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The Standardization of Inorganic Crystal-Structure Data*

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Abstract

This paper describes a proposal for a standardized presentation of inorganic crystal-structure data with the aim to recognize identical or nearly identical structures from the similarity of the numerical values of the atom coordinates.

Introduction

For the classification of crystal structures and for various crystal-chemical considerations of inorganic and alloy structures it is important to recognize different compounds which have identical or nearly identical atom arrangements.† Owing to the lack of standards for the description of crystal structures, the lists of positional coordinates of two identical structures may not show any correspondence whatsoever. There are numerous examples in the literature where isotypic‡ crystal structures were described as different structure types. This happened even in *Strukturberichte* (1937) where, for example, the types *B*16 (GeS) and *B*29 (SnS) correspond to the same structure type and where the types $D0_{11}$ (Fe_3C) and $D0_{20}$ ($NiAl_3$) are nearly identical.

As a simple demonstration, in the upper part of Table 1(*a*) the structural data for $CeCu_2$ and KHg_2 according to Pearson (1967) are given. From a comparison of the numerical data the isotypy of the two structures cannot be recognized immediately although both are described with the *same* Hermann–Mauguin space-group symbol. Not only are the axes interchanged and the positional coordinates quite different, but also the Wyckoff letters of the positions differ. The isotypy was probably recognized only after drawings of the two structures had been compared.

In this paper a set of rules is proposed for the standardization of crystal-structure data, the aim of which is to simplify the task of recognizing identical or nearly identical structures.§

Previous proposals to standardize crystal-structure data

To our knowledge there exists only one paper on the standardization of the description of crystal structures. Schwarzenbach (1963) proposed a set of rules which were applied to the monoclinic and orthorhombic structure types listed in Smithells (1955). A more extensive paper in *Z. Kristallogr.* was announced but never published.

Other proposals refer only to one aspect of the standardization problem, namely the cell reduction for triclinic and monoclinic crystals and the labelling of the axes. A unique description of a lattice is the reduced set of basis vectors defined by Niggli (1928) and re-introduced by Buerger (1960). The definition of this reduced cell can also be found in Mighell (1976) and in *International Tables for Crystallography* (1983), Vol. A, § 9.3; this reference gives for each of the 44 types of reduced cell the reduced form and the transformation matrices relating the reduced cell to a corresponding conventional cell; see also Mighell & Rodgers (1980).

The Hermann–Mauguin space group in a standard setting as given in *International Tables for X-ray Crystallography* (1983), Vol. A (see later) permits in certain cases the labelling of one or more axes without ambiguity. However, for the labelling of the axes in the absence of requirements imposed by the standard space group, two different conventions can be found in the literature:

(1) $a<b<c$ (*abc* rule) was proposed by Buerger (1942) and Balashov (1956);

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† This is not a problem for organic structures as there are rarely compounds with identical or nearly identical atom arrangements.

‡ In the Angloamerican literature often called isomorphic.

§ No efforts will be made here to define the limits of isotypy; however, the results of a standardization of crystal-structure data could serve as basis for further discussions on isotypy. Some structures may not really be isotypic but only isopuntal, which means they have the same space group and the same occupation of Wyckoff positions with the same adjustable parameters, but different unit-cell ratios and different atom coordinations.

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(2) $c < a < b$ (*cab* rule) was proposed by Donnay, Tunell & Barth (1934) and Donnay (1943). It was intended to smoothen the transition from the older morphological to the newer structural description of minerals.

However, no generally accepted rules exist for the labelling of axes.

There exist two extensive compilations of lattice parameters. In *Crystal Data Determinative Tables* (1973–1981), the *cab* rule has been applied to all triclinic, monoclinic and orthorhombic unit cells, whereas in the National Bureau of Standards Single Crystal Identification Data Base (1981) the *abc* rule is adopted for the description of Niggli reduced cells. In both compilations many structures are thus described with a non-standard space-group setting.

Some general considerations

It is evident that in the absence of any (arbitrary) rules there exist an infinite number of possible structure descriptions. The rules can be based either on the geometry of the structure or on the symmetry of the atom arrangement.

In the view of a crystal chemist the most appropriate description would be one which allows geometrical relationships to other structures to be seen. Unfortunately, this cannot serve as a basis for a standard description since, depending on the structures to be compared, different descriptions might be needed.* Furthermore, the recognition of relationships between structures is exposed to subjective interpretation.

Geometrical relationships between structures with different symmetry might be discovered by comparing the atomic positions in the Niggli reduced cells of the structures. This method has the disadvantage of imposing a structure description which deviates completely from our conventional way of describing crystal structures and therefore does not seem appropriate for application on a large scale.

The symmetry of the atom arrangement, together with the conventions of the *International Tables of Crystallography* (1983) of putting the symmetry axes along **a**, **b**, **c** and the way the Wyckoff positions are written down, can serve as a basis for a standard. However, as demonstrated above with $CeCu_2$ and KHg_2, even here different equivalent structure descriptions are possible, depending on the choice of the basis vectors (origin, length and direction). Thus, in addition to the logical choice of describing a structure with the standard Hermann–Mauguin space group it will be necessary in certain cases to have extra rules.

* As an example we can consider the cubic face-centred Cu structure. For comparison with other close-packed structures like Mg, Nd or Sm one would choose the triple hexagonal cell, for a comparison with Cu_3Au or CuAu the conventional cubic cell. Thus there would not even be an agreement on what kind of unit cell one should use for the standard.

Different ways to describe a crystal structure in a standard Hermann–Mauguin space group

In order to find out which extra rules are needed for standardization, it is necessary to study the different possibilities of describing a structure with different numerical values for the positional coordinates after having decided on the space group, the basis vectors of the unit cell and the choice of the representative triplet from a given Wyckoff position (to be discussed later).

Different structure descriptions can be obtained by

(1) shift of origin of the coordinate system (unit cell);

(2) rotation of the coordinate system (unit cell);

(3) inversion of the basis-vector triplet (or reflection of one basis vector).

The last operation needs a special comment. Since we use by convention a right-handed coordinate system, the *inversion* of the basis vectors is in principle not permitted. However, it corresponds to a representation of the inverted original structure in a right-hand coordinate system.

The different possible descriptions of a crystal structure in a standard space-group setting can be derived from the corresponding Cheshire group (Hirshfeld, 1968) [also called Euclidean normalizer (Fischer & Koch, 1983)]. The elements of the Cheshire group describe the symmetry of the arrangement of symmetry elements in a given space group. A group theoretical definition of a Euclidean normalizer can be found in appropriate text books, such as, for example, Schenkman (1975), and has been discussed by Gubler (1982). As the details of the application of Euclidean normalizers have been treated by Fischer & Koch (1983), we give here only the results and simple checks on the number of possible descriptions.

In columns *E* and *F* of Table 6 are summarized the different possibilities of describing a crystal structure assuming a choice of space group and unit cell as given in columns *B*, *C* and *D*. The possible shifts of origin of the coordinate system (Giacovazzo, 1980) are listed in column *F*. In column *E* are given non-redundant *xyz* triplets. An *xyz* triplet obtained from another triplet by a permitted rotation or inversion of the coordinate system is called non-redundant if it cannot be obtained either by the symmetry operations of the space group or by a permitted origin shift.

The prefixes in column *E* give information on the chirality of the corresponding space group. The disposition of atom sites in a chiral space group (prefixes *C* or *E* in column *E*) cannot be brought into congruence with its mirror image by translation and/or rotation of the coordinate system. The only symmetry elements present are proper rotation axes (with or without translation components). The *xyz* triplets on the same line are related by rotations of the coordinate system without change of chirality. An enantiomorphic structure setting corresponding to a mirror image can be obtained by changing the signs of the *x*, *y* and *z* coordinates of all atoms (second line for each entry in column *E*). For three space groups, however, ($I4_1$, $I4_122$, $F4_132$) a shift of origin is also necessary. In space groups with prefix *C* the enantiomorphic structure setting is possible with the same space group; however, in those with prefix *E* the enantiomorph structure setting is possible only with the other space group of the enantiomorphic space-group pair.

The disposition of atom sites in an achiral space group (prefix *A* or no prefix in column *E*) can be brought into congruence with its mirror image by translation and/or rotation of the coordinate system. Achiral space groups have at least one improper rotation axis. All chiral and all achiral, non-centrosymmetric space groups (prefixes *C*, *E* and *A*) are polar space groups in a broader sense (to be distinguished from the special case of space groups with axial polarity, discussed below) which means they contain a direction and its opposite which are not related by symmetry. Centrosymmetric space groups (those *without* prefix in column *E*) are non-polar because the symmetry centre relates every direction with its opposite. In column *E* the *xyz* triplets on the same line are related by those rotations of the coordinate system which do not lead to a change of polarity. The polarity can be changed by changing the signs of the *x*, *y* and *z* coordinates of all atoms (second line of each entry in column *E*). In four space groups, however, ($Fdd2$, $I4_1md$, $I4_1cd$, $I\bar{4}2d$) an origin shift is also necessary. Contrary to the case of chiral space groups, where the change of chirality requires an inversion of the coordinate system, in achiral non-centrosymmetric space groups the structure setting with changed polarity could also be obtained by a rotation and translation of the coordinate system.

A particular case of the polar space groups concerns the space groups with axial polarity which is defined here to mean those space groups where one or more polar directions coincide with one or more axes and where the origin of at least one coordinate axis cannot be related to the positions of symmetry elements. The permitted origins (column *F*) have at least one freely adjustable parameter and correspondingly at least one of the unit cell vectors of the Cheshire group (column *H*) has a factor ε. The Cheshire group (column *G*) has in this case a 'degenerate Bravais lattice' denoted by Z^1, Z^2, Z^3 with the superscript denoting the number of polar coordinate axes.

A space group as well as its Cheshire group (column *G* of Table 6) is based on a point group (ignoring translation and glide components) and a translation subgroup. The point group of the Cheshire group has at least the same order as the point group of the space group. The ratio of the two orders (index) corresponds to the number of non-redundant *xyz* triplets given in column *E* of Table 6.* For enantiomorphic space-group pairs this calculation gives the total number of non-redundant *xyz* triplets for both space groups. In Table 6 only the *xyz* triplets for one of the two space groups are listed.

In general, the number of possible origins (column *F* of Table 6) can be obtained by dividing the volume of the space-group unit cell by the volume of the unit cell of the corresponding Cheshire group (to be calculated from the unit-cell vectors of the Cheshire group listed in column *H* of Table 6). If, however, the types of their Bravais lattices differ, each volume has first to be divided by the number of lattice points in its unit cell. In space groups with axial polarity, characterized by degenerate Bravais lattices of the corresponding Cheshire groups, the origin shifts are continuous in one, two or three directions, but are discrete in the remaining direction(s). For each such space group, the number of entries in column *F* of Table 6 can be obtained by a procedure similar to that for the general case, but disregarding the degenerate direction(s).

Example for space group No. 20

	Corresponding point group	Point-group order	Basic vectors	Bravais-lattice points	Unit-cell volume
Space group $C222_1$	222	4	**a**, **b**, **c**	2	abc
Cheshire group $Pmmm$	mmm	8	$\frac{1}{2}$**a**, $\frac{1}{2}$**b**, $\frac{1}{2}$**c**	1	$\frac{1}{8}(abc)$

Number of non-redundant *xyz* triplets: $\frac{8}{4}=2$.

Number of possible origins: $\dfrac{abc}{2}\Big/\dfrac{\frac{1}{8}(abc)}{1}=4.$

These numbers correspond to the number of entries in columns *E* and *F*, respectively, of Table 6 for space group $C222_1$.

The total number of different descriptions (different numerical values of the representative atom coordinates) can be obtained by multiplying the number of non-redundant *xyz* triplets (column *E* of Table 6) by the number of permitted origins (column *F*). Note that space groups with axial polarity have an infinite number of possible origins. The maximum number

* In the list of non-redundant *xyz* triplets it is found for certain space groups that the rotation or inversion of the coordinate system requires a translation component (for example in space group $Ia\bar{3}$). This can only occur if the corresponding Cheshire group is asymmorphic, *i.e.* contains at least a glide plane or a screw axis in its symbol.

of different descriptions for non-polar space groups is 24 (space groups $P312$, $P\bar{6}$). For the $CeCu_2$ structure mentioned above with space group *Imma* (see Table 1(*a*) there are according to Table 6 four different descriptions. This applies for a given choice of axes. The four descriptions for $a < b$ are listed in Table 1(*b*). There are four more descriptions with axes **a** and **b** interchanged.

A special case occurs for structures with atoms on positions which differ by a permitted origin shift (column F of Table 6). Some of the descriptions may yield identical atom positions. For example, for CsCl with space group $Pm\bar{3}m$ the two descriptions are:

first description	second description with origin shift $\frac{1}{2}\frac{1}{2}\frac{1}{2}$
1Cl in 1(*b*) $\frac{1}{2}\frac{1}{2}\frac{1}{2}$	1Cs in 1(*b*) $\frac{1}{2}\frac{1}{2}\frac{1}{2}$
1Cs in 1(*a*) 000	1Cl in 1(*a*) 000.

Proposal for structure data standardization

The following proposal for the standardization of crystal-structure data* is the result of our efforts to establish an alloy structure-type file of limited size for use in our laboratory. The flow chart of the standardization procedure is presented in Fig. 1.

* The following standards apply to structures which can be described with the regular space groups given in *International Tables for Crystallography* (1983). No efforts have been made to include 'non-commensurate' charge-density or spin-wave modulations and other unusual structure variations which do not fall into a three-dimensional lattice.

Choice of unit-cell and space-group setting with the principal conventions
(*a*) standard setting of *International Tables for Crystallography* (1983) (*b*-axis unique, triple hexagonal unit cell, symmetry centre at origin)
(*b*) Niggli reduced cell or cell with $a < b < c$ if not defined otherwise by symmetry

↓

Choice of representative coordinate triplet for all atoms, taking into account
(*a*) the permitted origins
(*b*) the permitted rotations of the coordinate system
(*c*) the enantiomorphic structure representation

↓

Ordering and renumbering of the atoms in the final list

Fig. 1. Flow chart of the standardization procedure.

