: it occurs for *P*2, $P2_1$, *Pm*, *P*2/*m* and $P2_1/m$. The reflection conditions of the symmorphic groups are not affected by class II*B* twinning, while the effect on $P2_1$ and $P2_1/m$ is the same as that on the orthorhombic group $P222_1$, which in fact has the same diffraction symbol if the monoclinic unique axis is oriented to coincide with the orthorhombic *c* axis. For all the other monoclinic groups, this metric specialization corresponds to a normalizer that is only orthorhombic. The non-trivial tetragonal metric specialization is realized in two different ways, depending on whether the conventional unit cell is primitive or centred ($c = a^{1/2}$, β = 135° for *Pc*, *P*2/*c* and $P2_1/c$; $a = c^{1/2}$, β = 135° for *C*2, *Cm*, *Cc*, *C*2/*m* and *C*2/*c*): the fourfold axis of the normalizer is now along the monoclinic *b* axis. These groups have the same reflection conditions of tetragonal groups (when expressed in the tetragonal setting) and thus undergo the same effect of class II*B* twinning.

(i) *Pc* and *P*2/*c* on the one hand, and *Cc* and *C*2/*c* on the other hand, have diffraction symbols *P*1*c*1 and *C*1*c*1, respectively (in the *b*-unique setting); in the tetragonal setting

Table 8
Effect of class II*B* twinning on the reflection conditions of orthorhombic or monoclinic crystals with a tetragonal or cubic metric.

A fourfold rotation about an axis is possible only in correspondence with a metric specialization in the plane perpendicular to that axis. When a cubic or tetragonal Euclidean normalizer exists in correspondence with the metric specialization, that normalizer is indicated and the corresponding twin operation has no effect on the reflection conditions. The basis vectors of the Euclidean normalizer are always ***a***/2, ***b***/2, ***c***/2 except when the Euclidean normalizer has a continuous translation along one or two axes (symbol containing P^1 or P^2), in which case the basis vectors contain an infinitesimal translation along one or two directions. Symmorphic types of space groups with a conventional unit cell of type *P*, *I* or *F* are not shown because they only have integral reflection conditions that are not affected by the twin operations. The same conventions are adopted as for Table 7. Entries are ordered according to the diffraction symbol in the lower crystal family (crystal family of the individual), as given in LVB.

Diffraction symbol in the lower crystal family	*H*	No.	Twin operation (coset representative)	Diffraction symbol in the different crystal family	*hkl*	*hk*0	0*kl*	*h*0*l*	00*l*	0*k*0	*h*00	Specialized metric	Euclidean normalizer
P--2_1	$P112_1$	4							*l*			$a = b$, $\gamma = 90°$	P^14/mmm
	$P112_1/m$	11										$a = b$, $\gamma = 90°$	$P4/mmm$
	$P222_1$	17										$a = b$	$P4_2/mmc$
			any	*P*---					***ann***				
$P2_12_1$-	$P2_12_12$	18								*k*	*h*	$a = b$	$P4/mmm$
			$4_{[001]}$	P-2_1-						*k*	*h*		
			$4_{[100]}$	$P4_2$--						***ann***	*h*		
			$4_{[010]}$	$P4_2$--						*k*	***ann***		
			all	*P*---						***ann***	***ann***		
$P2_12_12_1$	$P2_12_12_1$	19							*l*	*k*	*h*	$a = b \neq c$	$P4_2/mmc$
												$a = b = c$	$Pm\bar{3}n$
			any	$P4_22_1$-					*l*	*k*	*h*		
P--*a*	*Pmma*	51				*h*					*h*	---	*Pmmm*
			$\mathbf{4_{[001]}}$	incompatible		***h/k***					***ann***		
			$4_{[100]}$	$P4_2$--		***ann***					*h*		
			$4_{[010]}$	*P*---		***ann***					***ann***		
			all	*P*---		***ann***					***ann***		
P--*n*	*Pmmn*	59				*h*+*k*				*k*	*h*	$a = b$	$P4/mmm$
			$4_{[001]}$	*Pn*--		*h*+*k*				*k*	*h*		
			$4_{[100]}$	$P4_2$--		***ann***				***ann***	*h*		
			$4_{[010]}$	$P4_2$--		***ann***				*k*	***ann***		
			all	*P*---		***ann***				***ann***	***ann***		
P-*a*-	*Pma*2	28						*h*			*h*	---	P^1mmm
			$4_{[001]}$	*P*---				***ann***			***ann***		
			$4_{[100]}$	$P4_2$--				***ann***			*h*		
			$\mathbf{4_{[010]}}$	incompatible				***h/l***			***ann***		
			all	*P*---				***ann***			***ann***		
P-*c*-	*P*1*c*1	7						*l*	*l*			$\beta = 90°$	P^2mmm
	*P*12/*c*1	13										$\beta = 90°$	*Pmmm*
	$Pmc2_1$	26										---	P^1mmm
			$4_{[001]}$	$P4_2$--				***ann***	*l*				
			$4_{[100]}$	*P*---				***ann***	***ann***				
			$\mathbf{4_{[010]}}$	incompatible				***h/l***	***ann***				
			all	*P*---				***ann***	***ann***				
P-$2_1/c$-	$P12_1/c1$	14						*l*	*l*	*k*		$\beta = 90°$	*Pmmm*
			$4_{[001]}$	$P4_2$--				***ann***	*l*	***ann***			
			$\mathbf{4_{[100]}}$	incompatible				***ann***	*l*	*k*			
			$\mathbf{4_{[010]}}$	incompatible				***h/l***	***ann***	*k*			
			all	*P*---				***ann***	***ann***	***ann***			
P-*n*-	$Pmn2_1$	31						*h*+*l*	*l*		*h*	---	P^1mmm
			$4_{[001]}$	$P4_2$--				***ann***	*l*		***ann***		
			$4_{[100]}$	$P4_2$--				***ann***	***ann***		*h*		
			$4_{[010]}$	*Pn*--				*h*+*l*	*l*		*h*		
			all	*P*---				***ann***	***ann***		***ann***		
P-*na*	*Pmna*	53				*h*		*h*+*l*	*l*		*h*	---	*Pmmm*
			$\mathbf{4_{[001]}}$	incompatible		***h/k***		***ann***	*l*		***ann***		
			$\mathbf{4_{[100]}}$	incompatible		***h/h+k***		***h/h+l***	***ann***		*h*		
			$4_{[010]}$	*Pn*--		***ann***		*h*+*l*	*l*		*h*		
			all	*P*---		***ann***		***ann***	***ann***		***ann***		
Pba-	*Pba*2	32					*k*	*h*		*k*	*h*	$a = b$	P^14/mmm
	Pbam	55											$P4/mmm$
			$4_{[001]}$	*P*-*b*-			*k*	*h*		*k*	*h*		
			$\mathbf{4_{[100]}}$	incompatible			***k/l***	***ann***		***ann***	*h*		
			$\mathbf{4_{[010]}}$	incompatible			***ann***	***h/l***		*k*	***ann***		
			all	*P*---			***ann***	***ann***		***ann***	***ann***		

