Standardization of crystal structure data as an aid to the classification of crystal structure types

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Abstract

Owing to the different ways in which crystal structures may be described, isotypic compounds are often not identified as such. To remedy this situation, crystal structure data can be standardized by means of the STRUCTURE TIDY program. In the standardized data of isotypic structures, occupied sites have the same Wyckoff representation. This makes it possible to use the Wyckoff sequence (the letters of occupied Wyckoff sites) to classify crystal structure types. This classification is much finer than the previously used classification based on the Pearson code and is of great help if one wants to know whether a particular atom arrangement is already known. The standardization has enabled us not only to demonstrate new cases of isotypism, but also to discover structural relationships between different structure types with the same space group, for example substitution, vacancy or filled-in variants.

1. Introduction

As a base for crystal chemical studies one requires compilations of structure type data as well as lists of isotypic compounds. The recognition of isotypic compounds is not always simple because there are so many different ways of describing crystal structures, and as a consequence many isotypic compounds have not been identified as such but have been considered as crystallizing in different structure types. Conversely, some different structures with the same space group and Pearson classification code were erroneously considered as being isotypic because their reported unit cell parameters are similar. This complicated the work of crystal chemists who, using lists of isotypic compounds, were trying to explain the reasons for the formation of particular atom arrangements. We shall discuss here some of the problems which make it difficult to recognize isotypism, the application of a standardization procedure, designed to remedy this undesirable situation, and a new classification system of structure types, based on standardized data, which allows the recognition of certain structural relationships.

2. Definition of isotypism and problems with its recognition

Two structures are called (configurationally) isotypic if they have the same stoichiometry (for fully ordered structures), the same space group, the same Wyckoff sites (fully or partially occupied at random) with the same or similar positional coordinates (x, y, z) and the same or similar values of the unit cell axial ratios $(c/a, a/b, b/c)$ and cell angles (α, β, γ) [1]. Isotypism is found particularly with inorganic compounds. To explain why two compounds adopt the same atom arrangement is not always simple. For some structure types we believe we understand the reasons for isotypism, but there are also structure types (mostly simple) where many different unrelated effects, not all understood as yet, may lead to the formation of the same atom arrangement.

Let us consider a few examples of isotypism and some of the crystal chemical interpretations.

The isotypism of $Gd_4Ni_6Al_{23}$ with $Y_4Ni_6Al_{23}$ is not surprising because Gd and Y are from the same group of the periodic table, have comparable electron configurations and nearly the same size.

Li_2SiO_3 and $LiSi_2N_3$ both adopt the same structure type, a normal adamantane structure type. The corresponding elements here are not all from the same groups in the periodic table. However, the observed isotypism* seems plausible because the particular structural features of adamantane structures can be related

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*A detailed study of these two structures shows that the tetrahedra are deformed, but in Li_2SiO_3 and $LiSi_2N_3$ in a different way (*e.g.*, three short and one long Li–O, but one short and three long Si–N distances). These differences in the distances within a given tetrahedron are to be expected according to the bond valence concept. The two structures are thus not isotypic in a rigorous sense, but constitute two branches of a common hypothetical structure type with undeformed tetrahedra.

TABLE 1. The four equivalent descriptions of the diamond type which differ owing to a different choice of origin

1	(227) $Fd\bar{3}m$,	origin choice 1	C 8(a) (0 0 0, 3/4 1/4 3/4)+[F][a]
2	(227) $Fd\bar{3}m$,	origin choice 1	C 8(b) (1/2 1/2 1/2, 1/4 3/4 1/4)+[F]
3	(227) $Fd\bar{3}m$,	origin choice 2	C 8(a) (1/8 1/8 1/8, 7/8 3/8 3/8)+[F]
4	(227) $Fd\bar{3}m$,	origin choice 2	C 8(b) (3/8 3/8 3/8, 1/8 5/8 1/8)+[F]

[a][F]=0 0 0, 0 1/2 1/2, 1/2 0 1/2, 1/2 1/2 0.

to particular values of the total and partial valence electron concentration and for the two compounds under consideration one obtains the same values (VEC=4, VEC_A=8) (for more details see ref. 2).

GdNi and NiB both crystallize with the CrB type structure, characterized by trigonal prisms formed by the elements given in the first position of the chemical formula and centred by the element in the second position. Thus in the first compound the Ni atoms centre the trigonal prisms, whereas in the second they form the prisms. One can conclude that, besides other reasons, the size difference of the elements is of importance for the existence of this structure type.