Table 1. *Structural data for* $CeCu_2$ *and* KHg_2

(*a*) Comparison of the structure data for $CeCu_2$ and KHg_2
Non-standardized data after Pearson (1967)

$CeCu_2$				KHg_2			
Imma, $a = 4{\cdot}425$, $b = 7{\cdot}057$, $c = 7{\cdot}475$ Å				*Imma*, $a = 8{\cdot}10$, $b = 5{\cdot}16$, $c = 8.77$ Å			
	x	y	z		x	y	z
Ce in 4(*e*)	0	$\frac{1}{4}$	0·5377	K in 4(*e*)	0	$\frac{1}{4}$	0·703
Cu in 8(*h*)	0	0·051	0·1648	Hg in 8(*i*)	0·190	$\frac{1}{4}$	0·087

Standardized data

$CeCu_2$				KHg_2			
Standardization parameter $\Gamma = 0{\cdot}7655$				Standardization parameter $\Gamma = 0{\cdot}7751$			
Imma, $a = 4{\cdot}425$, $b = 7{\cdot}057$, $c = 7{\cdot}475$ Å				*Imma*, $a = 5{\cdot}16$, $b = 8{\cdot}10$, $c = 8{\cdot}77$ Å			
	x	y	z		x	y	z
Cu in 8(*h*)	0	0·051	0·1648	Hg in 8(*h*)	0	0·06	0·163
Ce in 4(*e*)	0	$\frac{1}{4}$	0·5377	K in 4(*e*)	0	$\frac{1}{4}$	0·547

KHg_2 had first to be transformed to a cell where $a < b$ while retaining the standard *Imma* space-group setting (shift of origin by $\frac{1}{4}\frac{1}{4}\frac{1}{4}$ and interchange of a and b axes) and then different origins (000, $\frac{1}{2}\frac{1}{2}0$) were tried to find the lowest standardization parameter.

(*b*) Structure data for $CeCu_2$: the four possible descriptions for a unit cell with $a < b$. The coordinate triplets given here have been chosen from the Wyckoff positions according to the rules explained in the text

		x	y	z
(1) Origin shift 000	$\Gamma = 0{\cdot}7655$	x	y	z
	Cu in 8(*h*)	0	0·051	0·1648
	Ce in 4(*e*)	0	$\frac{1}{4}$	0·5377
(2) Origin shift $00\frac{1}{2}$	$\Gamma = 0{\cdot}8978$	x	y	z
	Cu in 8(*h*)	0	0·551	0·3352
	Ce in 4(*e*)	0	$\frac{1}{4}$	0·0377
(3) Origin shift $0\frac{1}{2}0$	$\Gamma = 1{\cdot}1007$	x	y	z
	Cu in 8(*h*)	0	0·551	0·1648
	Ce in 4(*e*)	0	$\frac{1}{4}$	0·4623
(4) Origin shift $0\frac{1}{2}\frac{1}{2}$	$\Gamma = 1{\cdot}3333$	x	y	z
	Cu in 8(*h*)	0	0·051	0·3352
	Ce in 4(*e*)	0	$\frac{1}{4}$	0·9623

Choice of unit cell and space-group setting

(1) Right-handed coordinate system.

(2) Standard space-group setting, as given in the 1983 edition of *International Tables for Crystallography*, Vol. *A*, with the following additional restrictions:

(*a*) *b*-axis setting for monoclinic space groups;†

(*b*) obverse triple hexagonal unit cell for trigonal *R* space groups;

(*c*) the setting with the symmetry centre at the origin in all cases where two origin choices are given in *International Tables for Crystallography*;

(*d*) for the enantiomorphic space-group pairs, the space group with the smallest index for the relevant screw axis is normally taken as standard (for

† For each monoclinic space group six descriptions are given in *International Tables for Crystallography* (1983), three with *b* unique and three with *c* unique. They are characterized by only *one standard short symbol* (it appears in large letters at the top of all pages devoted to a particular space group) which corresponds to the space-group setting with axis *b* unique and which has already been given in the 1935 and 1952 editions.

example $P4_132$ instead of $P4_332$). However, if the absolute configuration has been determined, it is important not to lose this information. In this case a special procedure will be applied which will be discussed below.

(3)(*a*) Triclinic cells are chosen such that **a**, **b** and **c** are the shortest three non-coplanar lattice translation vectors that define the Niggli reduced cell in a right-handed coordinate system. The cell edges are labelled so as to have $a < b < c$. There are two kinds of triclinic cells. Those of type II have $\alpha \geq 90°$, $\beta \geq 90°$, $\gamma \geq 90°$ and those of type I $\alpha < 90°$, $\beta < 90°$ and $\gamma < 90°$.

(*b*) For monoclinic space groups with a primitive Bravais lattice and without a glide plane a 'reset' Niggli reduced cell is used which we define in the following way: the axes of the Niggli reduced cell of type II are relabelled so as to obtain a cell with $a < c$ and $\beta \geq 90°$.

For monoclinic space groups with centred Bravais lattices or glide planes we select **a** and **c** as the shortest non-parallel lattice translation vectors perpendicular to **b** – under the condition that β is non-acute – which allow the structure to be described with the standard monoclinic space-group symbol (for details see Gelato & Parthé, 1984).

(*c*) Orthorhombic structures where the space-group symbols do not prescribe a particular labelling of any of the three unit-cell axes have to be described with a unit cell where $a < b < c$. These space groups have cubic affine normalizers (Burzlaff & Zimmermann, 1980). If the space-group symmetry prescribes a label of one unit-cell axis (it is always the c axis in *International Tables for Crystallography*), the two other being free, unit cells with $a < b$ are used. These orthorhombic space groups have tetragonal affine normalizers. For all other orthorhombic structures (those with orthorhombic affine normalizers which in these cases are identical with the Euclidean normalizers) the standard space-group setting fixes the proper labelling of the three unit-cell axes.

All these conventions are listed in condensed form in Table 6. For a standard structure description, all valid descriptions have to be compared and a selection has to be made.

Choice of representative coordinate triplets

Having decided on the unit cell, we want to find a standard for the choice of the representative coordinate triplet of a Wyckoff position. This may be done in the following way: As representative positional coordinates for an atom those xyz values have to be chosen which satisfy $0 \leq x, y, z < 1$ and which correspond to the first xyz triplet printed in *International Tables for Crystallography* for its Wyckoff point set. For point sets with unspecialized coordinates, different symmetry-equivalent xyz triplets of the same point set may correspond to the first xyz triplet printed in *International Tables for Crystallography*, Vol. A. In this case a rule is needed to choose between the various possible triplets.* We adopt that triplet for which $(x^2+y^2+z^2)^{1/2}$ is a minimum.† If the same minimum square-root value is found with several xyz triplets, the triplet for which x has the smallest value and where necessary y also has the smallest value is adopted as standard.

The standardization parameter Γ

The sum of the minimal $(x^2+y^2+z^2)^{1/2}$ values of all standardized representative coordinates of the atoms in the unit cell of a structure is taken as a standardization parameter, Γ, to characterize the structure with a given choice of translation, rotation and inversion of the coordinate system.

For the standard description of a structure, that description is chosen for which the standardization parameter, Γ, is a minimum.‡ As an example we can see in Tables 1(*a*) and (*b*) that the description for $CeCu_2$ found in the literature is the description with the smallest standardization parameter. Only the order of the atoms had to be changed according to the further rules given below. If several possible descriptions lead to the same value of the standardization parameter, then that description is chosen where the sum of the x coordinates of all atoms is the smallest. If this procedure is equivocal, the sum of the y coordinates is used as well and then the sum of the z coordinates. If even this does not lead to a result one compares the sum of the three coordinates of the first atom in the different descriptions (after the ordering of the atom list). The description with

* Our original idea to choose as representative coordinates those corresponding to sites which are within the asymmetric unit, as defined in *International Tables for Crystallography* (1983) had to be abandoned. Data points within the given asymmetric unit do not necessarily correspond to the first xyz triplet given for each point set in *International Tables for Crystallography* (1983) but to a symmetry-equivalent point. For example, for $Pn\bar{3}n$, origin choice 2 with symmetry centre at origin, the asymmetric unit with $\frac{1}{4} \leq x \leq \frac{3}{4}$, $\frac{1}{4} \leq y \leq \frac{3}{4}$, $\frac{1}{4} \leq z \leq \frac{3}{4}$, $y \leq x$, $z \leq y$ does not contain point 000, the first entry for Wyckoff letter 2(*a*), but instead the symmetry equivalent $\frac{1}{2}\frac{1}{2}\frac{1}{2}$. An additional difficulty exists with a data point which is on the surface of the asymmetric unit since it may appear more than once. Special rules would be needed for each space group to make the proper choice.

† We choose this formula because in 'fractional space', *i.e.* not considering the cell parameters, it corresponds to the distance from the origin of an atom with coordinates xyz.

‡ For space groups with axial polarity we have the additional difficulty that in at least one direction the origin cannot be fixed by the symmetry elements. Continuing in the same manner as above, we choose the origin for these groups to be based on the coordinates themselves in such a way as to minimize Γ, which requires summing over all atoms (not only the representative atoms) in the unit cell. The mathematical formulation is discussed in the *STRUCTURE TIDY* program description (Gelato & Parthé, 1984).

the smallest sum is taken as standard. If this is ambiguous one compares the sum of the *x*, *y* and *z* values of the second atom and so on.

If, as in the case of CsCl, the different possible descriptions lead to the same numerical values of the atom positions, either description may be taken as standard.

Ordering and renumbering of atoms

For the presentation of atomic coordinates in the final list the following convention is adopted. The atoms are listed in the order of their Wyckoff letters, as given in *International Tables for Crystallography* (1983) (from top to bottom), regardless of the atomic species involved. This deviates from the usual convention of ordering the atoms, but permits types and antitypes as well as alloys with mixed site occupation to be described in a uniform way and avoids any controversy concerning the proper sequence of the elements in the chemical formula. However, in order to be able to take in at a glance the different positions occupied by one particular element in a structure, the different element symbols in the final atom list are displaced sideways by different amounts (see examples). If different coordinate triplets with the same Wyckoff letter appear, they are arranged according to increasing *x*, then increasing *y* and finally increasing *z* values.

The numbering of atoms of one kind which occupy the same or different Wyckoff positions in a structure is to follow the sequence of their representative *xyz* triplets in the final structure data list.*

Once the atoms are properly numbered and the order of all atoms in the final list has been established, the numerical values for *y* (and *z*) have to be replaced by their analytical expression provided they are listed as such in *International Tables for Crystallography* (1983). For examples see Tables 2 and 5.

Occupation factors are given in the final list as in the unstandardized data since only the structure sites are affected by a standardization.

The errors of the atom coordinates in the standardized structure description are calculated from the original data by the propagation of errors. Details will be discussed by Gelato & Parthé (1984).

Procedure to be adopted to indicate the chirality and polarity in the standardized structure data

A study of Bijvoet differences should, in appropriate circumstances, permit determination of the chirality and polarity of all non-centrosymmetric structures. To indicate these results in the standardized structure data the following procedure is proposed:

Structures based on a space group which has an enantiomorph are always standardized in the space group with the smallest index for the relevant screw axis (groups with prefix *E* of Table 6) if necessary, by changing the signs of all coordinates to perform the change to the enantiomorphic space group. If the experimental data indicate that the correct space group is the one with the higher index, minus signs are placed in front of the standardized atom coordinates and the real space group with higher index is listed. As an example we consider low-quartz (Donnay & Le Page, 1978) for which the standardized descriptions of the two enantiomorphs are as follows:

	Laevoquartz $P3_121$		
6O in 6(*c*)	0·41	0·14	0·12
3Si in 3(*a*)	0·53	0	$\frac{1}{3}$
	Dextroquartz $P3_221$		
6O in 6(*c*)	−0·41	−0·14	−0·12
3Si in 3(*a*)	−0·53	0	$-\frac{1}{3}$

The procedure is similar for all other non-centrosymmetric structures. The structures are first standardized in the normal way considering all rotations and inversion of the coordinate system. If the chirality or the polarity of the standardized structure data are different from that found by experimental evidence, minus signs are placed in front of the standardized atom coordinates. For seven space groups, however, ($Fdd2$, $I4_1$, $I4_122$, $I4_1md$, $I4_1cd$, $I\bar{4}2d$ and $F4_132$) also the necessary translation component has to be given (Table 6, column *E*, first entry on the second line for the corresponding space group). This origin shift has to be given separately for all atom coordinates. For example, for $F4_132$: $-x_s+\frac{1}{4}$, $-y_s+\frac{1}{4}$, $-z_s+\frac{1}{4}$ where x_s, y_s and z_s are the atom coordinates obtained by normal standardization.

The adopted procedure allows an easy comparison of the atom coordinates of identical structures which differ only in chirality or polarity.

Examples for standardized isotypic structures

(*a*) $CeCu_2$ and KHg_2 are two isotypic structures, for which the non-standardized data are given in the upper part of Table 1(*a*). Inspection of the standardized data, given in the lower part, makes the isotypy of the two structures evident.

(*b*) The published and the standardized structure data for $Ca_{31}Sn_{20}$ and $Pu_{31}Rh_{20}$ can be found in Table 2. Both compounds have moderately complicated alloy structures with 15 different atom sites. The isotypy of these two compounds was not expected.

* Rotation of the coordinate system as well as a change of the origin needed for standardization will lead to a Wyckoff position having the same point symmetry but which may have a different Wyckoff letter. This may have an effect on the sequence of the representative atom coordinates and on the numbering of the atoms of one kind.