Table 8 (continued)

Diffraction symbol in the lower crystal family	H	No.	Twin operation (coset representative)	Diffraction symbol in the different crystal family	hkl	hk0	0kl	h0l	00l	0k0	h00	Specialized metric	Euclidean normalizer
Pban	Pban	50				h+k	k	h		k	h	a = b	P4/mmm
			$4_{[001]}$	Pnb-		h+k	k	h		k	h		
			$\mathbf{4}_{[100]}$	incompatible		**h/h+k**	**k/l**	**h/h+l**		**ann**	h		
			$\mathbf{4}_{[010]}$	incompatible		**k/h+k**	**k/k+l**	**h/l**		k	**ann**		
			all	P---		**ann**	**ann**	**ann**		**ann**	**ann**		
Pbc-	Pbcm	57					k	l	l	k		---	Pmmm
			$\mathbf{4}_{[001]}$	incompatible			**k/l**	**h/l**	l	**ann**			
			$\mathbf{4}_{[100]}$	incompatible			**k/l**	**ann**	l	k			
			$\mathbf{4}_{[010]}$	incompatible			**ann**	**h/l**	**ann**	k			
			all	P---			**ann**	**ann**	**ann**	**ann**			
Pbca	Pbca	61				h	k	l	l	k	h	a = b = c	$Pm\bar{3}$
			any	incompatible		**h/k**	**k/l**	**h/l**	l	k	h		
Pbcn	Pbcn	60				h+k	k	l	l	k	h	---	Pmmm
			$\mathbf{4}_{[001]}$	incompatible		h+k	**k/l**	**h/l**	l	k	h		
			$\mathbf{4}_{[100]}$	incompatible		**k/h+k**	**k/l**	**l/h+l**	l	k	h		
			$\mathbf{4}_{[010]}$	incompatible		**k/h+k**	**k/k+l**	**h/l**	l	k	h		
			all	incompatible		**k/h+k**	**ann**	**ann**	l	k	h		
Pca-	$Pca2_1$	29					l	h	l		h	---	P^1mmm
			$\mathbf{4}_{[001]}$	incompatible			**k/l**	**h/l**	l		**ann**		
			$\mathbf{4}_{[100]}$	incompatible			**k/l**	**ann**	**ann**		h		
			$\mathbf{4}_{[010]}$	incompatible			**ann**	**h/l**	l		h		
			all	P---			**ann**	**ann**	**ann**		**ann**		
Pcc-	Pcc2	27					l	l	l			a = b	P^14/mmm
	Pccm	49											P4/mmm
			$4_{[001]}$	P-c-			l	l	l				
			$\mathbf{4}_{[100]}$	incompatible			**k/l**	**ann**	**ann**				
			$\mathbf{4}_{[010]}$	incompatible			**ann**	**h/l**	**ann**				
			all	P---			**ann**	**ann**	**ann**				
Pcca	Pcca	54				h	l	l	l		h	---	Pmmm
			$\mathbf{4}_{[001]}$	incompatible		**h/k**	l	l	l		**ann**		
			$\mathbf{4}_{[100]}$	incompatible		**h/k**	**k/l**	**h/l**	**ann**		h		
			$\mathbf{4}_{[010]}$	incompatible		h	l	**h/l**	l		h		
			all	incompatible		**h/k**	**k/l**	**h/l**	**ann**		**ann**		
Pccn	Pccn	56				h+k	l	l	l	k	h	a = b	P4/mmm
			$4_{[001]}$	Pnc-		h+k	l	l	l	k	h		
			$\mathbf{4}_{[100]}$	incompatible		**k/h+k**	**k/l**	**l/h+l**	l	k	h		
			$\mathbf{4}_{[010]}$	incompatible		**h/k**	**l/k+l**	**h/l**	l	k	h		
			all	$P2_1$--, $P4_2/$--		**ann**	**ann**	**ann**	l	k	h		
Pn-a	Pnma	62				h	k+l		l	k	h	---	Pmmm
			$\mathbf{4}_{[001]}$	incompatible		**h/k**	**ann**		l	k	h		
			$4_{[100]}$	$P4_2/n$--		**ann**	k+l		l	k	h		
			$\mathbf{4}_{[010]}$	incompatible		**h/h+k**	**l/k+l**		l	k	h		
			all	$P2_1$--, $P4_2/$--		**ann**	**ann**		l	k	h		
Pna-	$Pna2_1$	33					k+l	h	l	k	h	---	P^1mmm
			$\mathbf{4}_{[001]}$	incompatible			**k/k+l**	**h/h+l**	l	k	h		
			$4_{[100]}$	$P4_2/n$--			k+l	**ann**	l	k	h		
			$\mathbf{4}_{[010]}$	incompatible			**ann**	**h/l**	l	k	h		
			all	$P2_1$--, $P4_2/$--			**ann**	**ann**	l	k	h		
Pnc-	Pnc2	30					k+l	l	l	k		---	P^1mmm
			$\mathbf{4}_{[001]}$	incompatible			**l/k+l**	**l/h+l**	l	**ann**			
			$4_{[100]}$	Pn--			k+l	**ann**	l	k			
			$\mathbf{4}_{[010]}$	incompatible			**ann**	**l/h+l**	**ann**	k			
			all	P---			**ann**	**ann**	**ann**	**ann**			
Pnn-	Pnn2	34					k+l	h+l	l	k	h	a = b	P^14/mmm
	Pnnm	58											P4/mmm
			$\mathbf{4}_{[001]}$	P-n-			k+l	h+l	l	k	h		
			$\mathbf{4}_{[100]}$	$P4_2/n$--			k+l	**ann**	l	k	h		
			$\mathbf{4}_{[010]}$	$P4_2/n$--			**ann**	h+l	l	k	h		
			all	$P2_1$--, $P4_2/$--			**ann**	**ann**	l	k	h		
Pnna	Pnna	52				h	k+l	h+l	l	k	h	---	Pmmm
			$\mathbf{4}_{[001]}$	incompatible		**h/k**	k+l	h+l	l	k	h		
			$\mathbf{4}_{[100]}$	incompatible		**h/h+k**	k+l	**h/h+l**	l	k	h		
			$\mathbf{4}_{[010]}$	incompatible		**h/h+k**	**l/k+l**	h+l	l	k	h		
			all	$P2_1$--, $P4_2/$--		**ann**	**ann**	**ann**	l	k	h		