$Pu_{31}Rh_{20}$ is isotypic with $Ca_{31}Sn_{20}$. The isotypism of these two compounds of unusual stoichiometry was not expected and we do not understand the reasons for it. This should be a topic for further study.

It is evident that as a base for crystal chemical studies one needs lists of all structure types as well as lists of the isotypic compounds. Unfortunately, such lists are not as simple to establish as one might think because there are so many different ways of describing crystal structures. This led to the regrettable fact that many isotypic compounds were not recognized as such. Such oversight occurred even in the very first published structure type compilation, the *Strukturberichte* [3] (henceforth abbreviated SB) where, for example, the B16 (GeS) type and the B29 (SnS) type structures actually refer to the same atom arrangement and where the correspondence between the DO_{11} (Fe_3C) and DO_{20} ($NiAl_3$) types is not mentioned.

Let us investigate more closely the different possibilities of describing a crystal structure. We assume beforehand that all structure descriptions are based on the symmetry equivalent *xyz* triplets listed in the *International Tables for Crystallography* [4]*. Even then there may be, depending on the space group, ambiguities with reference to the following five points: the space group setting, the coordinate system basis vectors, the

*There are even some very recent publications where the conventions of the *International Tables* are not taken into consideration. Historical reasons are often quoted, as for example in a 1992 paper on the structure determination of the quartz-type phases of SiO_2 and GeO_2 [5]. However, since not everyone feels bound by historical reasons, there are in effect now different descriptions of the same structure in the literature.

TABLE 2. Original structure data of $CeCu_2$ (SR 26, 107) and KHg_2 (SR 19, 231) and the standardized data of KHg_2 [6] which demonstrate the isotypism

$CeCu_2$ (74) *Imma*				KHg_2 (74) *Imma*		
a=4.43, b=7.05, c=7.45 Å				a=8.10, b=5.16, c=8.77 Å		
	x	y	z		x	y	z
Cu 8(h)	0	0.0510	0.1648	Hg 8(i)	0.190	1/4	0.087
Ce 4(e)	0	1/4	0.5377	K 4(e)	0	1/4	0.703
				a=5.16, b=8.10, c=8.77 Å		
					x	y	z
				Hg 8(h)	0	0.060	0.163
				K 4(e)	0	1/4	0.547

origin of the coordinate system, the representative atom coordinates, and the order and numbering of the atom sites.

A few simple demonstrations will be useful.

As examples of different descriptions due to a different choice of origin, we give in Table 1 four equivalent descriptions of the diamond structure type, all in agreement with the *International Tables for Crystallography* [4].

For many years no one realized that $CeCu_2$ and KHg_2 are isotypic. This was because in the original publications the a and b axes were chosen differently (Table 2).

The number of possible descriptions due to a different permitted choice of origin, rotation of the coordinate system and/or inversion of the coordinate triplet depends on the space group (see complete list in Table 6 in ref. 6). For example, for the structure of $Zr_2Fe_{12}P_7$ (SR 33A, 103**) with space group (174) $P\bar{6}$, without polar axes, there are 24 possible, different but equivalent, descriptions. In fact there are only two space groups where only one description is possible: (229) $Im\bar{3}m$ and (230) $Ia\bar{3}d$.

In the case of monoclinic structures the number of cases where isotypism has been missed is particularly

**SR stands for *Structure Reports* [7]. The references given here generally refer to the most recent refinement reported in the SR. For compounds defining structure types the data are taken directly from the original publication, whereas for isotypic compounds they are quoted from SB or SR.

high. This is due to different space group settings which lead to different unit cells and consequently to positional atom coordinates which show no correspondence whatsoever.

3. Standardization of crystal structure data

To avoid all these pitfalls in the description of structure types and the identification of isotypic structures, a standardization procedure was developed by Parthé and Gelato [6, 8], where the five above-mentioned points, which may give rise to ambiguity in the structure description, are regulated.

The criteria for space group setting and unit cell parameters used in the standardization process are as follows:

(1) right-handed coordinate system;

(2) standard space group setting as given in the *International Tables for Crystallography* [4] with the following restrictions: (a) monoclinic space groups, b-axis unique and cell choice 1 where applicable; (b) trigonal space groups with R-type Bravais lattice, obverse triple hexagonal unit cell; (c) centrosymmetric structures, symmetry centre at the origin, *i.e.* origin choice 2 when two origin choices are proposed in ref. 4; (d) enantiomorphic space groups, space group with the smallest index for the relevant screw axis;

(3) (a) triclinic structures, Niggli reduced cell; (b) monoclinic structures, "best cell" with $\beta \geqslant 90°$ [8];

(4) orthorhombic structures, $a \leqslant b$ or $a \leqslant b \leqslant c$.