Table 2. *Published and standardized structure data of* $Ca_{31}Sn_{20}$ *and* $Pu_{31}Rh_{20}$

Data for $Ca_{31}Sn_{20}$
(Fornasini & Franceschi, 1977)

*I*4/*mcm*, *c*/*a* = 3·189
Γ = 6·6780

	x	*y*	*z*
Ca(1) in 8(*h*)	0·3405	$\frac{1}{2}+x$	0
Ca(2) in 32(*m*)	0·2103	0·0519	0·0533
Ca(3) in 8(*g*)	0	$\frac{1}{2}$	0·0716
Ca(4) in 32(*m*)	0·0808	0·2161	0·1365
Ca(5) in 8(*g*)	0	$\frac{1}{2}$	0·1678
Ca(6) in 32(*m*)	0·2138	0·0861	0·2125
Ca(7) in 4(*b*)	0	$\frac{1}{2}$	$\frac{1}{4}$
Sn(1) in 4(*c*)	0	0	0
Sn(2) in 8(*h*)	0·0859	$\frac{1}{2}+x$	0
Sn(3) in 16(*l*)	0·3019	$\frac{1}{2}+x$	0·0748
Sn(4) in 8(*f*)	0	0	0·0949
Sn(5) in 16(*l*)	0·1617	$\frac{1}{2}+x$	0·1231
Sn(6) in 8(*f*)	0	0	0·1733
Sn(7) in 16(*l*)	0·3469	$\frac{1}{2}+x$	0·2087
Sn(8) in 4(*a*)	0	0	$\frac{1}{4}$

Data for $Pu_{31}Rh_{20}$
(Cromer & Larson, 1977)

*I*4/*mcm*, *c*/*a* = 3·334
Γ = 6·7647

	x	*y*	*z*
Pu(1) in 4(*b*)	0	$\frac{1}{2}$	$\frac{1}{4}$
Pu(2) in 8(*g*)	0	$\frac{1}{2}$	0·0756
Pu(3) in 8(*g*)	0	$\frac{1}{2}$	0·1656
Pu(4) in 8(*h*)	0·1586	$x+\frac{1}{2}$	0
Pu(5) in 32(*m*)	0·2947	0·4299	0·0500
Pu(6) in 32(*m*)	0·2855	0·5774	0·1346
Pu(7) in 32(*m*)	0·2819	0·4125	0·2114
Rh(1) in 4(*c*)	0	0	0
Rh(2) in 4(*a*)	0	0	$\frac{1}{4}$
Rh(3) in 8(*f*)	0	0	0·0940
Rh(4) in 8(*f*)	0	0	0·1734
Rh(5) in 8(*h*)	0·4035	$x+\frac{1}{2}$	0
Rh(6) in 16(*l*)	0·1812	$x+\frac{1}{2}$	0·0726
Rh(7) in 16(*l*)	0·3417	$x+\frac{1}{2}$	0·1269
Rh(8) in 16(*l*)	0·1536	$x+\frac{1}{2}$	0·2109

Standardized data for $Ca_{31}Sn_{20}$
Γ = 6·6780

	x	*y*	*z*
Ca(1) in 32(*m*)	0·0808	0·2161	0·1365
Ca(2) in 32(*m*)	0·2103	0·0519	0·0533
Ca(3) in 32(*m*)	0·2138	0·0861	0·2125
Sn(1) in 16(*l*)	0·1531	$\frac{1}{2}+x$	0·2913
Sn(2) in 16(*l*)	0·1617	$\frac{1}{2}+x$	0·1231
Sn(3) in 16(*l*)	0·1981	$\frac{1}{2}+x$	0·4252
Sn(4) in 8(*h*)	0·0859	$\frac{1}{2}+x$	0
Ca(4) in 8(*h*)	0·3405	$\frac{1}{2}+x$	0
Ca(5) in 8(*g*)	0	$\frac{1}{2}$	0·0716
Ca(6) in 8(*g*)	0	$\frac{1}{2}$	0·1678
Sn(5) in 8(*f*)	0	0	0·0949
Sn(6) in 8(*f*)	0	0	0·1733
Sn(7) in 4(*c*)	0	0	0
Ca(7) in 4(*b*)	0	$\frac{1}{2}$	$\frac{1}{4}$
Sn(8) in 4(*a*)	0	0	$\frac{1}{4}$

Standardized data for $Pu_{31}Rh_{20}$
Γ = 6·6688

	x	*y*	*z*
Pu(1) in 32(*m*)	0·0774	0·2145	0·1346
Pu(2) in 32(*m*)	0·2053	0·0701	0·0500
Pu(3) in 32(*m*)	0·2181	0·0875	0·2114
Rh(1) in 16(*l*)	0·1536	$\frac{1}{2}+x$	0·2891
Rh(2) in 16(*l*)	0·1583	$\frac{1}{2}+x$	0·1269
Rh(3) in 16(*l*)	0·1812	$\frac{1}{2}+x$	0·4274
Rh(4) in 8(*h*)	0·0965	$\frac{1}{2}+x$	0
Pu(4) in 8(*h*)	0·3414	$\frac{1}{2}+x$	0
Pu(5) in 8(*g*)	0	$\frac{1}{2}$	0·0756
Pu(6) in 8(*g*)	0	$\frac{1}{2}$	0·1656
Rh(5) in 8(*f*)	0	0	0·0940
Rh(6) in 8(*f*)	0	0	0·1734
Rh(7) in 4(*c*)	0	0	0
Pu(7) in 4(*b*)	0	$\frac{1}{2}$	$\frac{1}{4}$
Rh(8) in 4(*a*)	0	0	$\frac{1}{4}$

In the case of $Pu_{31}Rh_{20}$ an origin shift of $00\frac{1}{2}$ leads to the smallest standardization parameter. No origin shift was necessary for $Ca_{31}Sn_{20}$; however, the atoms had to be relabelled and put into a different order.

Table 3. *Standardized structure data of R-phase* Mo–Co–Cr (*Komura, Sly & Shoemaker*, 1960)

$R\bar{3}$, *a* = 10·903, *c* = 19·342 Å

M = Cr + Co	*x*	*y*	*z*
M(1) in 18(*f*)	0·10523	0·38767	0·06667
Mo(1) in 18(*f*)	0·11153	0·39957	0·28887
$Mo_{0.62}M_{0.38}$ in 18(*f*)	0·1265	0·1759	0·1031
$Mo_{0.11}M_{0.89}$ in 18(*f*)	0·1393	0·0212	0·3038
M(2) in 18(*f*)	0·1969	0·2250	0·2315
M(3) in 18(*f*)	0·24593	0·41967	0·16467
$Mo_{0.76}M_{0.24}$ in 18(*f*)	0·2579	0·0330	0·1817
$Mo_{0.53}M_{0.47}$ in 18(*f*)	0·2687	0·1132	0·0348
M(4) in 6(*c*)	0	0	0·1956
Mo(2) in 6(*c*)	0	0	0·4265
$Mo_{0.11}M_{0.89}$ in 3(*a*)	0	0	0

To obtain this standardized description with the lowest value of the standardization parameter (Γ = 3·6121) the coordinate system had to be rotated ($xyz \rightarrow yx\bar{z}$) and the origin shifted by $00\frac{1}{2}$.

(*c*) The *R*-phase Mo–Cr–Co, for which the standardized data are found in Table 3, represents an example of a complicated alloy structure with sites having mixed occupation. The standardization leads here to a rotation of the coordinate system.

(*d*) The standardized data of Y_3Co_2 and Mo_2IrB_2, shown in Table 4, make it evident that the ternary compound is a substitution derivative of the binary structure type.

(*e*) The non-standardized literature descriptions of the η-carbide, Ti_4Ni_2O and Ti_2Ni structures, presented in the upper part of Table 5, do not allow the relation between these structures to be recognized. However, the standardized descriptions given in the lower part of Table 5 show immediately that W_4Co_2C, W_3Fe_3C and Ti_4Ni_2O are isotypic and that Ti_2Ni has the same atom arrangement except for one structure site which is not occupied.

Problems with the proposed standardization

There are two kinds of problems which can arise with the proposed standardization. One concerns the proper choice of basis vectors for those space groups where the cell metric is used as a guide for the choice

Table 4. *Published and standardized data for* Y_3Co_2 *and* Mo_2IrB_2

Y_3Co_2
(Moreau, Parthé & Paccard, 1975)

Pnnm, $a = 12{\cdot}248$, $b = 9{\cdot}389$, $c = 3{\cdot}975$ Å

	x	*y*	*z*
Y(1) in 4(*g*)	0·128	0·193	0
Y(2) in 4(*g*)	0·387	0·373	0
Y(3) in 4(*g*)	0·137	0·574	0
Co(1) in 4(*g*)	0·269	0·860	0
Co(2) in 4(*g*)	0·462	0·883	0

Standardized data
$\Gamma = 2{\cdot}2469$

Pnnm, $a = 9{\cdot}389$, $b = 12{\cdot}248$, $c = 3{\cdot}975$ Å

	x	*y*	*z*
Co(1) in 4(*g*)	0·117	0·038	0
Co(2) in 4(*g*)	0·14	0·231	0
Y(1) in 4(*g*)	0·193	0·628	0
Y(2) in 4(*g*)	0·426	0·363	0
Y(3) in 4(*g*)	0·627	0·113	0

Mo_2IrB_2
(Rogl, Benesovsky & Nowotny, 1972)

Pnnm, $a = 9{\cdot}422$, $b = 7{\cdot}356$, $c = 3{\cdot}231$ Å

	x	*y*	*z*
Ir in 4(*g*)	0·11	0·12	0
Mo(1) in 4(*g*)	0·37	0·32	0
Mo(2) in 4(*g*)	0·64	0·07	0
B(1) in 4(*g*)	(0·04	0·61	0)*
B(2) in 4(*g*)	(0·25	0·61	0)*

Standardized data
$\Gamma = 2{\cdot}2359$

Pnnm, $a = 7{\cdot}356$, $b = 9{\cdot}422$, $c = 3{\cdot}231$ Å

	x	*y*	*z*
B(1) in 4(*g*)	(0·11	0·04	0)*
B(2) in 4(*g*)	(0·11	0·25	0)*
Mo(1) in 4(*g*)	0·18	0·63	0
Mo(2) in 4(*g*)	0·43	0·36	0
Ir in 4(*g*)	0·62	0·11	0

For Y_3Co_2 the *a* and *b* axes had to be interchanged and the origin shifted by $0\frac{1}{2}0$, while in the case of Mo_2IrB_2 after an interchange of *a* and *b* the origin was shifted by $\frac{1}{2}00$.

* The B positions have been estimated using space considerations.

Table 5. *Published and standardized structure data for* W_4Co_2C, W_3Fe_3C, Ti_4Ni_2O *and* Ti_2Ni

W_4Co_2C
[*SR* (1954) **18**, 81]*

$Fd\bar{3}m$, origin away from symmetry centre

		x	*y*	*z*
16C	in 16(*c*)	$\frac{1}{8}$	$\frac{1}{8}$	$\frac{1}{8}$
16W(1)	in 16(*d*)	$\frac{5}{8}$	$\frac{5}{8}$	$\frac{5}{8}$
48W(2)	in 48(*f*)	0·195	0	0
32Co	in 32(*e*)	0·825	*x*	*x*

Standardized data
$\Gamma = 1{\cdot}6774$

	x	*y*	*z*
W(1) in 48(*f*)	0·430	$\frac{1}{8}$	$\frac{1}{8}$
Co in 32(*e*)	0·200	*x*	*x*
C in 16(*d*)	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$
W(2) in 16(*c*)	0	0	0

Shift of origin from published data $\frac{5}{8}\frac{5}{8}\frac{5}{8}$

W_3Fe_3C
[*SR* (1967) **32A**, 45]

$Fd\bar{3}m$, symmetry centre at origin

		x	*y*	*z*
16Fe(1)	in 16(*d*)	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$
32Fe(2)	in 32(*e*)	0·7047	*x*	*x*
48W	in 48(*f*)	0·3228	$\frac{1}{8}$	$\frac{1}{8}$
16C	in 16(*c*)	0	0	0

Standardized data
$\Gamma = 1{\cdot}6829$

	x	*y*	*z*
W in 48(*f*)	0·4272	$\frac{1}{8}$	$\frac{1}{8}$
Fe(1) in 32(*e*)	0·2047	*x*	*x*
C in 16(*d*)	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$
Fe(2) in 16(*c*)	0	0	0

Shift of origin from published data $\frac{1}{2}\frac{1}{2}\frac{1}{2}$

Ti_4Ni_2O
[*SR* (1963) **28**, 140]

$Fd\bar{3}m$, origin away from symmetry centre

		x	*y*	*z*
16Ti(1)	in 16(*c*)	$\frac{1}{8}$	$\frac{1}{8}$	$\frac{1}{8}$
48Ti(2)	in 48(*f*)	0·312	0	0
32Ni	in 32(*e*)	0·916	*x*	*x*
16O	in 16(*d*)	$\frac{5}{8}$	$\frac{5}{8}$	$\frac{5}{8}$

Standardized data
$\Gamma = 1{\cdot}7069$

	x	*y*	*z*
Ti(1) in 48(*f*)	0·437	$\frac{1}{8}$	$\frac{1}{8}$
Ni in 32(*e*)	0·209	*x*	*x*
O in 16(*d*)	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$
Ti(2) in 16(*c*)	0	0	0

Shift of origin from published data $\frac{1}{8}\frac{1}{8}\frac{1}{8}$

Ti_2Ni
[*SR* (1963) **28**, 21]

$Fd\bar{3}m$, origin away from symmetry centre

		x	*y*	*z*
16Ti(1)	in 16(*c*)	$\frac{1}{8}$	$\frac{1}{8}$	$\frac{1}{8}$
48Ti(2)	in 48(*f*)	0·311	0	0
32Ni	in 32(*e*)	0·912	*x*	*x*

Standardized data
$\Gamma = 0{\cdot}839$

	x	*y*	*z*
Ti(1) in 48(*f*)	0·436	$\frac{1}{8}$	$\frac{1}{8}$
Ni in 32(*e*)	0·213	*x*	*x*
Ti(2) in 16(*c*)	0	0	0

Shift of origin from published data $\frac{1}{8}\frac{1}{8}\frac{1}{8}$

* References to *Structure Reports*, giving date, volume number and page number.

of the unit cell. The second concerns the standardization of nearly isotypic structures where one or several positional parameters vary around a special value.

In Table 6 are listed 53 space groups where the numerical values of the lattice parameters are used to find a reduced cell and/or to label the axes for a standard description. If by chance the cell parameters are not significantly different, a special procedure is necessary for the standardization. In this case one applies the regular standardization procedure to each of the equivalent structure descriptions and the final selection is made according to the smallest value of the standardization parameter.

A second problem exists with closely related but slightly different structures which each can be formally standardized, but show no correspondence in their standardized descriptions. This arises because there is a discontinuity in the numerical *x*, *y*, *z* values at the limit of the unit cell (or any other chosen translation period) and *any* standardization procedure would be affected by this difficulty. A similar case, a discontinuity close to a special value, was found for Pu_3Co, Zr_3Co, $PuBr_3$ and $TbCl_3$. The first two compounds have similar standardized descriptions as shown in the lower part of Table 7, while the two nearly isotypic halogenides have standardized

Table 6. *Hermann–Mauguin symbols of space groups in standard setting, extra conditions for choice of unit cell, extra condition for the labelling of the axes, list of non-redundant xyz triplets, permitted origins of unit cell, symbols and basis vectors of corresponding Cheshire groups.*

The prefix in column *E* indicates if the space group is chiral (*C*) with its special case of enantiomorphic (*E*) or achiral (*A*) with its special case of centrosymmetric (without prefix). *xyz* triplets in the second line correspond to a changed chirality and polarity.