Table 8 (continued)

Diffraction symbol in the lower crystal family	H	No.	Twin operation (coset representative)	Diffraction symbol in the different crystal family	hkl	hk0	0kl	h0l	00l	0k0	h00	Specialized metric	Euclidean normalizer
Pnnn	Pnnn	48				h+k	k+l	h+l	l	k	h	$a = b \neq c$	P4/mmm
												$a = b = c$	$Pm\bar{3}m$
			all	Pnn-		h+k	k+l	h+l	l	k	h		
C---†	C121	5			h+k	h+k	k	h		k	h	$\beta = 90^\circ$	P^1mmm
	C1m1	8											P^2mmm
	C12/m1	12											Pmmm
	C222	21										$a = b$	P4/mmm
	Cmm2	35											P^14/mmm
	Cmmm	65											P4/mmm
			$4_{[001]}$	P---‡	h+k	h+k	k	h		k	h		
			$4_{[100]}$	incompatible	**h+k/h+l**	**h/h+k**	**k/l**	**h/h+l**		**ann**	h		
			$4_{[010]}$	incompatible	**h+k/k+l**	**k/h+k**	**k/k+l**	**h/l**		k	**ann**		
			all	P---	**ann**	**ann**	**ann**	**ann**		**ann**	**ann**		
$C\text{--}2_1$	$C222_1$	20			h+k	h+k	k	h	l	k	h	$a = b$	$P4_2/mmc$
			$4_{[001]}$	incompatible	h+k	h+k	k	h	l	k	h		
			$4_{[100]}$	incompatible	**h+k/h+l**	**h/h+k**	**k/l**	**h/h+l**	l	k	h		
			$4_{[010]}$	incompatible	**h+k/k+l**	**k/h+k**	**k/k+l**	**h/l**	l	k	h		
			all	$P2_1\text{--}$, $P4_2\text{--}$	**ann**	**ann**	**ann**	**ann**	l	k	h		
C--(ab)	Cmme	67			h+k	h,k	k	h		k	h	$a = b$	P4/mmm
			$4_{[001]}$	Pn--	h+k	h,k	k	h		k	h		
			$4_{[100]}$	incompatible	**h+k,h+l**	**h**	**k/l**	h		**ann**	h		
			$4_{[010]}$	incompatible	**h+k,k+l**	**k**	k	**h/l**		k	**ann**		
			all	incompatible	**ann**	**h/k**	**k/l**	**h/l**		**ann**	**ann**		
C-c-	C1c1	9			h+k	h+k	k	h,l	l	k	h	$\beta = 90^\circ$	P^2mmm
	C12/c1	15										$\beta = 90^\circ$	Pmmm
	$Cmc2_1$	36										---	P^1mmm
	Cmcm	63										---	Pmmm
			$4_{[001]}$	$P4_2\text{--}$	h+k	h+k	k	**h**	l	k	h		
			$4_{[100]}$	incompatible	**h+k/h+l**	h+k	**k/l**	**h+l**	l	k	h		
			$4_{[010]}$	incompatible	**h+k/k+l**	**k/h+k**	**k/k+l**	h,l	l	k	h		
			all	incompatible	**ann**	**k/h+k**	**ann**	**h/h+l**	l	k	h		
C-c(ab)	Cmce	64			h+k	h,k	k	h,l	l	k	h	---	Pmmm
			$4_{[001]}$	$P4_2/n\text{--}$	h+k	h,k	k	**h**	l	k	h		
			$4_{[100]}$	incompatible	**h+k,h+l**	h,k	**k/l**	h,l	l	k	h		
			$4_{[010]}$	incompatible	**h+k,k+l**	**k**	k	h,l	l	k	h		
			all	incompatible	**ann**	**k**	**k/l**	**h**	l	k	h		
Ccc-	Ccc2	37			h+k	h+k	k,l	h,l	l	k	h	$a = b$	P^14/mmm
	Cccm	66										$a = b$	P4/mmm
			$4_{[001]}$	P-c-	h+k	h+k	k,l	h,l	l	k	h		
			$4_{[100]}$	incompatible	**h+k/h+l**	h+k	k,l	**h+l**	l	k	h		
			$4_{[010]}$	incompatible	**h+k/k+l**	h+k	**k+l**	h,l	l	k	h		
			all	Pnn-	**ann**	h+k	**k+l**	**h+l**	l	k	h		
Ccc(ab)	Ccce	68			h+k	h,k	k,l	h,l	l	k	h	$a = b$	P4/mmm
			$4_{[001]}$	Pn-c	h+k	h,k	k,l	h,l	l	k	h		
			$4_{[100]}$	incompatible	**h+k,h+l**	h,k	k,l	h,l	l	k	h		
			$4_{[010]}$	incompatible	**h+k,k+l**	h,k	k,l	h,l	l	k	h		
			all	incompatible	**ann**	h,k	k,l	h,l	l	k	h		
A---	Amm2	38			k+l	k	k+l	l	l	k		---	P^1mmm
			$4_{[001]}$	incompatible	**h+l/k+l**	**h/k**	**l/k+l**	**l/h+l**	l	**ann**			
			$4_{[100]}$	P---	k+l	k	k+l	l	l	k			
			$4_{[010]}$	incompatible	**h+k/k+l**	**k/h+k**	**k/k+l**	**h/l**	**ann**	k			
			all	P---	**ann**	**ann**	**ann**	**ann**	**ann**	**ann**			
A-a-	Ama2	40			k+l	k	k+l	h,l	l	k	h	---	P^1mmm
			$4_{[001]}$	incompatible	**h+l/k+l**	**h/k**	k+l	**h+l**	l	k	h		
			$4_{[100]}$	$P4_2/n\text{--}$	k+l	k	k+l	**l**	l	k	h		
			$4_{[010]}$	incompatible	**h+k/k+l**	**k/h+k**	**k/k+l**	h,l	l	k	h		
			all	incompatible	**ann**	**k/h+k**	**k/k+l**	**h/h+l**	l	k	h		
A(bc)--	Aem2	39			k+l	k	k,l	l	l	k		---	P^1mmm
			$4_{[001]}$	incompatible	**h+l/k+l**	**h/k**	**l**	l	l	**ann**			
			$4_{[100]}$	Pn--	k+l	k	k,l	l	l	k			
			$4_{[010]}$	incompatible	**h+k/k+l**	k	**k**	**h/l**	**ann**	k			
			all	incompatible	**ann**	**h/k**	**k/l**	**h/l**	**ann**	**ann**			
A(bc)a-	Aea2	41			k+l	k	k,l	h,l	l	k	h	---	P^1mmm
			$4_{[001]}$	incompatible	**h+l/k+l**	**h/k**	k,l	h,l	l	k	h		
			$4_{[100]}$	P--c	k+l	k	k,l	**l**	l	k	h		