These conditions are applied in an eliminative way, *i.e.* if condition (2) is not sufficient to define the cell parameters, conditions (3) or (4) are applied.

Also, the following criteria for the representative atom coordinates of each site are applied in an eliminative way:

(1) $0 \leqslant x, y, z < 1$;

(2) coordinates for atoms at special positions should correspond to the first xyz triplet of its Wyckoff site given in ref. 4;

(3) special rules for the origin choice in polar groups;

(4) minimum value of $(x^2 + y^2 + z^2)$;

(5) minimum value of x-coordinate;

(6) minimum value of y-coordinate.

Once a structure has been described according to these criteria, the problem is generally not yet solved. One has now to compare the different descriptions due to a possible shift of origin and/or to a rotation and/ or to an inversion of the coordinate system. In order to be able to compare all equivalent data sets the standardization parameter Γ was introduced:

$$\Gamma = \sum_{i=1}^{N} (x_i^2 + y_i^2 + z_i^2)^{1/2} \tag{1}$$

where N is the number of atom sites. This parameter is calculated for each data set and, as a first condition, the set(s) with the lowest value of Γ will be selected for the standardized description. The complete list of eliminative conditions applied to the data sets is given below:

(1) minimum value of Γ;

(2) minimum value of Σx;

(3) minimum value of Σy;

(4) minimum value of Σz;

(5) minimum value $(x + y + z)$.

With the help of the STRUCTURE TIDY computer program, written by Gelato and Parthé [9], the standardization procedure can now be performed in practice. The output consists of the standardized unit cell parameters, a list of the standardized atom coordinates together with the Wyckoff sites, and the value of the standardization parameter Γ.

The program also calculates a second parameter called CG (centre of gravity) [9]. In distinction to the standardization parameter Γ, which is determined exclusively from the fractional coordinates, in the calculation of CG the differences in the shape of the unit cell (one-dimensional contractions, variations in angles, etc.) are accounted for. The expression for CG is similar to that of the parameter Γ, but is calculated in direct space. To avoid the influence of the size of the atoms, it is further divided by the cube root of the cell volume:

$$\begin{aligned} CG = \Bigg[& a^2 \left(\sum_{i=1}^{N} x_i \right)^2 + b^2 \left(\sum_{i=1}^{N} y_i \right)^2 \\ & + c^2 \left(\sum_{i=1}^{N} z_i \right)^2 + 2ab(\cos \gamma) \left(\sum_{i=1}^{N} x_i y_i \right)^2 \\ & + 2ac(\cos \beta) \left(\sum_{i=1}^{N} x_i z_i \right)^2 \\ & + 2bc(\cos \alpha) \left(\sum_{i=1}^{N} y_i z_i \right)^2 \Bigg]^{1/2} \Bigg/ NV^{1/3} \end{aligned} \tag{2}$$

where N is the number of atom sites. As will be shown below the CG value can be used as an additional parameter for a first rough differentiation of structures with the same space group and the same Wyckoff sequence.

The usefulness of the standardization procedure for the recognition of isotypic crystal structures of course depends on the starting data. There can be found in the literature a number of cases where even the space group chosen by the authors is incorrect, in so far as it does not consider all symmetry elements contained in the structure (for more details see ref. 10). To be able to identify isotypic structures, it is necessary that

the structures to be standardized be described in the correct space groups.

4. Examples of standardized structure data

As a simple example where the standardization procedure can be followed easily, we shall derive the standardized description of the diamond type. In the case of space group (227) $Fd\bar{3}m$, as well as in 23 other centrosymmetric space groups, two settings are proposed in the *International Tables for Crystallography* [4] which correspond to two different origin choices. The standardization program selects, as stated above, the setting with the symmetry centre at the origin (origin choice 2), which for diamond eliminates description variants 1 and 2 of Table 1. A further selection between variants 3 and 4 is based on the criterion of minimum value of the standardization parameter Γ:

for variant 3 $\Gamma = [(1/8)^2 + (1/8)^2 + (1/8)^2]^{1/2}$

$= 3^{1/2} \times 1/8 = 0.22$

for variant 4 $\Gamma = [(3/8)^2 + (3/8)^2 + (3/8)^2]^{1/2}$

$= 3^{1/2} \times 3/8 = 0.65$

The standardized description of the diamond structure type thus corresponds to variant 3.