A No.	B Standard space-group symbol	C Extra condition for choice of unit cell	D Labels of axes	E Non-redundant *xyz* triplets	F Permitted origins	G Cheshire group	H Basis vectors of Cheshire group
TRICLINIC Either type I cell, positive reduced form: $\alpha<90$, $\beta<90$, $\gamma<90°$ or type II cell, negative reduced form: $\alpha\geq90$, $\beta\geq90$, $\gamma\geq90°$							
1	$P1$	Niggli reduced cell	$a<b<c$	*C* *xyz* $\bar{x}\bar{y}\bar{z}$	*xyz*	$Z^3\bar{1}$	εa, εb, εc
2	$P\bar{1}$	Niggli reduced cell	$a<b<c$	*xyz*	000, ½00, 0½0, 00½, 0½½, ½0½, ½½0, ½½½	$P\bar{1}$	½a, ½b, ½c
MONOCLINIC *b*-axis unique; $\beta\geq90$, $\alpha=\gamma=90°$							
3	$P2$	Reset Niggli reduced cell of type II	$a<c$	*C* *xyz* $\bar{x}\bar{y}\bar{z}$	0*y*0, 0*y*½, ½*y*0, ½*y*½	Z^12/m	½a, εb, ½c
4	$P2_1$	Reset Niggli reduced cell of type II	$a<c$	*C* *xyz* $\bar{x}\bar{y}\bar{z}$	0*y*0, 0*y*½, ½*y*0, ½*y*½	Z^12/m	½a, εb, ½c
5	$C2$	**a** and **c** shortest translation vectors which agree with space group		*C* *xyz* $\bar{x}\bar{y}\bar{z}$	0*y*0, 0*y*½	Z^12/m	½a, εb, ½c
6	Pm	Reset Niggli reduced cell of type II	$a<c$	*A* *xyz* $\bar{x}\bar{y}\bar{z}$	*x*0*z*, *x*½*z*	Z^22/m	εa, ½b, εc
7	Pc	**a** and **c** shortest translation vectors which agree with space group		*A* *xyz* $\bar{x}\bar{y}\bar{z}$	*x*0*z*, *x*½*z*	Z^22/m	εa, ½b, εc
8	Cm	**a** and **c** shortest translation vectors which agree with space group		*A* *xyz* $\bar{x}\bar{y}\bar{z}$	*x*0*z*	Z^22/m	εa, ½b, εc
9	Cc	**a** and **c** shortest translation vectors which agree with space group*		*A* *xyz* $\bar{x}\bar{y}\bar{z}$	*x*0*z*	Z^22/m	εa, ½b, εc
10	$P2/m$	Reset Niggli reduced cell of type II	$a<c$	*xyz*	000, ½00, 0½0, 00½, 0½½, ½0½, ½½0, ½½½	$P2/m$	½a, ½b, ½c
11	$P2_1/m$	Reset Niggli reduced cell of type II	$a<c$	*xyz*	000, ½00, 0½0, 00½, 0½½, ½0½, ½½0, ½½½	$P2/m$	½a, ½b, ½c
12	$C2/m$	**a** and **c** shortest translation vectors which agree with space group		*xyz*	000, 00½, 0½0, 0½½	$P2/m$	½a, ½b, ½c
13	$P2/c$	**a** and **c** shortest translation vectors which agree with space group		*xyz*	000, ½00, 0½0, 00½, 0½½, ½0½, ½½0, ½½½	$P2/m$	½a, ½b, ½c
14	$P2_1/c$	**a** and **c** shortest translation vectors which agree with space group		*xyz*	000, ½00, 0½0, 00½, 0½½, ½0½, ½½0, ½½½	$P2/m$	½a, ½b, ½c
15	$C2/c$	**a** and **c** shortest translation vectors which agree with space group†		*xyz*	000, 00½, 0½0, 0½½	$P2/m$	½a, ½b, ½c
ORTHORHOMBIC $\alpha=\beta=\gamma=90°$							
16	$P222$		$a<b<c$	*C* *xyz* $\bar{x}\bar{y}\bar{z}$	000, ½00, 0½0, 00½, 0½½, ½0½, ½½0, ½½½	$Pmmm$	½a, ½b, ½c
17	$P222_1$		$a<b$ [00¼]‡	*C* *xyz* $\bar{x}\bar{y}\bar{z}$	000, ½00, 0½0, 00½, 0½½, ½0½, ½½0, ½½½	$Pmmm$	½a, ½b, ½c
18	$P2_12_12$		$a<b$	*C* *xyz* $\bar{x}\bar{y}\bar{z}$	000, ½00, 0½0, 00½, 0½½, ½0½, ½½0, ½½½	$Pmmm$	½a, ½b, ½c
19	$P2_12_12_1$		$a<b<c$ [¼¼¼]§	*C* *xyz* $\bar{x}\bar{y}\bar{z}$	000, ½00, 0½0, 00½, 0½½, ½0½, ½½0, ½½½	$Pmmm$	½a, ½b, ½c
20	$C222_1$		$a<b$ [00¼]‡	*C* *xyz* $\bar{x}\bar{y}\bar{z}$	000, 00½, 0½0, 0½½	$Pmmm$	½a, ½b, ½c
21	$C222$		$a<b$	*C* *xyz* $\bar{x}\bar{y}\bar{z}$	000, 00½, 0½0, 0½½	$Pmmm$	½a, ½b, ½c
22	$F222$		$a<b<c$	*C* *xyz* $\bar{x}\bar{y}\bar{z}$	000, ¼¼¼, ½½½, ¾¾¾	$Immm$	½a, ½b, ½c
23	$I222$		$a<b<c$	*C* *xyz* $\bar{x}\bar{y}\bar{z}$	000, 00½, 0½0, 0½½	$Pmmm$	½a, ½b, ½c
24	$I2_12_12_1$		$a<b<c$ [¼¼¼]§	*C* *xyz* $\bar{x}\bar{y}\bar{z}$	000, 00½, 0½0, 0½½	$Pmmm$	½a, ½b, ½c
25	$Pmm2$		$a<b$	*A* *xyz* $\bar{x}\bar{y}\bar{z}$	00*z*, 0½*z*, ½0*z*, ½½*z*	Z^1mmm	½a, ½b, εc
26	$Pmc2_1$			*A* *xyz* $\bar{x}\bar{y}\bar{z}$	00*z*, 0½*z*, ½0*z*, ½½*z*	Z^1mmm	½a, ½b, εc
27	$Pcc2$		$a<b$	*A* *xyz* $\bar{x}\bar{y}\bar{z}$	00*z*, 0½*z*, ½0*z*, ½½*z*	Z^1mmm	½a, ½b, εc
28	$Pma2$			*A* *xyz* $\bar{x}\bar{y}\bar{z}$	00*z*, 0½*z*, ½0*z*, ½½*z*	Z^1mmm	½a, ½b, εc
29	$Pca2_1$			*A* *xyz* $\bar{x}\bar{y}\bar{z}$	00*z*, 0½*z*, ½0*z*, ½½*z*	Z^1mmm	½a, ½b, εc
30	$Pnc2$			*A* *xyz* $\bar{x}\bar{y}\bar{z}$	00*z*, 0½*z*, ½0*z*, ½½*z*	Z^1mmm	½a, ½b, εc
31	$Pmn2_1$			*A* *xyz* $\bar{x}\bar{y}\bar{z}$	00*z*, 0½*z*, ½0*z*, ½½*z*	Z^1mmm	½a, ½b, εc

Table 6 (*cont.*)