Table 8 (continued)

Diffraction symbol in the lower crystal family	*H*	No.	Twin operation (coset representative)	Diffraction symbol in the different crystal family	*hkl*	*hk*0	0*kl*	*h*0*l*	00*l*	0*k*0	*h*00	Specialized metric	Euclidean normalizer
			$\mathbf{4_{[010]}}$	incompatible	***h+k/k+l***	*k*	***k***	*h,l*	*l*	*k*	*h*		
			all	incompatible	***ann***	***h/k***	*k*	*l*	*l*	*k*	*h*		
I---	$I2_12_12_1$	24			*h+k+l*	*h+k*	*k+l*	*h+l*	*l*	*k*	*h*	$a = b \neq c$	$P4_2/mmc$
												$a = b = c$	$Pm\bar{3}n$
			any	*I---*	*h+k+l*	*h+k*	*k+l*	*h+l*	*l*	*k*	*h*		
I--(ab)	*Imma*	74			*h+k+l*	*h,k*	*k+l*	*h+l*	*l*	*k*	*h*	$a = b$	$P4_2/mmc$
			$\mathbf{4_{[001]}}$	incompatible	*h+k+l*	*h,k*	*k+l*	*h+l*	*l*	*k*	*h*		
			$4_{[100]}$	*I---*	*h+k+l*	***h+k***	*k+l*	*h+l*	*l*	*k*	*h*		
			$4_{[010]}$	*I---*	*h+k+l*	***h+k***	*k+l*	*h+l*	*l*	*k*	*h*		
			all	*I---*	*h+k+l*	***h+k***	*k+l*	*h+l*	*l*	*k*	*h*		
I-(ac)-	*Ima*2	46			*h+k+l*	*h+k*	*k+l*	*h,l*	*l*	*k*	*h*	---	P^1mmm
			$\mathbf{4_{[001]}}$	*I---*	*h+k+l*	*h+k*	*k+l*	***h+l***	*l*	*k*	*h*		
			$\mathbf{4_{[100]}}$	*I---*	*h+k+l*	*h+k*	*k+l*	***h+l***	*l*	*k*	*h*		
			$\mathbf{4_{[010]}}$	incompatible	*h+k+l*	*h+k*	*k+l*	*h,l*	*l*	*k*	*h*		
			all	*I---*	*h+k+l*	*h+k*	*k+l*	***h+l***	*l*	*k*	*h*		
Iba-	*Iba*2	45			*h+k+l*	*h+k*	*k,l*	*h,l*	*l*	*k*	*h*	$a = b$	P^14/mmm
	Ibam	72										$a = b$	$P4/mmm$
			$4_{[001]}$	*I-c-*	*h+k+l*	*h+k*	*k,l*	*h,l*	*l*	*k*	*h*		
			$\mathbf{4_{[100]}}$	incompatible	*h+k+l*	*h+k*	*k,l*	***h+l***	*l*	*k*	*h*		
			$\mathbf{4_{[010]}}$	incompatible	*h+k+l*	*h+k*	***k+l***	*h,l*	*l*	*k*	*h*		
			all	*I---*	*h+k+l*	*h+k*	***k+l***	***h+l***	*l*	*k*	*h*		
Ibca	*Ibca*	73			*h+k+l*	*h,k*	*k,l*	*h,l*	*l*	*k*	*h*	$a = b \neq c$	$P4_2/mmc$
			$\mathbf{4_{[001]}}$	incompatible	*h+k+l*	*h,k*	*k,l*	*h,l*	*l*	*k*	*h*	$a = b = c$	$Pm\bar{3}n$
			$\mathbf{4_{[100]}}$	incompatible	*h+k+l*	*h,k*	*k,l*	*h,l*	*l*	*k*	*h*		
			$\mathbf{4_{[010]}}$	incompatible	*h+k+l*	*h,k*	*k,l*	*h,l*	*l*	*k*	*h*		
			all	*Ia--*	*h+k+l*	*h,k*	*k,l*	*h,l*	*l*	*k*	*h*		
Fdd-	*Fdd*2	43			*h+k,h+l,k+l*	*h,k*	$k+l = 4n$, *k,l*	$h+l = 4n$, *h,l*	$l = 4n$	$k = 4n$	$h = 4n$	$a = b$	P^14/nbm
			$\mathbf{4_{[001]}}$	incompatible	*h+k,h+l,k+l*	*h,k*	$k+l = 4n$, *k,l*	$h+l = 4n$, *h,l*	$l = 4n$	$k = 4n$	$h = 4n$		
			$\mathbf{4_{[100]}}$	incompatible	*h+k,h+l,k+l*	*h,k*	$k+l = 4n$, *k,l*	***h,l***	$l = 4n$	$k = 4n$	$h = 4n$		
			$\mathbf{4_{[010]}}$	incompatible	*h+k,h+l,k+l*	*h,k*	***k,l***	$h+l = 4n$, *h,l*	$l = 4n$	$k = 4n$	$h = 4n$		