An application of the standardization procedure to the data of $CeCu_2$ and KHg_2, listed in Table 2, shows that the original data of $CeCu_2$ with $a < b$ already fulfil all conditions for standardized data and will thus not be changed by the STRUCTURE TIDY program. In the case of KHg_2 the standardization leads to an interchange of the a and b axes, which for space group (74) *Imma* requires, however, an origin shift of 1/4 1/4 1/4. Figure 1 shows the structure of KHg_2 with two unit cells, one corresponding to the original and the other to the standardized description. The final standardized data, given in the lower right part of Table 2, demonstrate isotypism with $CeCu_2$.

As a third example we want to discuss the simple structures (only four atoms in the unit cell) of $TaTl_{0.33}Se_2$, $TaIn_{0.67}S_2$ and $NbInS_2$ which are considered in the data compilation by Villars and Calvert [11] as crystallizing with three different structure types. The upper right corner of Table 3 shows the data as found in the literature for $TaTl_{0.33}Se_2$ (except for a rounded-off z parameter for the Se atoms). If we consider the six possible origin shifts and in addition a possible inversion of the coordinate system we obtain the 12 possible structure descriptions, listed in Table 3, where the letters of the occupied Wyckoff sites vary greatly from one description to another. The 12 different settings

KHg_2, $oI12$, *Imma - he*
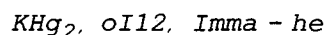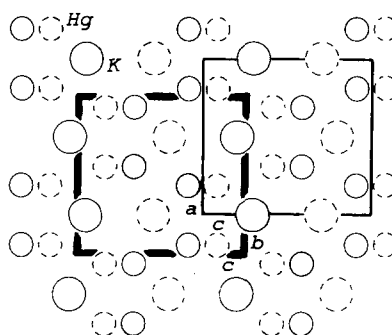
$a = 5.16$, $b = 8.10$, $c = 8.77\,\text{Å}$

Fig. 1. The structure of KHg_2 with two unit cells, the cell indicated with thin lines corresponding to the original description, and the cell drawn with heavy lines corresponding to the standardized description. Fully drawn and dashed circles distinguish atoms which differ by 1/2 in height; in the original description they are at 1/4 and 3/4, but in the standardized description at 0 and 1/2.

of the $TaTl_{0.33}Se_2$ structure are presented in Fig. 2, where the atom arrangement in the (11$\bar{2}$0) plane of the hexagonal cell is shown. The two descriptions of $TaTl_{0.33}Se_2$ in the second row of Table 3 with an origin shift of 0 0 1/2 correspond to the published data of $NbInS_2$ and $TaIn_{0.67}S_2$ respectively. All three structures are thus isotypic, and after using the STRUCTURE TIDY program one obtains for all three compounds equivalent standardized descriptions, which correspond to that shown in italic.

5. The Wyckoff sequence, the Γ and CG values and their use for the classification of structure types

Since in the standardized structure data the Wyckoff sites are uniquely determined, we can formulate for each structure type the so-called Wyckoff sequence [9] and use it for classification purposes. The Wyckoff sequence is the sequence of the letters of all, fully or partially occupied, Wyckoff sites in the standardized structure description. The Wyckoff letters are ordered as in the *International Tables for Crystallography* [4]*, i.e. in reverse alphabetical order. The number of times that a particular Wyckoff site appears in the list of atom coordinates is indicated as a superscript (if greater than one) after the corresponding Wyckoff letter. The Wyckoff sequence is written after the standard space group symbol.

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*The unintentional differences in the Wyckoff letters assigned to particular sites between the 1983 edition and the 1952 edition have no influence on the Wyckoff sequence of the standardized data, since they occur only in monoclinic space groups with unique c-axis (see ref. 13).