A No.	B Standard space-group symbol	C Extra condition for choice of unit cell	D Labels of axes	E Non-redundant *xyz* triplets	F Permitted origins	G Cheshire group	H Basis vectors of Cheshire group
32	$Pba2$		$a<b$	$A\ xyz$ $\bar{x}\bar{y}\bar{z}$	$00z, 0\frac{1}{2}z, \frac{1}{2}0z, \frac{1}{2}\frac{1}{2}z$	Z^1mmm	$\frac{1}{2}a, \frac{1}{2}b, \varepsilon c$
33	$Pna2_1$			$A\ xyz$ $\bar{x}\bar{y}\bar{z}$	$00z, 0\frac{1}{2}z, \frac{1}{2}0z, \frac{1}{2}\frac{1}{2}z$	Z^1mmm	$\frac{1}{2}a, \frac{1}{2}b, \varepsilon c$
34	$Pnn2$		$a<b$	$A\ xyz$ $\bar{x}\bar{y}\bar{z}$	$00z, 0\frac{1}{2}z, \frac{1}{2}0z, \frac{1}{2}\frac{1}{2}z$	Z^1mmm	$\frac{1}{2}a, \frac{1}{2}b, \varepsilon c$
35	$Cmm2$		$a<b$	$A\ xyz$ $\bar{x}\bar{y}\bar{z}$	$00z, 0\frac{1}{2}z$	Z^1mmm	$\frac{1}{2}a, \frac{1}{2}b, \varepsilon c$
36	$Cmc2_1$			$A\ xyz$ $\bar{x}\bar{y}\bar{z}$	$00z, 0\frac{1}{2}z$	Z^1mmm	$\frac{1}{2}a, \frac{1}{2}b, \varepsilon c$
37	$Ccc2$		$a<b$	$A\ xyz$ $\bar{x}\bar{y}\bar{z}$	$00z, 0\frac{1}{2}z$	Z^1mmm	$\frac{1}{2}a, \frac{1}{2}b, \varepsilon c$
38	$Amm2$			$A\ xyz$ $\bar{x}\bar{y}\bar{z}$	$00z, \frac{1}{2}0z$	Z^1mmm	$\frac{1}{2}a, \frac{1}{2}b, \varepsilon c$
39	$Abm2$			$A\ xyz$ $\bar{x}\bar{y}\bar{z}$	$00z, \frac{1}{2}0z$	Z^1mmm	$\frac{1}{2}a, \frac{1}{2}b, \varepsilon c$
40	$Ama2$			$A\ xyz$ $\bar{x}\bar{y}\bar{z}$	$00z, \frac{1}{2}0z$	Z^1mmm	$\frac{1}{2}a, \frac{1}{2}b, \varepsilon c$
41	$Aba2$			$A\ xyz$ $\bar{x}\bar{y}\bar{z}$	$00z, \frac{1}{2}0z$	Z^1mmm	$\frac{1}{2}a, \frac{1}{2}b, \varepsilon c$
42	$Fmm2$		$a<b$	$A\ xyz$ $\bar{x}\bar{y}\bar{z}$	$00z$	Z^1mmm	$\frac{1}{2}a, \frac{1}{2}b, \varepsilon c$
43	$Fdd2$		$a<b$ $[\frac{1}{4}\frac{1}{4}\frac{1}{4}]$¶	$A\ xyz$ $\frac{1}{4}-x\frac{1}{4}-y\frac{1}{4}-z$	$00z$	Z^1ban	$\frac{1}{2}a, \frac{1}{2}b, \varepsilon c$
44	$Imm2$		$a<b$	$A\ xyz$ $\bar{x}\bar{y}\bar{z}$	$00z, 0\frac{1}{2}z$	Z^1mmm	$\frac{1}{2}a, \frac{1}{2}b, \varepsilon c$
45	$Iba2$		$a<b$	$A\ xyz$ $\bar{x}\bar{y}\bar{z}$	$00z, 0\frac{1}{2}z$	Z^1mmm	$\frac{1}{2}a, \frac{1}{2}b, \varepsilon c$
46	$Ima2$			$A\ xyz$ $\bar{x}\bar{y}\bar{z}$	$00z, 0\frac{1}{2}z$	Z^1mmm	$\frac{1}{2}a, \frac{1}{2}b, \varepsilon c$
47	$Pmmm$		$a<b<c$	xyz	$000, \frac{1}{2}00, 0\frac{1}{2}0, 00\frac{1}{2}, 0\frac{1}{2}\frac{1}{2}, \frac{1}{2}0\frac{1}{2}, \frac{1}{2}\frac{1}{2}0, \frac{1}{2}\frac{1}{2}\frac{1}{2}$	$Pmmm$	$\frac{1}{2}a, \frac{1}{2}b, \frac{1}{2}c$
48	$Pnnn$	Origin at centre of symmetry	$a<b<c$	xyz	$000, \frac{1}{2}00, 0\frac{1}{2}0, 00\frac{1}{2}, 0\frac{1}{2}\frac{1}{2}, \frac{1}{2}0\frac{1}{2}, \frac{1}{2}\frac{1}{2}0, \frac{1}{2}\frac{1}{2}\frac{1}{2}$	$Pmmm$	$\frac{1}{2}a, \frac{1}{2}b, \frac{1}{2}c$
49	$Pccm$		$a<b$	xyz	$000, \frac{1}{2}00, 0\frac{1}{2}0, 00\frac{1}{2}, 0\frac{1}{2}\frac{1}{2}, \frac{1}{2}0\frac{1}{2}, \frac{1}{2}\frac{1}{2}0, \frac{1}{2}\frac{1}{2}\frac{1}{2}$	$Pmmm$	$\frac{1}{2}a, \frac{1}{2}b, \frac{1}{2}c$
50	$Pban$	Origin at centre of symmetry	$a<b$	xyz	$000, \frac{1}{2}00, 0\frac{1}{2}0, 00\frac{1}{2}, 0\frac{1}{2}\frac{1}{2}, \frac{1}{2}0\frac{1}{2}, \frac{1}{2}\frac{1}{2}0, \frac{1}{2}\frac{1}{2}\frac{1}{2}$	$Pmmm$	$\frac{1}{2}a, \frac{1}{2}b, \frac{1}{2}c$
51	$Pmma$			xyz	$000, \frac{1}{2}00, 0\frac{1}{2}0, 00\frac{1}{2}, 0\frac{1}{2}\frac{1}{2}, \frac{1}{2}0\frac{1}{2}, \frac{1}{2}\frac{1}{2}0, \frac{1}{2}\frac{1}{2}\frac{1}{2}$	$Pmmm$	$\frac{1}{2}a, \frac{1}{2}b, \frac{1}{2}c$
52	$Pnna$			xyz	$000, \frac{1}{2}00, 0\frac{1}{2}0, 00\frac{1}{2}, 0\frac{1}{2}\frac{1}{2}, \frac{1}{2}0\frac{1}{2}, \frac{1}{2}\frac{1}{2}0, \frac{1}{2}\frac{1}{2}\frac{1}{2}$	$Pmmm$	$\frac{1}{2}a, \frac{1}{2}b, \frac{1}{2}c$
53	$Pmna$			xyz	$000, \frac{1}{2}00, 0\frac{1}{2}0, 00\frac{1}{2}, 0\frac{1}{2}\frac{1}{2}, \frac{1}{2}0\frac{1}{2}, \frac{1}{2}\frac{1}{2}0, \frac{1}{2}\frac{1}{2}\frac{1}{2}$	$Pmmm$	$\frac{1}{2}a, \frac{1}{2}b, \frac{1}{2}c$
54	$Pcca$			xyz	$000, \frac{1}{2}00, 0\frac{1}{2}0, 00\frac{1}{2}, 0\frac{1}{2}\frac{1}{2}, \frac{1}{2}0\frac{1}{2}, \frac{1}{2}\frac{1}{2}0, \frac{1}{2}\frac{1}{2}\frac{1}{2}$	$Pmmm$	$\frac{1}{2}a, \frac{1}{2}b, \frac{1}{2}c$
55	$Pbam$		$a<b$	xyz	$000, \frac{1}{2}00, 0\frac{1}{2}0, 00\frac{1}{2}, 0\frac{1}{2}\frac{1}{2}, \frac{1}{2}0\frac{1}{2}, \frac{1}{2}\frac{1}{2}0, \frac{1}{2}\frac{1}{2}\frac{1}{2}$	$Pmmm$	$\frac{1}{2}a, \frac{1}{2}b, \frac{1}{2}c$
56	$Pccn$		$a<b$	xyz	$000, \frac{1}{2}00, 0\frac{1}{2}0, 00\frac{1}{2}, 0\frac{1}{2}\frac{1}{2}, \frac{1}{2}0\frac{1}{2}, \frac{1}{2}\frac{1}{2}0, \frac{1}{2}\frac{1}{2}\frac{1}{2}$	$Pmmm$	$\frac{1}{2}a, \frac{1}{2}b, \frac{1}{2}c$
57	$Pbcm$			xyz	$000, \frac{1}{2}00, 0\frac{1}{2}0, 00\frac{1}{2}, 0\frac{1}{2}\frac{1}{2}, \frac{1}{2}0\frac{1}{2}, \frac{1}{2}\frac{1}{2}0, \frac{1}{2}\frac{1}{2}\frac{1}{2}$	$Pmmm$	$\frac{1}{2}a, \frac{1}{2}b, \frac{1}{2}c$
58	$Pnnm$		$a<b$	xyz	$000, \frac{1}{2}00, 0\frac{1}{2}0, 00\frac{1}{2}, 0\frac{1}{2}\frac{1}{2}, \frac{1}{2}0\frac{1}{2}, \frac{1}{2}\frac{1}{2}0, \frac{1}{2}\frac{1}{2}\frac{1}{2}$	$Pmmm$	$\frac{1}{2}a, \frac{1}{2}b, \frac{1}{2}c$
59	$Pmmn$	Origin at centre of symmetry	$a<b$	xyz	$000, \frac{1}{2}00, 0\frac{1}{2}0, 00\frac{1}{2}, 0\frac{1}{2}\frac{1}{2}, \frac{1}{2}0\frac{1}{2}, \frac{1}{2}\frac{1}{2}0, \frac{1}{2}\frac{1}{2}\frac{1}{2}$	$Pmmm$	$\frac{1}{2}a, \frac{1}{2}b, \frac{1}{2}c$
60	$Pbcn$			xyz	$000, \frac{1}{2}00, 0\frac{1}{2}0, 00\frac{1}{2}, 0\frac{1}{2}\frac{1}{2}, \frac{1}{2}0\frac{1}{2}, \frac{1}{2}\frac{1}{2}0, \frac{1}{2}\frac{1}{2}\frac{1}{2}$	$Pmmm$	$\frac{1}{2}a, \frac{1}{2}b, \frac{1}{2}c$
61	$Pbca$		$a<b<c$ [↻]**	xyz	$000, \frac{1}{2}00, 0\frac{1}{2}0, 00\frac{1}{2}, 0\frac{1}{2}\frac{1}{2}, \frac{1}{2}0\frac{1}{2}, \frac{1}{2}\frac{1}{2}0, \frac{1}{2}\frac{1}{2}\frac{1}{2}$	$Pmmm$	$\frac{1}{2}a, \frac{1}{2}b, \frac{1}{2}c$
62	$Pnma$			xyz	$000, \frac{1}{2}00, 0\frac{1}{2}0, 00\frac{1}{2}, 0\frac{1}{2}\frac{1}{2}, \frac{1}{2}0\frac{1}{2}, \frac{1}{2}\frac{1}{2}0, \frac{1}{2}\frac{1}{2}\frac{1}{2}$	$Pmmm$	$\frac{1}{2}a, \frac{1}{2}b, \frac{1}{2}c$
63	$Cmcm$			xyz	$000, 00\frac{1}{2}, 0\frac{1}{2}0, 0\frac{1}{2}\frac{1}{2}$	$Pmmm$	$\frac{1}{2}a, \frac{1}{2}b, \frac{1}{2}c$
64	$Cmca$			xyz	$000, 00\frac{1}{2}, 0\frac{1}{2}0, 0\frac{1}{2}\frac{1}{2}$	$Pmmm$	$\frac{1}{2}a, \frac{1}{2}b, \frac{1}{2}c$
65	$Cmmm$		$a<b$	xyz	$000, 00\frac{1}{2}, 0\frac{1}{2}0, 0\frac{1}{2}\frac{1}{2}$	$Pmmm$	$\frac{1}{2}a, \frac{1}{2}b, \frac{1}{2}c$
66	$Cccm$		$a<b$	xyz	$000, 00\frac{1}{2}, 0\frac{1}{2}0, 0\frac{1}{2}\frac{1}{2}$	$Pmmm$	$\frac{1}{2}a, \frac{1}{2}b, \frac{1}{2}c$
67	$Cmma$		$a<b$ $[\frac{1}{4}\frac{1}{4}0]$††	xyz	$000, 00\frac{1}{2}, 0\frac{1}{2}0, 0\frac{1}{2}\frac{1}{2}$	$Pmmm$	$\frac{1}{2}a, \frac{1}{2}b, \frac{1}{2}c$
68	$Ccca$	Origin at centre of symmetry	$a<b$ $[\frac{1}{4}\frac{1}{4}0]$††	xyz	$000, 00\frac{1}{2}, 0\frac{1}{2}0, 0\frac{1}{2}\frac{1}{2}$	$Pmmm$	$\frac{1}{2}a, \frac{1}{2}b, \frac{1}{2}c$
69	$Fmmm$		$a<b<c$	xyz	$000, \frac{1}{2}\frac{1}{2}\frac{1}{2}$	$Pmmm$	$\frac{1}{2}a, \frac{1}{2}b, \frac{1}{2}c$
70	$Fddd$	Origin at centre of symmetry	$a<b<c$ $[\frac{1}{4}\frac{1}{4}0$↻$]$‡‡	xyz	$000, \frac{1}{2}\frac{1}{2}\frac{1}{2}$	$Pnnn$	$\frac{1}{2}a, \frac{1}{2}b, \frac{1}{2}c$
71	$Immm$		$a<b<c$	xyz	$000, 00\frac{1}{2}, 0\frac{1}{2}0, 0\frac{1}{2}\frac{1}{2}$	$Pmmm$	$\frac{1}{2}a, \frac{1}{2}b, \frac{1}{2}c$
72	$Ibam$		$a<b$	xyz	$000, 00\frac{1}{2}, 0\frac{1}{2}0, 0\frac{1}{2}\frac{1}{2}$	$Pmmm$	$\frac{1}{2}a, \frac{1}{2}b, \frac{1}{2}c$
73	$Ibca$		$a<b<c$ $[\frac{1}{4}\frac{1}{4}\frac{1}{4}]$§	xyz	$000, 00\frac{1}{2}, 0\frac{1}{2}0, 0\frac{1}{2}\frac{1}{2}$	$Pmmm$	$\frac{1}{2}a, \frac{1}{2}b, \frac{1}{2}c$
74	$Imma$		$a<b$ $[\frac{1}{4}\frac{1}{4}\frac{1}{4}]$¶	xyz	$000, 00\frac{1}{2}, 0\frac{1}{2}0, 0\frac{1}{2}\frac{1}{2}$	$Pmmm$	$\frac{1}{2}a, \frac{1}{2}b, \frac{1}{2}c$
TETRAGONAL $a=b$, $\alpha=\beta=\gamma=90°$, no extra conditions for the labelling of axes							
75	$P4$			$C\ xyz, \bar{x}y\bar{z}$ $\bar{x}\bar{y}\bar{z}, x\bar{y}z$	$00z, \frac{1}{2}\frac{1}{2}z$	Z^14/mmm	$\frac{1}{2}(a-b), \frac{1}{2}(a+b), \varepsilon c$
76	$P4_1$			$E\ xyz, \bar{x}y\bar{z}$	$00z, \frac{1}{2}\frac{1}{2}z$	Z^1422	$\frac{1}{2}(a-b), \frac{1}{2}(a+b), \varepsilon c$
77	$P4_2$			$C\ xyz, \bar{x}y\bar{z}$ $\bar{x}\bar{y}\bar{z}, x\bar{y}z$	$00z, \frac{1}{2}\frac{1}{2}z$	Z^14/mmm	$\frac{1}{2}(a-b), \frac{1}{2}(a+b), \varepsilon c$
78	$P4_3$	Enantiomorph of $P4_1$					
79	$I4$			$C\ xyz, \bar{x}y\bar{z}$ $\bar{x}\bar{y}\bar{z}, x\bar{y}z$	$00z$	Z^14/mmm	$\frac{1}{2}(a-b), \frac{1}{2}(a+b), \varepsilon c$
80	$I4_1$			$C\ xyz, yx\bar{z}$ $\bar{x}\frac{1}{2}-y\bar{z}, \bar{y}\frac{1}{2}-xz$	$00z$	Z^14/nbm	$\frac{1}{2}(a-b), \frac{1}{2}(a+b), \varepsilon c$
81	$P\bar{4}$			$A\ xyz, \bar{y}\bar{x}\bar{z}$ $\bar{x}\bar{y}\bar{z}, yxz$	$000, 00\frac{1}{2}, \frac{1}{2}\frac{1}{2}0, \frac{1}{2}\frac{1}{2}\frac{1}{2}$	$P4/mmm$	$\frac{1}{2}(a-b), \frac{1}{2}(a+b), \frac{1}{2}c$

Table 6 (*cont.*)