			all	$F4_1$--	*h+k,h+l,k+l*	*h,k*	***k,l***	***h,l***	$l = 4n$	$k = 4n$	$h = 4n$		
Fddd	*Fddd*	70			*h+k,h+l,k+l*	$h+k = 4n$, *k,k*	$k+l = 4n$, *k,l*	$h+l = 4n$, *h,l*	$l = 4n$	$k = 4n$	$h = 4n$	$a = b \neq c$	$P4_2/nnm$
												$a = b = c$	$Pn\bar{3}m$
			$4_{[001]}$	*I--d*	*h+k,h+l,k+l*	$h+k = 4n$, *h,k*	$k+l = 4n$, *k,l*	$h+l = 4n$, *h,l*	$l = 4n$	$k = 4n$	$h = 4n$		
			$4_{[100]}$	*I--d*	*h+k,h+l,k+l*	$h+k = 4n$, *h,k*	$k+l = 4n$, *k,l*	$h+l = 4n$, *h,l*	$l = 4n$	$k = 4n$	$h = 4n$		
			$4_{[010]}$	*I--d*	*h+k,h+l,k+l*	$h+k = 4n$, *h,k*	$k+l = 4n$, *k,l*	$h+l = 4n$, *h,l*	$l = 4n$	$k = 4n$	$h = 4n$		
			all	*Fd--*	*h+k,h+l,k+l*	$h+k = 4n$, *h,k*	$k+l = 4n$, *k,l*	$h+l = 4n$, *h,l*	$l = 4n$	$k = 4n$	$h = 4n$		

† A trivial tetragonal metric specialization for these monoclinic groups corresponds only to an orthorhombic normalizer (see §6.2), but because these are symmorphic groups the effect of class II*B* twinning on their reflection conditions is the same as for their orthorhombic supergroups, which have instead a tetragonal normalizer. ‡ In the presence of a tetragonal metric, the integral reflection conditions of a space-group type with *oC* conventional cell disappear when expressed in the conventional *tP* cell. Furthermore, the zonal reflection conditions on *h*0*l* and 0*kl* lose their *h* and *k* components, respectively. Ditto for space-group types with an *oA* orthorhombic conventional cell when the tetragonal metric is realized in the (100) plane.

corresponding to the specialized metric both become *Pn*-- and the effect of class II*B* twinning on these four groups is the same as that on $P4/n$.

(ii) $P2_1/c$ has diffraction symbol $P12_1/c1$ (in the *b*-unique setting); in the tetragonal setting corresponding to the specialized metric it becomes $P4_2/n$-- and the effect of class II*B* twinning on this group is the same as that on $P4_2/n$.

(iii) *C*2, *Cm* and *C*2/*m* are symmorphic groups; in the tetragonal setting corresponding to the specialized metric the conventional cell is primitive and the diffraction symbol becomes *P*--. No effect of class II*B* twinning appears from the reflection conditions.

(*g*) Triclinic space-group types do not give reflection conditions and class II*B* twinning cannot be recognized from the reflection conditions; the only indication one may get, if diffraction enhancement of symmetry is not realized, comes from the discrepancy between the metric symmetry and the symmetry of the intensity distribution.