TABLE 3. The 12 different possible descriptions of TaTl$_{0.33}$Se$_2$ (SR 40A, 94), NbInS$_2$ [12] and TaIn$_{0.67}$S$_2$ (SR 55A, 52), all crystallizing with the same space group (187) $P\bar{6}m2$ and similar unit cells; a compound formula is written above a structure description when it corresponds to the way the structure of the compound is described in the literature; all compounds are isotypic, the standardized description of the structure type is shown in italics

		Setting							Origin shift		
		x	y	z		$-x$	$-y$	$-z$			
					$TaTl_{0.33}Se_2$						
Ta	1(a)	0	0	0	1(a)	0	0	0	0	0	0
Tl	1(b)	0	0	1/2	1(b)	0	0	1/2			
Se	2(h)	1/3	2/3	0.20	2(i)	2/3	1/3	0.20			
		$NbInS_2$				$TaIn_{0.67}S_2$					
Ta	1(b)	0	0	1/2	1(b)	0	0	1/2	0	0	1/2
Tl	1(a)	0	0	0	1(a)	0	0	0			
Se	2(h)	1/3	2/3	0.30	2(i)	2/3	1/3	0.30			
Ta	1(e)	2/3	1/3	0	1(e)	2/3	1/3	0	1/3	2/3	0
Tl	1(f)	2/3	1/3	1/2	1(f)	2/3	1/3	1/2			
Se	2(g)	0	0	0.20	2(h)	1/3	2/3	0.20			
Ta	1(f)	2/3	1/3	1/2	1(f)	2/3	1/3	1/2	1/3	2/3	1/2
Tl	1(e)	2/3	1/3	0	1(e)	2/3	1/3	0			
Se	2(g)	0	0	0.30	2(h)	1/3	2/3	0.30			
Ta	1(c)	1/3	2/3	0	1(c)	1/3	2/3	0	2/3	1/3	0
Tl	1(d)	1/3	2/3	1/2	1(d)	1/3	2/3	1/2			
Se	2(i)	2/3	1/3	0.20	2(g)	0	0	0.20			
Ta	1(d)	1/3	2/3	1/2	1(d)	1/3	2/3	1/2	2/3	1/3	1/2
Tl	1(c)	1/3	2/3	0	1(c)	1/3	2/3	0			
Se	2(i)	2/3	1/3	0.30	2(g)	0	0	0.30			

$TaTl_{0.33}Se_2$, hP4-0.67, $P\bar{6}m2$ - hba
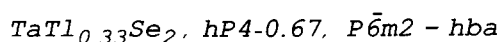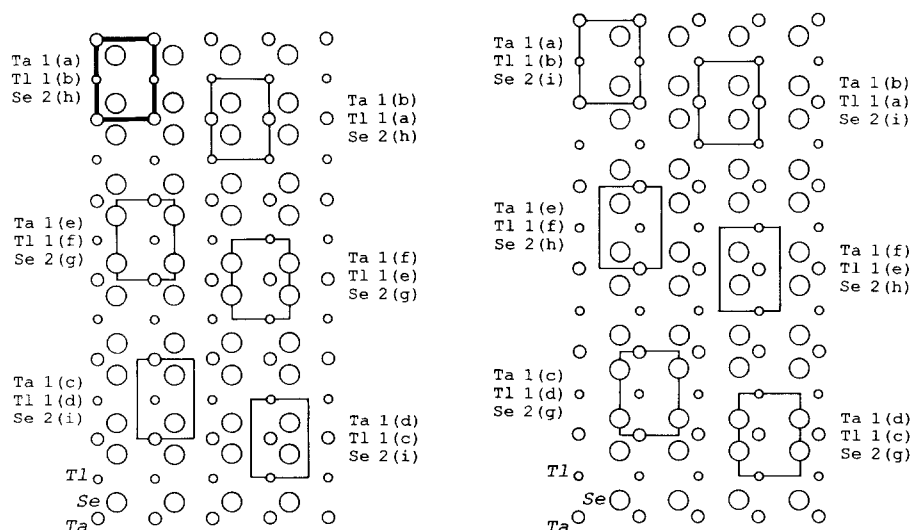
$a = 3.473$, $c = 8.393$ Å

Fig. 2. Atom arrangement in the (11$\bar{2}$0) plane of the hexagonal cell of TaTl$_{0.33}$Se$_2$, described in 12 different ways. The Wyckoff letters added to each cell projection simplify the search for the corresponding data in Table 3. The standardized structure description is indicated with heavy lines.