A No.	*B* Standard space-group symbol	*C* Extra condition for choice of unit cell	*D* Labels of axes	*E* Non-redundant *xyz* triplets	*F* Permitted origins	*G* Cheshire group	*H* Basis vectors of Cheshire group
82	$I\bar{4}$			*A* $xyz, \bar{y}\bar{x}\bar{z}$ $\bar{x}\bar{y}\bar{z}, yxz$	$000, 00\frac{1}{2}, 0\frac{1}{2}\frac{1}{4}, 0\frac{1}{2}\frac{3}{4}$	$I4/mmm$	$\frac{1}{2}(a-b), \frac{1}{2}(a+b), \frac{1}{2}c$
83	$P4/m$			$xyz, \bar{x}y\bar{z}$	$000, 00\frac{1}{2}, \frac{1}{2}\frac{1}{2}0, \frac{1}{2}\frac{1}{2}\frac{1}{2}$	$P4/mmm$	$\frac{1}{2}(a-b), \frac{1}{2}(a+b), \frac{1}{2}c$
84	$P4_2/m$			$xyz, \bar{x}y\bar{z}$	$000, 00\frac{1}{2}, \frac{1}{2}\frac{1}{2}0, \frac{1}{2}\frac{1}{2}\frac{1}{2}$	$P4/mmm$	$\frac{1}{2}(a-b), \frac{1}{2}(a+b), \frac{1}{2}c$
85	$P4/n$	Origin at centre of symmetry		$xyz, yx\bar{z}$	$000, 00\frac{1}{2}, \frac{1}{2}\frac{1}{2}0, \frac{1}{2}\frac{1}{2}\frac{1}{2}$	$P4/mmm$	$\frac{1}{2}(a-b), \frac{1}{2}(a+b), \frac{1}{2}c$
86	$P4_2/n$	Origin at centre of symmetry		$xyz, yx\bar{z}$	$000, 00\frac{1}{2}, \frac{1}{2}\frac{1}{2}0, \frac{1}{2}\frac{1}{2}\frac{1}{2}$	$P4/mmm$	$\frac{1}{2}(a-b), \frac{1}{2}(a+b), \frac{1}{2}c$
87	$I4/m$			$xyz, \bar{x}y\bar{z}$	$000, 00\frac{1}{2}$	$P4/mmm$	$\frac{1}{2}(a-b), \frac{1}{2}(a+b), \frac{1}{2}c$
88	$I4_1/a$	Origin at centre of symmetry		$xyz, x\bar{y}\bar{z}$	$000, 00\frac{1}{2}$	$P4_2/nnm$	$\frac{1}{2}(a-b), \frac{1}{2}(a+b), \frac{1}{2}c$
89	$P422$			*C* xyz $\bar{x}\bar{y}\bar{z}$	$000, 00\frac{1}{2}, \frac{1}{2}\frac{1}{2}0, \frac{1}{2}\frac{1}{2}\frac{1}{2}$	$P4/mmm$	$\frac{1}{2}(a-b), \frac{1}{2}(a+b), \frac{1}{2}c$
90	$P42_12$			*C* xyz $\bar{x}\bar{y}\bar{z}$	$000, 00\frac{1}{2}, \frac{1}{2}\frac{1}{2}0, \frac{1}{2}\frac{1}{2}\frac{1}{2}$	$P4/mmm$	$\frac{1}{2}(a-b), \frac{1}{2}(a+b), \frac{1}{2}c$
91	$P4_122$			*E* xyz	$000, 00\frac{1}{2}, \frac{1}{2}\frac{1}{2}0, \frac{1}{2}\frac{1}{2}\frac{1}{2}$	$P4_222$	$\frac{1}{2}(a-b), \frac{1}{2}(a+b), \frac{1}{2}c$
92	$P4_12_12$			*E* xyz	$000, 00\frac{1}{2}, \frac{1}{2}\frac{1}{2}0, \frac{1}{2}\frac{1}{2}\frac{1}{2}$	$P4_222$	$\frac{1}{2}(a-b), \frac{1}{2}(a+b), \frac{1}{2}c$
93	$P4_222$			*C* xyz $\bar{x}\bar{y}\bar{z}$	$000, 00\frac{1}{2}, \frac{1}{2}\frac{1}{2}0, \frac{1}{2}\frac{1}{2}\frac{1}{2}$	$P4/mmm$	$\frac{1}{2}(a-b), \frac{1}{2}(a+b), \frac{1}{2}c$
94	$P4_22_12$			*C* xyz $\bar{x}\bar{y}\bar{z}$	$000, 00\frac{1}{2}, \frac{1}{2}\frac{1}{2}0, \frac{1}{2}\frac{1}{2}\frac{1}{2}$	$P4/mmm$	$\frac{1}{2}(a-b), \frac{1}{2}(a+b), \frac{1}{2}c$
95	$P4_322$	Enantiomorph of $P4_122$					
96	$P4_32_12$	Enantiomorph of $P4_12_12$					
97	$I422$			*C* xyz $\bar{x}\bar{y}\bar{z}$	$000, 00\frac{1}{2}$	$P4/mmm$	$\frac{1}{2}(a-b), \frac{1}{2}(a+b), \frac{1}{2}c$
98	$I4_122$			*C* xyz $\bar{x}\frac{1}{2}-y\frac{1}{4}-z$	$000, 00\frac{1}{2}$	$P4_2/nnm$	$\frac{1}{2}(a-b), \frac{1}{2}(a+b), \frac{1}{2}c$
99	$P4mm$			*A* xyz $\bar{x}\bar{y}\bar{z}$	$00z, \frac{1}{2}\frac{1}{2}z$	Z^14/mmm	$\frac{1}{2}(a-b), \frac{1}{2}(a+b), \varepsilon c$
100	$P4bm$			*A* xyz $\bar{x}\bar{y}\bar{z}$	$00z, \frac{1}{2}\frac{1}{2}z$	Z^14/mmm	$\frac{1}{2}(a-b), \frac{1}{2}(a+b), \varepsilon c$
101	$P4_2cm$			*A* xyz $\bar{x}\bar{y}\bar{z}$	$00z, \frac{1}{2}\frac{1}{2}z$	Z^14/mmm	$\frac{1}{2}(a-b), \frac{1}{2}(a+b), \varepsilon c$
102	$P4_2nm$			*A* xyz $\bar{x}\bar{y}\bar{z}$	$00z, \frac{1}{2}\frac{1}{2}z$	Z^14/mmm	$\frac{1}{2}(a-b), \frac{1}{2}(a+b), \varepsilon c$
103	$P4cc$			*A* xyz $\bar{x}\bar{y}\bar{z}$	$00z, \frac{1}{2}\frac{1}{2}z$	Z^14/mmm	$\frac{1}{2}(a-b), \frac{1}{2}(a+b), \varepsilon c$
104	$P4nc$			*A* xyz $\bar{x}\bar{y}\bar{z}$	$00z, \frac{1}{2}\frac{1}{2}z$	Z^14/mmm	$\frac{1}{2}(a-b), \frac{1}{2}(a+b), \varepsilon c$
105	$P4_2mc$			*A* xyz $\bar{x}\bar{y}\bar{z}$	$00z, \frac{1}{2}\frac{1}{2}z$	Z^14/mmm	$\frac{1}{2}(a-b), \frac{1}{2}(a+b), \varepsilon c$
106	$P4_2bc$			*A* xyz $\bar{x}\bar{y}\bar{z}$	$00z, \frac{1}{2}\frac{1}{2}z$	Z^14/mmm	$\frac{1}{2}(a-b), \frac{1}{2}(a+b), \varepsilon c$
107	$I4mm$			*A* xyz $\bar{x}\bar{y}\bar{z}$	$00z$	Z^14/mmm	$\frac{1}{2}(a-b), \frac{1}{2}(a+b), \varepsilon c$
108	$I4cm$			*A* xyz $\bar{x}\bar{y}\bar{z}$	$00z$	Z^14/mmm	$\frac{1}{2}(a-b), \frac{1}{2}(a+b), \varepsilon c$
109	$I4_1md$			*A* xyz $\bar{x}\frac{1}{2}-y\bar{z}$	$00z$	Z^14/nbm	$\frac{1}{2}(a-b), \frac{1}{2}(a+b), \varepsilon c$
110	$I4_1cd$			*A* xyz $\bar{x}\frac{1}{2}-y\bar{z}$	$00z$	Z^14/nbm	$\frac{1}{2}(a-b), \frac{1}{2}(a+b), \varepsilon c$
111	$P\bar{4}2m$			*A* xyz $\bar{x}\bar{y}\bar{z}$	$000, 00\frac{1}{2}, \frac{1}{2}\frac{1}{2}0, \frac{1}{2}\frac{1}{2}\frac{1}{2}$	$P4/mmm$	$\frac{1}{2}(a-b), \frac{1}{2}(a+b), \frac{1}{2}c$
112	$P\bar{4}2c$			*A* xyz $\bar{x}\bar{y}\bar{z}$	$000, 00\frac{1}{2}, \frac{1}{2}\frac{1}{2}0, \frac{1}{2}\frac{1}{2}\frac{1}{2}$	$P4/mmm$	$\frac{1}{2}(a-b), \frac{1}{2}(a+b), \frac{1}{2}c$
113	$P\bar{4}2_1m$			*A* xyz $\bar{x}\bar{y}\bar{z}$	$000, 00\frac{1}{2}, \frac{1}{2}\frac{1}{2}0, \frac{1}{2}\frac{1}{2}\frac{1}{2}$	$P4/mmm$	$\frac{1}{2}(a-b), \frac{1}{2}(a+b), \frac{1}{2}c$
114	$P\bar{4}2_1c$			*A* xyz $\bar{x}\bar{y}\bar{z}$	$000, 00\frac{1}{2}, \frac{1}{2}\frac{1}{2}0, \frac{1}{2}\frac{1}{2}\frac{1}{2}$	$P4/mmm$	$\frac{1}{2}(a-b), \frac{1}{2}(a+b), \frac{1}{2}c$
115	$P\bar{4}m2$			*A* xyz $\bar{x}\bar{y}\bar{z}$	$000, 00\frac{1}{2}, \frac{1}{2}\frac{1}{2}0, \frac{1}{2}\frac{1}{2}\frac{1}{2}$	$P4/mmm$	$\frac{1}{2}(a-b), \frac{1}{2}(a+b), \frac{1}{2}c$
116	$P\bar{4}c2$			*A* xyz $\bar{x}\bar{y}\bar{z}$	$000, 00\frac{1}{2}, \frac{1}{2}\frac{1}{2}0, \frac{1}{2}\frac{1}{2}\frac{1}{2}$	$P4/mmm$	$\frac{1}{2}(a-b), \frac{1}{2}(a+b), \frac{1}{2}c$
117	$P\bar{4}b2$			*A* xyz $\bar{x}\bar{y}\bar{z}$	$000, 00\frac{1}{2}, \frac{1}{2}\frac{1}{2}0, \frac{1}{2}\frac{1}{2}\frac{1}{2}$	$P4/mmm$	$\frac{1}{2}(a-b), \frac{1}{2}(a+b), \frac{1}{2}c$
118	$P\bar{4}n2$			*A* xyz $\bar{x}\bar{y}\bar{z}$	$000, 00\frac{1}{2}, \frac{1}{2}\frac{1}{2}0, \frac{1}{2}\frac{1}{2}\frac{1}{2}$	$P4/mmm$	$\frac{1}{2}(a-b), \frac{1}{2}(a+b), \frac{1}{2}c$
119	$I\bar{4}m2$			*A* xyz $\bar{x}\bar{y}\bar{z}$	$000, 00\frac{1}{2}, 0\frac{1}{2}\frac{1}{4}, 0\frac{1}{2}\frac{3}{4}$	$I4/mmm$	$\frac{1}{2}(a-b), \frac{1}{2}(a+b), \frac{1}{2}c$
120	$I\bar{4}c2$			*A* xyz $\bar{x}\bar{y}\bar{z}$	$000, 00\frac{1}{2}, 0\frac{1}{2}\frac{1}{4}, 0\frac{1}{2}\frac{3}{4}$	$I4/mmm$	$\frac{1}{2}(a-b), \frac{1}{2}(a+b), \frac{1}{2}c$
121	$I\bar{4}2m$			*A* xyz $\bar{x}\bar{y}\bar{z}$	$000, 00\frac{1}{2}$	$P4/mmm$	$\frac{1}{2}(a-b), \frac{1}{2}(a+b), \frac{1}{2}c$
122	$I\bar{4}2d$			*A* xyz $\bar{x}\frac{1}{2}-y\frac{1}{4}-z$	$000, 00\frac{1}{2}$	$P4_2/nnm$	$\frac{1}{2}(a-b), \frac{1}{2}(a+b), \frac{1}{2}c$

Table 6 (*cont.*)

A No.	*B* Standard space-group symbol	*C* Extra condition for choice of unit cell	*D* Labels of axes	*E* Non-redundant *xyz* triplets	*F* Permitted origins	*G* Cheshire group	*H* Basis vectors of Cheshire group
123	$P4/mmm$			xyz	$000, 00\frac{1}{2}, \frac{1}{2}\frac{1}{2}0, \frac{1}{2}\frac{1}{2}\frac{1}{2}$	$P4/mmm$	$\frac{1}{2}(a-b), \frac{1}{2}(a+b), \frac{1}{2}c$
124	$P4/mcc$			xyz	$000, 00\frac{1}{2}, \frac{1}{2}\frac{1}{2}0, \frac{1}{2}\frac{1}{2}\frac{1}{2}$	$P4/mmm$	$\frac{1}{2}(a-b), \frac{1}{2}(a+b), \frac{1}{2}c$
125	$P4/nbm$	Origin at centre of symmetry		xyz	$000, 00\frac{1}{2}, \frac{1}{2}\frac{1}{2}0, \frac{1}{2}\frac{1}{2}\frac{1}{2}$	$P4/mmm$	$\frac{1}{2}(a-b), \frac{1}{2}(a+b), \frac{1}{2}c$
126	$P4/nnc$	Origin at centre of symmetry		xyz	$000, 00\frac{1}{2}, \frac{1}{2}\frac{1}{2}0, \frac{1}{2}\frac{1}{2}\frac{1}{2}$	$P4/mmm$	$\frac{1}{2}(a-b), \frac{1}{2}(a+b), \frac{1}{2}c$
127	$P4/mbm$			xyz	$000, 00\frac{1}{2}, \frac{1}{2}\frac{1}{2}0, \frac{1}{2}\frac{1}{2}\frac{1}{2}$	$P4/mmm$	$\frac{1}{2}(a-b), \frac{1}{2}(a+b), \frac{1}{2}c$
128	$P4/mnc$			xyz	$000, 00\frac{1}{2}, \frac{1}{2}\frac{1}{2}0, \frac{1}{2}\frac{1}{2}\frac{1}{2}$	$P4/mmm$	$\frac{1}{2}(a-b), \frac{1}{2}(a+b), \frac{1}{2}c$
129	$P4/nmm$	Origin at centre of symmetry		xyz	$000, 00\frac{1}{2}, \frac{1}{2}\frac{1}{2}0, \frac{1}{2}\frac{1}{2}\frac{1}{2}$	$P4/mmm$	$\frac{1}{2}(a-b), \frac{1}{2}(a+b), \frac{1}{2}c$
130	$P4/ncc$	Origin at centre of symmetry		xyz	$000, 00\frac{1}{2}, \frac{1}{2}\frac{1}{2}0, \frac{1}{2}\frac{1}{2}\frac{1}{2}$	$P4/mmm$	$\frac{1}{2}(a-b), \frac{1}{2}(a+b), \frac{1}{2}c$
131	$P4_2/mmc$			xyz	$000, 00\frac{1}{2}, \frac{1}{2}\frac{1}{2}0, \frac{1}{2}\frac{1}{2}\frac{1}{2}$	$P4/mmm$	$\frac{1}{2}(a-b), \frac{1}{2}(a+b), \frac{1}{2}c$
132	$P4_2/mcm$			xyz	$000, 00\frac{1}{2}, \frac{1}{2}\frac{1}{2}0, \frac{1}{2}\frac{1}{2}\frac{1}{2}$	$P4/mmm$	$\frac{1}{2}(a-b), \frac{1}{2}(a+b), \frac{1}{2}c$
133	$P4_2/nbc$	Origin at centre of symmetry		xyz	$000, 00\frac{1}{2}, \frac{1}{2}\frac{1}{2}0, \frac{1}{2}\frac{1}{2}\frac{1}{2}$	$P4/mmm$	$\frac{1}{2}(a-b), \frac{1}{2}(a+b), \frac{1}{2}c$
134	$P4_2/nnm$	Origin at centre of symmetry		xyz	$000, 00\frac{1}{2}, \frac{1}{2}\frac{1}{2}0, \frac{1}{2}\frac{1}{2}\frac{1}{2}$	$P4/mmm$	$\frac{1}{2}(a-b), \frac{1}{2}(a+b), \frac{1}{2}c$
135	$P4_2/mbc$			xyz	$000, 00\frac{1}{2}, \frac{1}{2}\frac{1}{2}0, \frac{1}{2}\frac{1}{2}\frac{1}{2}$	$P4/mmm$	$\frac{1}{2}(a-b), \frac{1}{2}(a+b), \frac{1}{2}c$
136	$P4_2/mnm$			xyz	$000, 00\frac{1}{2}, \frac{1}{2}\frac{1}{2}0, \frac{1}{2}\frac{1}{2}\frac{1}{2}$	$P4/mmm$	$\frac{1}{2}(a-b), \frac{1}{2}(a+b), \frac{1}{2}c$
137	$P4_2/nmc$	Origin at centre of symmetry		xyz	$000, 00\frac{1}{2}, \frac{1}{2}\frac{1}{2}0, \frac{1}{2}\frac{1}{2}\frac{1}{2}$	$P4/mmm$	$\frac{1}{2}(a-b), \frac{1}{2}(a+b), \frac{1}{2}c$
138	$P4_2/ncm$	Origin at centre of symmetry		xyz	$000, 00\frac{1}{2}, \frac{1}{2}\frac{1}{2}0, \frac{1}{2}\frac{1}{2}\frac{1}{2}$	$P4/mmm$	$\frac{1}{2}(a-b), \frac{1}{2}(a+b), \frac{1}{2}c$
139	$I4/mmm$			xyz	$000, 00\frac{1}{2}$	$P4/mmm$	$\frac{1}{2}(a-b), \frac{1}{2}(a+b), \frac{1}{2}c$
140	$I4/mcm$			xyz	$000, 00\frac{1}{2}$	$P4/mmm$	$\frac{1}{2}(a-b), \frac{1}{2}(a+b), \frac{1}{2}c$
141	$I4_1/amd$	Origin at centre of symmetry		xyz	$000, 00\frac{1}{2}$	$P4_2/nnm$	$\frac{1}{2}(a-b), \frac{1}{2}(a+b), \frac{1}{2}c$
142	$I4_1/acd$	Origin at centre of symmetry		xyz	$000, 00\frac{1}{2}$	$P4_2/nnm$	$\frac{1}{2}(a-b), \frac{1}{2}(a+b), \frac{1}{2}c$

TRIGONAL $a = b$, $\alpha = \beta = 90$, $\gamma = 120°$, no extra conditions for the labelling of axes