Hereafter, the normalizers are given according to the tables in Koch *et al.* (2006). When the twin operation leads to reflection conditions corresponding to those of some type of space group, the diffraction symbol is given, following Looijenga-Vos & Buerger (2006) (indicated as LVB in the tables); otherwise, the entry 'incompatible' already used in Table 6 is given.

6.2.1. Rhombohedral space-group types. Of the seven rhombohedral space-group types, five are symmorphic and show no reflection conditions in rhombohedral axes. The two non-symmorphic space-group types, *R*3*c* and $R\bar{3}c$, differ by an inversion centre, which does not affect the reflection conditions. It is therefore enough to investigate the effect of class II*B* twinning on one of the two, *i.e.* *R*3*c*, which is also an interesting study case illustrating the general procedure used to obtain Tables 7 and 8.

The cubic minimal supergroup of $3m$ is $43m$ and the index of P in P' is $[P'{:}P] = 4$. Therefore, three twin laws are obtained by coset decomposition, each of which can be represented by a fourfold rotation about a basis vector of the specialized cubic lattice. The reflection conditions for $R3c$ are hhl: $l = 2n$ and hhh: $h = 2n$, which is simply a specialization of the former. A fourfold rotation about c exchanges h and k, never superimposing present reflections from one individual with absent reflections for other individuals: the twin law represented by $4_{[001]}$ does not affect the reflection conditions. On the other hand, $4_{[100]}$ and $4_{[010]}$ annihilate all the reflection conditions by superposing hhl with hlh or lhh, respectively; only the special case of hhh: $h = 2n$ is not affected, but taken alone these reflection conditions are not characteristic of any space group. The two twin laws represented by $4_{[100]}$ and $4_{[010]}$ do affect the diffraction pattern and introduce non-space-group absences by annihilating part of the reflection conditions of H: this is enough to differentiate between the **H** and ***t*-H** models, provided that the investigator does not miss the systematic character of the absences on the very special class of reflections hhh.

6.2.2. Tetragonal space-group types. Class IIB twinning of tetragonal crystals is possible only in the presence of a cubic specialization of the lattice. The twin operation belongs to the cubic crystal family and therefore it is contained in a coset of the cubic P' with respect to a tetragonal subgroup $P_{\rm M}$ of lowest index in P'. In fact, if P is holohedral, P' is itself holohedral; it is a minimal supergroup of P and the index of P in P' is $[P'{:}P] = 3$. If P is merohedral, $[P'{:}P]$ can be 3, 6 or 12 while $[P'{:}P_{\rm M}] = 3$. This intermediate group $P_{\rm M}$ corresponds to twinning by syngonic merohedry (either class I or class IIA) that accompanies class IIB twinning in the case of a complete twin, but it is not necessarily present when the twin is incomplete.

The coset decomposition of P' in terms of $P_{\rm M}$ gives three cosets: the $P_{\rm M}$ subgroup and two twin laws, containing the $4_{[100]}$ and $4_{[010]}$ rotations, respectively. For example, a crystal belonging to the geometric crystal class 4 and having a cubic lattice may undergo class IIB twinning by a $4_{[100]}$ or $4_{[010]}$ rotation. The cubic extension of 4 is 432 and the index of 4 in 432 is 6. The intermediate group $P_{\rm M}$ is 422 and the coset decomposition of 432 in terms of 422 gives two twin laws, one containing the fourfold twin axis [100] and the other the fourfold twin axis [010]. The complete twin of six individuals is realized when class IIA twinning according to $2_{\langle 110\rangle}$ is also present, otherwise the twin is incomplete ($N < 6$).

Because the affine normalizer of a tetragonal space group is itself tetragonal, class IIB twinning does in general affect the reflection conditions of a tetragonal crystal. However, tetragonal space-group types have only two types of conventional unit cells (P and I) which are among the conventional unit cells of cubic crystals too (P, I and F): therefore, a class IIB twin operation belonging to a cubic lattice does not affect the reflection conditions of the 16 types of tetragonal symmorphic space groups. The symmetry of the diffraction intensities stays tetragonal unless the twin of H is complete and the individuals have all the same volume, in which case it becomes cubic. The measured diffractions are, however, the unphased sum of the intensities from each individual and the structure cannot be solved.

Class IIB twinning affects the reflection conditions of crystals belonging to the 52 non-symmorphic space-group types; the analysis is done by applying the two rotations $4_{[100]}$ and $4_{[010]}$, all the other operations being equivalent because they belong to the same cosets as these (Table 7).

In contrast to *International Tables for Crystallography,* in Table 7 the zonal reflection conditions for $0kl$ and $h0l$ are given explicitly, because they may be differently affected by incomplete twinning, therefore breaking the tetragonal symmetry of the reflection conditions (no similar effect appears for other symmetry-related reflection conditions, like those on hhl and $h\bar{h}l$, which are therefore not separated). This is for example the case for $P\bar{4}2_1m$ when only one twin law is active: the reflection conditions on either $0kl$ or $h0l$ are annihilated, but not both.