As examples, for the diamond structure, the KHg_2 (or $CeCu_2$) structure and the $TaTl_{0.33}Se_2$ (or $NbInS_2$ or $TaIn_{0.67}S_2$) structure, the Wyckoff sequences preceded by the space group symbols are denoted as

C (diamond)   (227) $Fd\bar{3}m$-a

KHg_2 ($CeCu_2$)   (74) $Imma$-he

$TaTl_{0.33}Se_2$($NbInS_2$, $TaIn_{0.67}S_2$)   (187) $P\bar{6}m2$-hba

During the standardization it may happen that the Wyckoff letters change, as for example with KHg_2, $NbInS_2$ and $TaIn_{0.67}S_2$. The result is that in the standardized description all isotypic structures have the same Wyckoff sequence.

A large research program has been under way in Geneva for 8 years to prepare a reference book on standardized data and crystal chemical characterization of inorganic structure types (oxides and halides only exceptionally included) [14] where the structure types are ordered within each space group according to their Wyckoff sequence. In earlier structure data compilations the structures were ordered by means of the Pearson code [15], which consists of a small letter characterizing the crystal system (*a*northic, *m*onoclinic, *o*rthorhombic, *t*etrahedral, *h*exagonal or trigonal, *c*ubic), a capital letter which stands for the Bravais lattice type (*P*, *S*, *I*, *R* or *F*) followed by the number of atoms in the unit cell.*

We found that the Wyckoff sequence is a very convenient parameter for the classification of structure types since the use of the space group and the Wyckoff sequence permits a much finer subdivision of structure types than the classification based on the simpler Pearson code. This is particularly true for space groups which have many different Wyckoff sites. There are 10 space groups with only one Wyckoff letter, whereas space group *Pmmm* has 27 different Wyckoff letters. In the triclinic space group *P*1 the superscript in the Wyckoff sequence simply corresponds to the number of atoms in the unit cell, however, most of the higher symmetry space groups have a sufficient number of Wyckoff letters to make these useful for classification purposes.

As an example we shall consider different orthorhombic structures with Pearson code *oP*20, which can be subdivided into 13 sections with different classification codes, as shown in Table 4. It is evident that the much finer graduation simplifies the identification of isotypic crystal structures, the search now being limited to structure types with same space group and Wyckoff sequence.

If the similarity between crystal structures is restricted only to the same space group and the same Wyckoff sequence the structures are called isopointal [1]. Isotypic structures are obviously always isopointal, the reciprocity, however, is not true. As seen in Table 4, there are 13 different isopointal structure types all with classification code (62) $Pnma$-c^5.

A further subdivision of a set of isopointal structures into individual structure types requires a detailed study of the unit cells and the atom coordinations, but can be very roughly approximated by an analysis of the Γ and CG values, calculated by the STRUCTURE TIDY program. Table 5 shows the further subdivision of the structures with Pearson code *oP*20 into 32 different structure types. In the case of the structures with classification code (62) $Pnma$-c^5, the CG values vary from 0.585 to 0.880, but it is possible to distinguish different sub-sets with similar values. A closer analysis of the real structures shows that these compounds crystallize in 13 different structure types and that isotypic compounds follow each other in the list. The subdivision into structure types, however, may be made differently depending on whether or not one considers certain end members of structure type branches as separate structure types.

An independent test of the usefulness of the standardization process is offered by a comparison of our lists of structure types, based on standardized structure data, with the lists of structure types given in the comprehensive handbook by Villars and Calvert [11]. There the structures were transformed to standard space group settings and origin choice 1 was adopted for centrosymmetric structures (where applicable), but

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*Following the recommendations of an IUCr commission [16], the side-face centred Bravais lattices should now be denoted by *S* instead of *C* (or *A* or *B*). In the case of structures with partially occupied sites a slightly modified code is used here where the number of atoms is expressed by two numbers, separated by a minus sign: (the sum of the multiplicities of all, fully and partially, occupied sites) minus (the difference between this number and the actual number of atoms in the unit cell). For trigonal space groups based on an *R* Bravais lattice the number in the Pearson code corresponds in our data compilation [14] (and also here) to the number of atoms in the triple-hexagonal cell, but in some others (see for example ref. 11) it corresponds to the number of atoms in the rhombohedral unit cell which is one third as large in volume.