A No.	*B*	*C*	*D*	*E*	*F*	*G*	*H*
143	$P3$			$C\ xyz, \bar{x}\bar{y}z, yx\bar{z}, \bar{y}\bar{x}\bar{z}$ $\bar{x}\bar{y}\bar{z}, xy\bar{z}, \bar{y}\bar{x}z, yxz$	$00z, \frac{1}{3}\frac{2}{3}z, \frac{2}{3}\frac{1}{3}z$	Z^16/mmm	$\frac{1}{3}(a-b), \frac{1}{3}(a+2b), \varepsilon c$
144	$P3_1$			$E\ xyz, \bar{x}\bar{y}z, yx\bar{z}, \bar{y}\bar{x}\bar{z}$	$00z, \frac{1}{3}\frac{2}{3}z, \frac{2}{3}\frac{1}{3}z$	Z^1622	$\frac{1}{3}(a-b), \frac{1}{3}(a+2b), \varepsilon c$
145	$P3_2$	Enantiomorph of $P3_1$					
146	$R3$	Hexagonal axes		$C\ xyz, yx\bar{z}$ $\bar{x}\bar{y}\bar{z}, \bar{y}\bar{x}z$	$00z$	$Z^1\bar{3}1m$	$\frac{1}{3}(a-b), \frac{1}{3}(a+2b), \varepsilon c$
147	$P\bar{3}$			$xyz, \bar{x}\bar{y}z, yx\bar{z}, \bar{y}\bar{x}\bar{z}$	$000, 00\frac{1}{2}$	$P6/mmm$	$a, b, \frac{1}{2}c$
148	$R\bar{3}$	Hexagonal axes		$xyz, yx\bar{z}$	$000, 00\frac{1}{2}$	$R\bar{3}m$	$-b, a+b, \frac{1}{2}c$
149	$P312$			$C\ xyz, \bar{x}\bar{y}z$ $\bar{x}\bar{y}\bar{z}, xy\bar{z}$	$000, 00\frac{1}{2}, \frac{1}{3}\frac{2}{3}0, \frac{1}{3}\frac{2}{3}\frac{1}{2}, \frac{2}{3}\frac{1}{3}0, \frac{2}{3}\frac{1}{3}\frac{1}{2}$	$P6/mmm$	$\frac{1}{3}(a-b), \frac{1}{3}(a+2b), \frac{1}{2}c$
150	$P321$			$C\ xyz, \bar{x}\bar{y}z$ $\bar{x}\bar{y}\bar{z}, xy\bar{z}$	$000, 00\frac{1}{2}$	$P6/mmm$	$a, b, \frac{1}{2}c$
151	$P3_112$			$E\ xyz, \bar{x}\bar{y}z$	$000, 00\frac{1}{2}, \frac{1}{3}\frac{2}{3}0, \frac{1}{3}\frac{2}{3}\frac{1}{2}, \frac{2}{3}\frac{1}{3}0, \frac{2}{3}\frac{1}{3}\frac{1}{2}$	$P6_222$	$\frac{1}{3}(a-b), \frac{1}{3}(a+2b), \frac{1}{2}c$
152	$P3_121$			$E\ xyz, \bar{x}\bar{y}z$	$000, 00\frac{1}{2}$	$P6_222$	$a, b, \frac{1}{2}c$
153	$P3_212$	Enantiomorph of $P3_112$					
154	$P3_221$	Enantiomorph of $P3_121$					
155	$R32$	Hexagonal axes		$C\ xyz$ $\bar{x}\bar{y}\bar{z}$	$000, 00\frac{1}{2}$	$R\bar{3}m$	$-b, a+b, \frac{1}{2}c$
156	$P3m1$			$A\ xyz, \bar{x}\bar{y}z$ $\bar{x}\bar{y}\bar{z}, xy\bar{z}$	$00z, \frac{1}{3}\frac{2}{3}z, \frac{2}{3}\frac{1}{3}z$	Z^16/mmm	$\frac{1}{3}(a-b), \frac{1}{3}(a+2b), \varepsilon c$
157	$P31m$			$A\ xyz, \bar{x}\bar{y}z$ $\bar{x}\bar{y}\bar{z}, xy\bar{z}$	$00z$	Z^16/mmm	$a, b, \varepsilon c$
158	$P3c1$			$A\ xyz, \bar{x}\bar{y}z$ $\bar{x}\bar{y}\bar{z}, xy\bar{z}$	$00z, \frac{1}{3}\frac{2}{3}z, \frac{2}{3}\frac{1}{3}z$	$Z^1/6mmm$	$\frac{1}{3}(a-b), \frac{1}{3}(a+2b), \varepsilon c$
159	$P31c$			$A\ xyz, \bar{x}\bar{y}z$ $\bar{x}\bar{y}\bar{z}, xy\bar{z}$	$00z$	Z^16/mmm	$a, b, \varepsilon c$
160	$R3m$	Hexagonal axes		$A\ xyz$ $\bar{x}\bar{y}\bar{z}$	$00z$	$Z^1\bar{3}1m$	$\frac{1}{3}(a-b), \frac{1}{3}(a+2b), \varepsilon c$
161	$R3c$	Hexagonal axes		$A\ xyz$ $\bar{x}\bar{y}\bar{z}$	$00z$	$Z^1\bar{3}1m$	$\frac{1}{3}(a-b), \frac{1}{3}(a+2b), \varepsilon c$
162	$P\bar{3}1m$			$xyz, \bar{x}\bar{y}z$	$000, 00\frac{1}{2}$	$P6/mmm$	$a, b, \frac{1}{2}c$
163	$P\bar{3}1c$			$xyz, \bar{x}\bar{y}z$	$000, 00\frac{1}{2}$	$P6/mmm$	$a, b, \frac{1}{2}c$
164	$P\bar{3}m1$			$xyz, \bar{x}\bar{y}z$	$000, 00\frac{1}{2}$	$P6/mmm$	$a, b, \frac{1}{2}c$
165	$P\bar{3}c1$			$xyz, \bar{x}\bar{y}z$	$000, 00\frac{1}{2}$	$P6/mmm$	$a, b, \frac{1}{2}c$
166	$R\bar{3}m$	Hexagonal axes		xyz	$000, 00\frac{1}{2}$	$R\bar{3}m$	$-b, a+b, \frac{1}{2}c$
167	$R\bar{3}c$	Hexagonal axes		xyz	$000, 00\frac{1}{2}$	$R\bar{3}m$	$-b, a+b, \frac{1}{2}c$

HEXAGONAL $a = b$, $\alpha = \beta = 90$, $\gamma = 120°$, no extra conditions for the labelling of axes

A No.	*B*	*C*	*D*	*E*	*F*	*G*	*H*
168	$P6$			$C\ xyz, yx\bar{z}$ $\bar{x}\bar{y}\bar{z}, \bar{y}\bar{x}z$	$00z$	Z^16/mmm	$a, b, \varepsilon c$
169	$P6_1$			$E\ xyz, yx\bar{z}$	$00z$	Z^1622	$a, b, \varepsilon c$
170	$P6_5$	Enantiomorph of $P6_1$					
171	$P6_2$			$E\ xyz, yx\bar{z}$	$00z$	Z^1622	$a, b, \varepsilon c$
172	$P6_4$	Enantiomorph of $P6_2$					
173	$P6_3$			$C\ xyz, yx\bar{z}$ $\bar{x}\bar{y}\bar{z}, \bar{y}\bar{x}z$	$00z$	Z^16/mmm	$a, b, \varepsilon c$
174	$P\bar{6}$			$A\ xyz, \bar{y}\bar{x}\bar{z}$ $\bar{x}\bar{y}\bar{z}, yxz$	$000, 00\frac{1}{2}, \frac{1}{3}\frac{2}{3}0, \frac{1}{3}\frac{2}{3}\frac{1}{2}, \frac{2}{3}\frac{1}{3}0, \frac{2}{3}\frac{1}{3}\frac{1}{2}$	$P6/mmm$	$\frac{1}{3}(a-b), \frac{1}{3}(a+2b), \frac{1}{2}c$
175	$P6/m$			$xyz, yx\bar{z}$	$000, 00\frac{1}{2}$	$P6/mmm$	$a, b, \frac{1}{2}c$
176	$P6_3/m$			$xyz, yx\bar{z}$	$000, 00\frac{1}{2}$	$P6/mmm$	$a, b, \frac{1}{2}c$

Table 6 (*cont.*)

A No.	*B* Standard space-group symbol	*C* Extra condition for choice of unit cell	*D* Labels of axes	*E* Non-redundant *xyz* triplets	*F* Permitted origins	*G* Cheshire group	*H* Basis vectors of Cheshire group
177	$P622$			$C\ xyz$ $\bar{x}\bar{y}\bar{z}$	$000, 00\tfrac{1}{2}$	$P6/mmm$	$a, b, \tfrac{1}{2}c$
178	$P6_122$			$E\ xyz$	$000, 00\tfrac{1}{2}$	$P6_222$	$a, b, \tfrac{1}{2}c$
179	$P6_522$	Enantiomorph of $P6_122$					
180	$P6_222$			$E\ xyz$	$000, 00\tfrac{1}{2}$	$P6_422$	$a, b, \tfrac{1}{2}c$
181	$P6_422$	Enantiomorph of $P6_222$					
182	$P6_322$			$C\ xyz$ $\bar{x}\bar{y}\bar{z}$	$000, 00\tfrac{1}{2}$	$P6/mmm$	$a, b, \tfrac{1}{2}c$
183	$P6mm$			$A\ xyz$ $\bar{x}\bar{y}\bar{z}$	$00z$	Z^16/mmm	$a, b, \varepsilon c$
184	$P6cc$			$A\ xyz$ $\bar{x}\bar{y}\bar{z}$	$00z$	Z^16/mmm	$a, b, \varepsilon c$
185	$P6_3cm$			$A\ xyz$ $\bar{x}\bar{y}\bar{z}$	$00z$	Z^16/mmm	$a, b, \varepsilon c$
186	$P6_3mc$			$A\ xyz$ $\bar{x}\bar{y}\bar{z}$	$00z$	Z^16/mmm	$a, b, \varepsilon c$
187	$P\bar{6}m2$			$A\ xyz$ $\bar{x}\bar{y}\bar{z}$	$000, 00\tfrac{1}{2}, \tfrac{1}{3}\tfrac{2}{3}0, \tfrac{1}{3}\tfrac{2}{3}\tfrac{1}{2}, \tfrac{2}{3}\tfrac{1}{3}0, \tfrac{2}{3}\tfrac{1}{3}\tfrac{1}{2}$	$P6/mmm$	$\tfrac{1}{3}(a-b), \tfrac{1}{3}(a+2b), \tfrac{1}{2}c$
188	$P\bar{6}c2$			$A\ xyz$ $\bar{x}\bar{y}\bar{z}$	$000, 00\tfrac{1}{2}, \tfrac{1}{3}\tfrac{2}{3}0, \tfrac{1}{3}\tfrac{2}{3}\tfrac{1}{2}, \tfrac{2}{3}\tfrac{1}{3}0, \tfrac{2}{3}\tfrac{1}{3}\tfrac{1}{2}$	$P6/mmm$	$\tfrac{1}{3}(a-b), \tfrac{1}{3}(a+2b), \tfrac{1}{2}c$
189	$P\bar{6}2m$			$A\ xyz$ $\bar{x}\bar{y}\bar{z}$	$000, 00\tfrac{1}{2}$	$P6/mmm$	$a, b, \tfrac{1}{2}c$
190	$P\bar{6}2c$			$A\ xyz$ $\bar{x}\bar{y}\bar{z}$	$000, 00\tfrac{1}{2}$	$P6/mmm$	$a, b, \tfrac{1}{2}c$
191	$P6/mmm$			xyz	$000, 00\tfrac{1}{2}$	$P6/mmm$	$a, b, \tfrac{1}{2}c$
192	$P6/mcc$			xyz	$000, 00\tfrac{1}{2}$	$P6/mmm$	$a, b, \tfrac{1}{2}c$
193	$P6_3/mcm$			xyz	$000, 00\tfrac{1}{2}$	$P6/mmm$	$a, b, \tfrac{1}{2}c$
194	$P6_3/mmc$			xyz	$000, 00\tfrac{1}{2}$	$P6/mmm$	$a, b, \tfrac{1}{2}c$
CUBIC $a=b=c$, $\alpha=\beta=\gamma=90°$, no extra conditions for the labelling of axes							
195	$P23$			$C\ xyz, yx\bar{z}$ $\bar{x}\bar{y}\bar{z}, \bar{y}\bar{x}z$	$000, \tfrac{1}{2}\tfrac{1}{2}\tfrac{1}{2}$	$Im\bar{3}m$	a, b, c
196	$F23$			$C\ xyz, yx\bar{z}$ $\bar{x}\bar{y}\bar{z}, \bar{y}\bar{x}z$	$000, \tfrac{1}{4}\tfrac{1}{4}\tfrac{1}{4}, \tfrac{1}{2}\tfrac{1}{2}\tfrac{1}{2}, \tfrac{3}{4}\tfrac{3}{4}\tfrac{3}{4}$	$Im\bar{3}m$	$\tfrac{1}{2}a, \tfrac{1}{2}b, \tfrac{1}{2}c$
197	$I23$			$C\ xyz, yx\bar{z}$ $\bar{x}\bar{y}\bar{z}, \bar{y}\bar{x}z$	000	$Im\bar{3}m$	a, b, c
198	$P2_13$			$C\ xyz, \tfrac{1}{4}-y\ \tfrac{1}{4}-x\ \tfrac{1}{4}-z$ $\bar{x}\bar{y}\bar{z}, \tfrac{3}{4}+y\ \tfrac{3}{4}+x\ \tfrac{3}{4}+z$	$000, \tfrac{1}{2}\tfrac{1}{2}\tfrac{1}{2}$	$Ia\bar{3}d$	a, b, c
199	$I2_13$			$C\ xyz, \tfrac{1}{4}-y\ \tfrac{1}{4}-x\ \tfrac{1}{4}-z$ $\bar{x}\bar{y}\bar{z}, \tfrac{3}{4}+y\ \tfrac{3}{4}+x\ \tfrac{3}{4}+z$	000	$Ia\bar{3}d$	a, b, c
200	$Pm\bar{3}$			$xyz, yx\bar{z}$	$000, \tfrac{1}{2}\tfrac{1}{2}\tfrac{1}{2}$	$Im\bar{3}m$	a, b, c
201	$Pn\bar{3}$	Origin at centre of symmetry		$xyz, \bar{y}\bar{x}\bar{z}$	$000, \tfrac{1}{2}\tfrac{1}{2}\tfrac{1}{2}$	$Im\bar{3}m$	a, b, c
202	$Fm\bar{3}$			$xyz, yx\bar{z}$	$000, \tfrac{1}{2}\tfrac{1}{2}\tfrac{1}{2}$	$Pm\bar{3}m$	$\tfrac{1}{2}a, \tfrac{1}{2}b, \tfrac{1}{2}c$
203	$Fd\bar{3}$	Origin at centre of symmetry		$xyz, \bar{y}\bar{x}\bar{z}$	$000, \tfrac{1}{2}\tfrac{1}{2}\tfrac{1}{2}$	$Pn\bar{3}m$	$\tfrac{1}{2}a, \tfrac{1}{2}b, \tfrac{1}{2}c$
204	$Im\bar{3}$			$xyz, yx\bar{z}$	000	$Im\bar{3}m$	a, b, c
205	$Pa\bar{3}$			xyz	$000, \tfrac{1}{2}\tfrac{1}{2}\tfrac{1}{2}$	$Ia\bar{3}$	a, b, c
206	$Ia\bar{3}$			$xyz, \tfrac{1}{4}-y\ \tfrac{1}{4}-x\ \tfrac{1}{4}-z$	000	$Ia\bar{3}d$	a, b, c
207	$P432$			$C\ xyz$ $\bar{x}\bar{y}\bar{z}$	$000, \tfrac{1}{2}\tfrac{1}{2}\tfrac{1}{2}$	$Im\bar{3}m$	a, b, c
208	$P4_232$			$C\ xyz$ $\bar{x}\bar{y}\bar{z}$	$000, \tfrac{1}{2}\tfrac{1}{2}\tfrac{1}{2}$	$Im\bar{3}m$	a, b, c
209	$F432$			$C\ xyz$ $\bar{x}\bar{y}\bar{z}$	$000, \tfrac{1}{2}\tfrac{1}{2}\tfrac{1}{2}$	$Pm\bar{3}m$	$\tfrac{1}{2}a, \tfrac{1}{2}b, \tfrac{1}{2}c$
210	$F4_132$			$C\ xyz$ $\tfrac{1}{4}-x\ \tfrac{1}{4}-y\ \tfrac{1}{4}-z$	$000, \tfrac{1}{2}\tfrac{1}{2}\tfrac{1}{2}$	$Pn\bar{3}m$	$\tfrac{1}{2}a, \tfrac{1}{2}b, \tfrac{1}{2}c$
211	$I432$			$C\ xyz$ $\bar{x}\bar{y}\bar{z}$	000	$Im\bar{3}m$	a, b, c
212	$P4_332$	Enantiomorph of $P4_132$					
213	$P4_132$			$E\ xyz$	$000, \tfrac{1}{2}\tfrac{1}{2}\tfrac{1}{2}$	$I4_132$	a, b, c
214	$I4_132$			$C\ xyz$ $\bar{x}\bar{y}\bar{z}$	000	$Ia\bar{3}d$	a, b, c
215	$P\bar{4}3m$			$A\ xyz$ $\bar{x}\bar{y}\bar{z}$	$000, \tfrac{1}{2}\tfrac{1}{2}\tfrac{1}{2}$	$Im\bar{3}m$	a, b, c
216	$F\bar{4}3m$			$A\ xyz$ $\bar{x}\bar{y}\bar{z}$	$000, \tfrac{1}{4}\tfrac{1}{4}\tfrac{1}{4}, \tfrac{1}{2}\tfrac{1}{2}\tfrac{1}{2}, \tfrac{3}{4}\tfrac{3}{4}\tfrac{3}{4}$	$Im\bar{3}m$	$\tfrac{1}{2}a, \tfrac{1}{2}b, \tfrac{1}{2}c$
217	$I\bar{4}3m$			$A\ xyz$ $\bar{x}\bar{y}\bar{z}$	000	$Im\bar{3}m$	a, b, c
218	$P\bar{4}3n$			$A\ xyz$ $\bar{x}\bar{y}\bar{z}$	$000, \tfrac{1}{2}\tfrac{1}{2}\tfrac{1}{2}$	$Im\bar{3}m$	a, b, c
219	$F\bar{4}3c$			$A\ xyz$ $\bar{x}\bar{y}\bar{z}$	$000, \tfrac{1}{4}\tfrac{1}{4}\tfrac{1}{4}, \tfrac{1}{2}\tfrac{1}{2}\tfrac{1}{2}, \tfrac{3}{4}\tfrac{3}{4}\tfrac{3}{4}$	$Im\bar{3}m$	$\tfrac{1}{2}a, \tfrac{1}{2}b, \tfrac{1}{2}c$