Inspection of Table 7 shows that:

(i) the twin operations sometimes produce annihilation of the reflection conditions, thus simulating the diffraction pattern of a symmorphic space-group type; this occurs for $P4_1$, $P4_2$, $P4_3$, $P4_122$, $P4_222$, $P4_322$, $P4_2/m$ for any of the two twin laws, and $P4/n$, $P42_12$, $P4bm$, $P\bar{4}2_1m$, $P\bar{4}c2$, $P\bar{4}b2$, $P4_2cm$, $P4/nmm$, $P4/mbm$, $P4_2/mcm$ when both twin laws are active;

(ii) the twin operations sometimes result in observed reflection conditions undergoing the cyclic h, k, l permutation typical of cubic crystals; this occurs for $I4_1$, $I4_122$, $P4_2/n$, $I4_1/a$, $P4_12_12$, $P4_22_12$, $P4_32_12$, $P4_2/nnm$ for any of the two twin laws, and for $P4_2nm$, $P\bar{4}n2$, $P4_2/mnm$, $I4cm$, $I\bar{4}c2$, $I4/mcm$ when both twin laws are active;

(iii) in all other cases, non-space-group absences occur in the diffraction pattern of the twin: the entry *incompatible* is then shown in the column giving the diffraction symbol. In fact, the reflection conditions produced by twinning are not compatible with a *cubic* space-group type, because the permutation of h, k, l indices does not occur (for example, $P4/n$ or $P4/nmm$ when only one twin law is active), or because the twin operation leaves only an unusual subset of the original reflection conditions: typical is the case of annihilation of the reflection conditions on hhl which leaves conditions only on $hh{\pm}h$ (reflection condition: $h = 2n$ or $h = 4n$: see Table 7) that we have already seen for the rhombohedral space groups.

For cases (i) and (ii) above, where the presence of twinning is not evident from the inspection of the diffraction pattern, the same arguments on the symmetry of the intensities hold as in the case of the symmorphic space-group types.

6.2.3. Orthorhombic space-group types. Class IIB twinning of orthorhombic crystals is possible only in the presence of tetragonal, cubic or hexagonal specializations of the lattice. The twin operation is contained in a coset of the hexagonal, cubic or tetragonal P' with respect to the orthorhombic subgroup P.

Orthorhombic types of space groups may have different types of metric specialization: three tetragonal specializations

($a = b$, $a = c$, and $b = c$), three hexagonal specializations ($a = b \times 3^{1/2}$ or $b = a \times 3^{1/2}$ for oC, $a = c \times 3^{1/2}$ or $c = a \times 3^{1/2}$ for oB, $c = b \times 3^{1/2}$ or $b = c \times 3^{1/2}$ for oA; any of them for oF) and a cubic specialization ($a = b = c$). Differently from the tetragonal case, class II*B* twinning can here also affect the diffraction pattern of some symmorphic types of space groups, namely those with a lattice type not compatible with the metric of the specialized lattice. This is the case for symmorphic space-group types with an *S* type of conventional unit cell; always, for a cubic specialized metric; in two out of three cases for a tetragonal specialized metric (*A* and *B* for $4_{[001]}$; *B* and *C* for $4_{[100]}$; *A* and *C* for $4_{[010]}$); and finally of *F* type if the metric is hexagonal. Table 8 gives the results for all types of orthorhombic space groups with cubic or tetragonal metric but with the symmorphic types with a *P*, *I* or *F* type of conventional unit cell, for which the integral reflection conditions are not affected by class II*B* twinning.

Space-group types with cubic affine normalizer. Eleven types of orthorhombic space groups ($P222$, $P2_12_12_1$, $F222$, $I222$, $I2_12_12_1$, *Pmmm, Pnnn, Fmmm, Fddd, Immm, Ibca*) have both tetragonal and cubic Euclidean normalizers, whose Laue class always corresponds to the holohedry: it follows that class II*B* twinning never affects the reflection conditions of a space group belonging to one of these 11 types.

The space-group type *Pbca* is particular in two respects: first of all, it has orthorhombic and cubic, but no tetragonal Euclidean normalizers: in fact, pairs of twofold screw axes are separated by $\frac{1}{4}$ along the three crystallographic axes and a tetragonal specialization of the metric does not produce a tetragonal normalizer. If, however, the metric is cubic, the basis vectors of the normalizer become half those of the space group along *all* the directions and the $\frac{1}{4}$ separation in the space group becomes $\frac{1}{2}$ in the normalizer, *i.e.* it is annihilated.

Secondly, the cubic affine normalizer of *Pbca* is $Pm\overline{3}$ (**a**/2, **b**/2, **c**/2), whose Laue class is $m\overline{3}$: a twin operation belonging to the coset of the cubic holohedry with respect to $m\overline{3}$ modifies the reflection condition of a crystal having a space group of type *Pbca*. In fact, the reflection conditions for *Pbca* are $0kl$: $k = 2n$, $h0l$: $l = 2n$, $hk0$: $h = 2n$, $h00$: $h = 2n$, $0k0$: $k = 2n$, $00l$: $l = 2n$. A $4_{[001]}$ rotation brings to overlap, for example, $u0e$ (present) reflections with $0ue$ (absent), $e0u$ (absent) with $0eu$ (present) and so on, resulting in the observed reflection conditions $h0l$: h or $l = 2n$, $0kl$: k or $l = 2n$, $hk0$: h or $k = 2n$, $h00$: $h = 2n$, $0k0$: $k = 2n$, $00l$: $l = 2n$. In contrast to that, a $3_{[111]}$ rotation, which belongs to the Laue class of the normalizer, brings to overlap $ek0$, $0el$ and $h0e$ reflections (all present) and $uk0$, $0ul$ and $h0u$ reflections (all absent), without affecting the observed reflection conditions.

Space-group types with tetragonal affine normalizer. Twenty-six types of orthorhombic space groups have a tetragonal affine normalizer ($P222_1$, $P2_12_12$, $C222_1$, $C222$, $Pmm2$, $Pcc2$, $Pba2$, $Pnn2$, $Cmm2$, $Ccc2$, $Fmm2$, $Fdd2$, $Imm2$, $Iba2$, *Pccm*, *Pban*, *Pbam*, *Pccn*, *Pnnm*, *Pmmn*, *Cmmm*, *Cccm*, *Cmme*, *Ccce*, *Ibam*, *Imma*). The Laue class of the normalizer is always the tetragonal holohedry: as a consequence, a fourfold rotation about the [001] orthorhombic axis when the crystal has a metric specialization $a = b$ never affects the reflection conditions and the presence of twinning cannot be inferred from the reflection conditions. A metric specialization in one of the two other planes never corresponds to a tetragonal normalizer and thus a $4_{[100]}$ or $4_{[010]}$ twin rotation always affects the reflection conditions.