TABLE 4. The 32 structure types with Pearson code *oP*20, classified according to space group and Wyckoff sequence which gives 13 sections; the number of different (isopointal) structure types with a given space group and Wyckoff sequence, is indicated within curly brackets

(31) $Pmn2_1$-a^{10}	{1}	(59) $Pmmn$-$e^3b^2a^2$	{1}
(33) $Pna2_1$-a^5	{1}	(59) $Pmmn$-fe^3ba	{1}
(53) $Pmna$-$ihge$	{1}	(60) $Pbcn$-d^2c	{1}
(55) $Pbam$-hg^4	{1}	(62) $Pnma$-c^5	{13}
(57) $Pbcm$-d^3c^2	{1}	(62) $Pnma$-dc^3	{4}
(57) $Pbcm$-ed^2c	{1}	(62) $Pnma$-dc^2a	{3}
(58) $Pnnm$-g^5	{3}		

TABLE 5. Classification of structures with Pearson code $oP20$, based on their space group, Wyckoff sequence and value of the CG parameter (centre of gravity)

Space group and Wyckoff sequence	Compound	Reference	Γ	CG	Structure type
(31) $Pmn2_1$-a^{10}	$Cd_2Sb_6S_{11}{}^a$	SR 48A,10	6.62	0.841	$Cd_2Sb_6S_{11}$
(33) $Pna2_1$-a^5	$ScYS_3{}^b$	SR 35A,101	2.21	0.428	$ScYS_3$
(53) $Pmna$-$ihge$	$CuSe_3Br$	SR 45A,206	1.77	0.369	$CuSe_3Br$
(55) $Pbam$-hg^4	ScB_2C_2	SR 30A,28	1.80	0.447	ScB_2C_2
(57) $Pbcm$-d^3c^2	$ScFe_2Si_2$	SR 45A,87	2.78	0.549	$HfFe_2Si_2$
	$HfFe_2Si_2$	SR 42A,95	2.78	0.553	$HfFe_2Si_2$
(57) $Pbcm$-ed^2c	$LaCu_{0.28}Te_2{}^c$	SR 50A,25	2.16	0.551	$LaCu_{0.28}Te_2$
(58) $Pnnm$-g^5	Er_2Pd_2Si	SR 50A,31	2.16	0.548	Er_2Pd_2Si
(58) $Pnnm$-g^5	Mo_2IrB_2	SR 38A,49	2.23	0.555	$Mo_2IrB_2{}^d$
	Y_3Co_2	SR 41A,54	2.25	0.570	Y_3Co_2
(59) $Pmmn$-$e^3b^2a^2$	$LaNi_3In_6$	SR 52A,56	4.65	0.728	$LaNi_3In_6$
(59) $Pmmn$-fe^3ba	$EuAl^e$	SR 52A,4	3.99	0.629	$EuAl$
(60) $Pbcn$-d^2c	Rh_2O_3 HP	SR 35A,211	1.25	0.386	Rh_2S_3
	Rh_2S_3	SR 32A,120	1.26	0.389	Rh_2S_3
(62) $Pnma$-c^5	α-$BaCu_2S_2$	SR 40A,31	2.69	0.585	α-$BaCu_2S_2$
	$BaCu_2Se_2$	SR 40A,31	2.70	0.586	α-$BaCu_2S_2$
	$BaZn_2Sb_2$	SR 45A,11	2.70	0.588	α-$BaCu_2S_2$
	$BaZn_2As_2$	SR 44A,18	2.70	0.588	α-$BaCu_2S_2$
(62) $Pnma$-c^5	$Pr_2ReC_2{}^f$	[17]	2.63	0.603	Pr_2ReC_2
	Y_2ReC_2	[17]	2.79	0.623	Pr_2ReC_2
	Er_2ReC_2	[17]	2.81	0.632	Pr_2ReC_2
(62) $Pnma$-c^5	$Pt_2Ge_3{}^g$	SR 24,111	3.04	0.654	Pt_2Ge_3
(62) $Pnma$-c^5	$YNiAl_3$	[18]	2.78	0.657	$YNiAl_3$
(62) $Pnma$-c^5	Bi_2S_3	SR 48A,31	2.96	0.674	Sb_2S_3
	Bi_2Se_3 II	SR 39A,34	2.96	0.676	Sb_2S_3
	Sb_2Se_3	SR 52A,10	2.96	0.683	Sb_2S_3
	Sb_2S_3	SR 42A,22	2.96	0.685	Sb_2S_3
(62) $Pnma$-c^5	Tm_2S_3 III	SR 41A,109	2.99	0.691	U_2S_3
	Sc_3As_2	SR 46A,21	2.98	0.692	$U_2S_3{}^h$
	U_2S_3	SR 12,180	3.00	0.692	U_2S_3
	Dy_2Se_3	SR 42A,80	3.00	0.693	U_2S_3
	Hf_3P_2	SR 33A,92	2.99	0.695	$U_2S_3{}^h$
	Th_2S_3	SR 12,180	3.01	0.707	U_2S_3
(62) $Pnma$-c^5	$InSbS_3$	[19]	2.84	0.749	$InSbS_3$
(62) $Pnma$-c^5	$CrGaSe_3$	SR 55A,56	2.84	0.750	$TaCuS_3$
	$TaCuS_3$	SR 54A,47	2.85	0.757	$TaCuS_3$
(62) $Pnma$-c^5	$CeCrSe_3$	SR 37A,61	2.81	0.775	$NH_4CdCl_3{}^i$
	$PbSnS_3$	SR 38A,116	2.84	0.784	NH_4CdCl_3
	$RbCdBr_3$	SR 43A,141	2.80	0.785	NH_4CdCl_3
	$NH_4CdCl_3{}^i$	SR 44A,160	2.80	0.786	NH_4CdCl_3
	$RbCdCl_3$	SR 44A,160	2.80	0.787	NH_4CdCl_3
	$(Ti,Sn)SnS_3$	SR 54A,53	2.83	0.801	NH_4CdCl_3
	$ZrPbS_3$	SR 44A,77	2.83	0.802	NH_4CdCl_3
	$HfSnS_3$	SR 56A,41	2.83	0.802	NH_4CdCl_3
	$HfPbS_3$	SR 56A,41	2.83	0.803	NH_4CdCl_3
(62) $Pnma$-c^5	Sn_2S_3	SR 32A,128	2.84	0.810	Sn_2S_3
(62) $Pnma$-c^5	$ZrAu_4$	SR 27,224	2.69	0.840	$ZrAu_4$