Table 6 (*cont.*)

A No.	*B* Standard space-group symbol	*C* Extra condition for choice of unit cell	*D* Labels of axes	*E* Non-redundant *xyz* triplets	*F* Permitted origins	*G* Cheshire group	*H* Basis vectors of Cheshire group
220	$I\bar{4}3d$			*A* xyz $\bar{x}\bar{y}\bar{z}$	000	$Ia\bar{3}d$	a, b, c
221	$Pm\bar{3}m$			xyz	000, $\frac{1}{2}\frac{1}{2}\frac{1}{2}$	$Im\bar{3}m$	a, b, c
222	$Pn\bar{3}n$	Origin at centre of symmetry		xyz	000, $\frac{1}{2}\frac{1}{2}\frac{1}{2}$	$Im\bar{3}m$	a, b, c
223	$Pm\bar{3}n$			xyz	000, $\frac{1}{2}\frac{1}{2}\frac{1}{2}$	$Im\bar{3}m$	a, b, c
224	$Pn\bar{3}m$	Origin at centre of symmetry		xyz	000, $\frac{1}{2}\frac{1}{2}\frac{1}{2}$	$Im\bar{3}m$	a, b, c
225	$Fm\bar{3}m$			xyz	000, $\frac{1}{2}\frac{1}{2}\frac{1}{2}$	$Pm\bar{3}m$	$\frac{1}{2}a, \frac{1}{2}b, \frac{1}{2}c$
226	$Fm\bar{3}c$			xyz	000, $\frac{1}{2}\frac{1}{2}\frac{1}{2}$	$Pm\bar{3}m$	$\frac{1}{2}a, \frac{1}{2}b, \frac{1}{2}c$
227	$Fd\bar{3}m$	Origin at centre of symmetry		xyz	000, $\frac{1}{2}\frac{1}{2}\frac{1}{2}$	$Pn\bar{3}m$	$\frac{1}{2}a, \frac{1}{2}b, \frac{1}{2}c$
228	$Fd\bar{3}c$	Origin at centre of symmetry		xyz	000, $\frac{1}{2}\frac{1}{2}\frac{1}{2}$	$Pn\bar{3}m$	$\frac{1}{2}a, \frac{1}{2}b, \frac{1}{2}c$
229	$Im\bar{3}m$			xyz	000	$Im\bar{3}m$	a, b, c
230	$Ia\bar{3}d$			xyz	000	$Ia\bar{3}d$	a, b, c

* To change $\mathbf{c} \rightarrow \mathbf{c}' = (\mathbf{a}+\mathbf{c})$ it is necessary to shift the origin by $0\frac{1}{4}0$.
† To change $\mathbf{c} \rightarrow \mathbf{c}' = (\mathbf{a}+\mathbf{c})$ it is necessary to shift the origin by $\frac{1}{4}\frac{3}{4}0$.
‡ The *a* and *b* axes may be interchanged if the origin is shifted by $00\frac{1}{4}$; the atomic coordinates then change from xyz to $y\,x\,\frac{1}{4}-z$.
§ A cyclic permutation of the axes is possible. For the permutations $ba\bar{c}$, $a\bar{c}b$ and $\bar{c}ba$, an origin shift of $\frac{1}{4}\frac{1}{4}\frac{1}{4}$ is necessary. The atomic coordinates then change from xyz to $y-\frac{1}{4}\,x-\frac{1}{4}\,\frac{1}{4}-z$, $x-\frac{1}{4}\,\frac{1}{4}-z\,y-\frac{1}{4}$ and $\frac{1}{4}-z\,y-\frac{1}{4}\,x-\frac{1}{4}$, respectively.
¶ The *a* and *b* axes may be interchanged if the origin is shifted by $\frac{1}{4}\frac{1}{4}\frac{1}{4}$; the atomic coordinates then change from xyz to $y-\frac{1}{4}\,x-\frac{1}{4}\,\frac{1}{4}-z$.
** Only cyclic permutations of the axes are possible. If $a<b<c$ cannot be obtained, then $a<b$ is taken.
†† The *a* and *b* axes may be interchanged if the origin is shifted by $\frac{1}{4}\frac{1}{4}0$. The atomic coordinates then change from xyz to $y-\frac{1}{4}\,x-\frac{1}{4}\,\bar{z}$.
‡‡ Cyclic permutations of the axes are possible. For the permutations $ba\bar{c}$, $a\bar{c}b$ and $\bar{c}ba$ origin shifts of $\frac{1}{4}\frac{1}{4}0$, $\frac{1}{4}0\frac{1}{4}$ and $0\frac{1}{4}\frac{1}{4}$, respectively, are necessary. The atomic coordinates then change from xyz to $y-\frac{1}{4}\,x-\frac{1}{4}\,\bar{z}$, $x-\frac{1}{4}\,\bar{z}\,y-\frac{1}{4}$ and $\bar{z}\,y-\frac{1}{4}\,x-\frac{1}{4}$, respectively.

Table 7. *Published and standardized structure data of* Pu_3Co *and* Zr_3Co

Pu_3Co [*SR* (1963) **28**, 17]

Cmcm, $a=3\cdot475$, $b=10\cdot976$, $c=9\cdot220$ Å

	x	*y*	*z*
4Pu(1) in 4(*c*)	0	0·0778	$\frac{1}{4}$
8Pu(2) in 8(*f*)	0	0·3678	0·0553
4Co in 4(*c*)	0	0·778	$\frac{1}{4}$

Standardized data
$\Gamma = 1\cdot398$

Cmcm, same unit cell

	x	*y*	*z*
Pu(1) in 8(*f*)	0	0·1322	0·0553
Pu(2) in 4(*c*)	0	0·4222	$\frac{1}{4}$
Co in 4(*c*)	0	0·722	$\frac{1}{4}$

Shift of origin of $0\frac{1}{2}\frac{1}{2}$ from published data

Zr_3Co [*SR* (1970) **35A**, 53]

Cmcm, $a=3\cdot27$, $b=10\cdot84$, $c=8\cdot95$ Å

	x	*y*	*z*
4Co in 4(*c*)	0	0·74	$\frac{1}{4}$
4Zr(1) in 4(*c*)	0	0·424	$\frac{1}{4}$
8Zr(2) in 8(*f*)	0	0·135	0·057

Standardized data
$\Gamma = 1\cdot4198$

Cmcm, same unit cell

	x	*y*	*z*
Zr(1) in 8(*f*)	0	0·135	0·057
Zr(2) in 4(*c*)	0	0·424	$\frac{1}{4}$
Co in 4(*c*)	0	0·74	$\frac{1}{4}$

No change of origin

Table 8. *Published, standardized and shifted structure data for* $PuBr_3$ *and* $TbCl_3$

$PuBr_3$ [*SR* (1948) **11**, 282]

Cmcm, $a=12\cdot65$, $b=4\cdot10$, $c=9\cdot15$ Å

	x	*y*	*z*
4Pu in 4(*c*)	0·25	0	$\frac{1}{4}$
4Br(1) in 4(*c*)	−0·07	0	$\frac{1}{4}$
8Br(2) in 8(*f*)	0·36	0	−0·05

Standardized data
$\Gamma = 1\cdot4136$

Ccmm, $a=4\cdot10$, $b=12\cdot65$, $c=9\cdot15$ Å

	x	*y*	*z*
Br(1) in 8(*f*)	0	0·36	0·05
Br(2) in 4(*c*)	0	0·07	$\frac{1}{4}$
Pu in 4(*c*)	0	0·75	$\frac{1}{4}$

Interchange of *a* and *b* axes to obtain standard space group setting

Shift of $0\frac{1}{2}\frac{1}{2}$ from standard
$\Gamma = 1\cdot4366$

	x	*y*	*z*
Br(1) in 8(*f*)	0	0·14	0·05
Br(2) in 4(*c*)	0	0·43	$\frac{1}{4}$
Pu in 4(*c*)	0	0·75	$\frac{1}{4}$

$TbCl_3$ [*SR* (1964) **29**, 274]

Cmcm, $a=3\cdot86$, $b=11\cdot71$, $c=8\cdot48$ Å

	x	*y*	*z*
4Tb in 4(*c*)	0	0·244	$\frac{1}{4}$
4Cl(1) in 4(*c*)	0	0·583	$\frac{1}{4}$
8Cl(2) in 8(*f*)	0	0·145	0·569

Standardized data
$\Gamma = 1\cdot4099$

Cmcm, same unit cell

	x	*y*	*z*
Cl(1) in 8(*f*)	0	0·355	0·069
Cl(2) in 4(*c*)	0	0·083	$\frac{1}{4}$
Tb in 4(*c*)	0	0·744	$\frac{1}{4}$

Shift of origin by $0\frac{1}{2}0$ from published data

Shift of $0\frac{1}{2}\frac{1}{2}$ from standard
$\Gamma = 1\cdot443$

	x	*y*	*z*
Cl(1) in 8(*f*)	0	0·145	0·069
Cl(2) in 4(*c*)	0	0·417	$\frac{1}{4}$
Tb in 4(*c*)	0	0·756	$\frac{1}{4}$

descriptions, given in the middle part of Table 8, which differ from those given in Table 7.*

However, a shift of $0\frac{1}{2}\frac{1}{2}$ from the standard (lower part of Table 8) allows the isotypy of all four compounds to be recognized. In this case the descriptions of structures in Table 8 have slightly higher standardization parameters. The two halogenides certainly have a different bonding type from the two alloy structures and probably form a different structure-type branch; however, a discussion of structure-type branches is not the object of this paper. As a general procedure for a comparison of different related structures consideration is recommended not only for the description with the lowest standardization parameter but also for those with higher values.

* In these particular structures a small variation of the *y* parameter of the last atom in the standardized data list can lead to a jump to another permitted origin ($y<0\cdot75$ or $y\geq 0\cdot75$).

Practical considerations

In view of the many possibilities of describing a crystal structure the normalization of crystal-structure data is not a simple procedure. For this reason a computer program *STRUCTURE TIDY* (Gelato &

Parthé, 1984) has been written which will standardize data.

Benefits and disadvantages

The proposed standardization allows each structure to be described in a unique way. Thus the structure data of the same structure determined in different laboratories will be strictly comparable. In the case of nearly isotypic structures the standardized data allow the isotypy to be recognized by simple inspection of the lists of atom coordinates provided that the numerical values of atomic coordinates of corresponding atoms are close.* The variations in atomic coordinates which still permit isotypy to be recognized depend on the structure in question.

There may be crystal chemical reasons which suggest that a non-standardized structure description is more appropriate. For example, in the case of low-symmetry deformation variants of basis structures with higher symmetry the standardized description may mask the structural relationship between these structures (for example rhombohedral variants of cubic structures which have to be described in the standardized way with a triple hexagonal cell). The crystallographer prefers here a description with unit-cell dimensions and atom coordinates which relate directly to the basis type. It is our belief that the standardized description should never replace any other description chosen to demonstrate a particular relationship to other structures, but should be given as an additional description. This presents a disadvantage as both descriptions would have to be printed. However, the benefits of a standardized structure description are sufficiently great that its publication should always be included. Last but not least, many inorganic structures are presented without any direct relationship to other known structures and the standard description thus provides an unequivocal way of describing the structure.

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* Four recent examples which were found by us using standardized descriptions: $U_3Fe_2Si_7$ (Akselrud, Yarmolyuk, Rozhdestvenskaya & Gladyshevskii, 1981) is isotypic with $La_3Co_2Sn_7$ (Dörrscheidt & Schäfer, 1980); $BaCuSn_2$ (May & Schäfer, 1974) is isotypic with $CeNiSi_2$ (Bodak & Gladyshevskii, 1970); $Gd_3Cu_4Ge_4$ (Rieger, 1970) is isotypic with $Li_4Sr_3Sb_4$ (Liebrich, Schäfer & Weiss, 1970); Y_3NiSi_3 (Klepp & Parthé, 1982) has the same atom sites with similar coordinates to $Ba_3Al_2Ge_2$ (Widera, Eisenmann, Schäfer & Turban, 1976).

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