Space-group types with orthorhombic affine normalizer. For the 21 types of orthorhombic space groups that have orthorhombic affine normalizers ($Pmc2_1$, $Pma2$, $Pca2_1$, $Pnc2$, $Pmn2_1$, $Pna2_1$, $Cmc2_1$, $Amm2$, $Aem2$, $Ama2$, $Aea2$, $Ima2$, *Pmma*, *Pnna*, *Pmna*, *Pcca*, *Pbcm*, *Pbcn*, *Pnma*, *Cmcm*, *Cmce*), class II*B* twinning in general does affect the reflection conditions of a crystal having a space group of this type. Two exceptions exist, however: for $Amm2$ and $Aem2$ the *A*-type of conventional unit cell combined with the *m*- or *e*-glide type of mirrors gives a diffraction pattern not affected by a fourfold twin operation about [100].

Space-group types with a specialized hexagonal lattice metric. An orthorhombic crystal with a hexagonal lattice has an orthohexagonal conventional unit cell base-centred in the plane perpendicular to the sixfold axis of the lattice. This means that only space-group types with the following types of conventional unit cells are compatible with a hexagonal lattice:

(i) oC with $a = b \times 3^{1/2}$ or $b = a \times 3^{1/2}$: the sixfold axis for the lattice is along the c axis of the crystal;

(ii) oA with $c = b \times 3^{1/2}$ or $b = c \times 3^{1/2}$: the sixfold axis for the lattice is along the a axis of the crystal;

(iii) oB with $a = c \times 3^{1/2}$ or $c = a \times 3^{1/2}$: the sixfold axis for the lattice is along the b axis of the crystal.[8]

The same argument applies to a monoclinic crystal with hexagonal lattice, the lower geometric crystal class having no influence on the effects of class II*B* twinning on the reflection conditions.

The coset decomposition of the hexagonal holohedry with respect to the orthorhombic holohedry gives two twin laws; the respective coset representatives can be taken as 3^+ and 3^- rotations, the other twin operations being equivalent under the point group *P* of the individual (if *H* is not holohedral, class II*A* may, but not necessarily does, accompany class II*B* twinning). Therefore, the effect of class II*B* twinning on an orthorhombic crystal with a hexagonal lattice can be studied through the effect of threefold rotations on the reflection conditions of non-symmorphic space-group types with *mP*, *mS* or *oS* types of conventional unit cells, *i.e.* 16 types of space groups ($P2_1$, *Pc*, *Cc*, $P2_1/m$, $P2/c$, $P2_1/c$, $C2/c$, $C222_1$, $Cmc2_1$, $Ccc2$, $Aem2$, $Ama2$, *Cmcm*, *Cccm*, *Cmme*, *Ccce*). A threefold rotation about the c axis exchanges planes $(h0l)^*$, $(hhl)^*$ and $(h\bar{h}l)^*$ on the one hand and planes $(0kl)^*$, $(3hhl)^*$ and $(3h\bar{h}l)^*$ on the other hand, or planes $(h0l)^*$, $(h3hl)^*$ and $(h\bar{3}hl)^*$ on the one hand and planes $(0kl)^*$, $(hhl)^*$ and $(h\bar{h}l)^*$ on the other hand (depending on whether $a > b$ or $b > a$; to obtain the results

[8] No space group is given with an oB conventional unit cell as standard setting in *International Tables for Crystallography*.

when the twin axis is along the *a* or *b* axis of the crystal one has to simply permute the indices). As a result, the zonal reflection conditions are annihilated and only the serial reflection conditions are left. Furthermore, some of the integral reflection conditions of the *F* type of unit cell are annihilated, the resulting diffraction pattern simulating the integral reflection conditions of an *S* type.

In conclusion, class II*B* twinning of an orthorhombic or monoclinic crystal with hexagonal lattice results in a diffraction pattern with only serial reflection conditions. No diffraction enhancement of symmetry is observed unless an equi-volume complete twin is realized.

7. Conclusions

Merohedric twinning corresponds to a single orientation for the lattice of the individuals and each measured diffraction actually corresponds to the weighted sum of diffractions from each individual. An ambiguity therefore arises on three structural models, that we have termed the **H**, the ***t*-H** and the **G** model. Nevertheless, the observed reflection conditions are compatible with the three models in 72 of 150 cases; for the other 78, either the **G** model is excluded because it is not compatible with the observed reflection conditions (71 cases), or it corresponds to a group which is not an extension $\langle H,s \rangle$ and thus the structure solution or at least the refinement would fail (seven cases). Furthermore, in one case of class II*A* twinning and several cases of class II*B* twinning, the twin operation may affect the observed reflection conditions, by bringing to overlap a present diffraction of an individual with an absent diffraction of another individual, which makes it easy to differentiate between the **H** and the ***t*-H** model. In the case of class II*B* twinning, the undistinguishable cases actually become a minority, and non-space-group absences, in particular those on the $hh\pm h$ diffractions, are an unambiguous sign of twinning. However, because they affect only a small subset of the diffraction pattern, they can be easily missed by the investigator. These reflection conditions, supplemented by a careful examination of the symmetry of the intensity distribution, allow one to recognize the presence of twinning at a pre-solution stage in a rather large number of cases.

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