(continued)

TABLE 5. *(continued)*

Space group and Wyckoff sequence	Compound	Reference	Γ	CG	Structure type
(62) $Pnma$-c^5	α-La_2S_3	SR 34A,98	2.86	0.866	$Cr_3C_2^h$
	$CeDyS_3$	SR 43A,45	2.86	0.871	$CeDyS_3^j$
	α-Nd_2S_3	SR 38A,127	2.86	0.871	$Cr_3C_2^h$
	α-Gd_2S_3	SR 33A,82	2.86	0.872	$Cr_3C_2^h$
	Cr_3C_2	SR 34A,56	2.84	0.880	Cr_3C_2
(62) $Pnma$-dc^3	Ni_3Sn_2 LT	SR 32A,107	1.92	0.462	Ni_3Sn_2 LT
(62) $Pnma$-dc^3	$BaTeS_3$	SR 42A,43	2.20	0.535	$BaTeS_3$
(62) $Pnma$-dc^3	K_2Te_3	SR 44A,94	2.26	0.595	K_2Te_3
(62) $Pnma$-dc^3	MgB_4	SR 38A,50	2.23	0.638	MgB_4
(62) $Pnma$-dc^2a	$AlSiP_3$	SR 45A,9	1.41	0.316	$AlSiP_3$
(62) $Pnma$-dc^2a	$UPdSe_3$	SR 56A,54	1.69	0.338	$UPdSe_3$
(62) $Pnma$-dc^2a	$BaZrS_3^k$	SR 46A,31	1.68	0.365	$GdFeO_3$
	$CaTiO_3$	SR 54A,155	1.70	0.370	$GdFeO_3$
	$SrZrS_3^k$	SR 46A,31	1.69	0.372	$GdFeO_3$
	$BaUS_3^k$	SR 46A,31	1.70	0.372	$GdFeO_3$
	$GdFeO_3$	SR 35A,218	1.71	0.376	$GdFeO_3$
	$URhS_3$	[20]	1.71	0.379	$GdFeO_3$
	$CaZrS_3^k$	SR 46A,31	1.72	0.380	$GdFeO_3$
	$ScCeS_3$	SR 46A,54	1.71	0.380	$GdFeO_3$
	$YFeO_3$	SR 30A,323	1.72	0.381	$GdFeO_3$
	α-$LaYbS_3$	SR 50A,46	1.72	0.382	$GdFeO_3$
	$UCrS_3$	SR 41A,48	1.71	0.384	$GdFeO_3$

^{a}oP20-1.
^{b}According to SR 46A,54 centrosymmetric structure type $GdFeO_3$ cannot be excluded.
^{c}oP20-6.88.
^{d}Ternary substitution variant of Y_3Co_2.
^{e}In the original paper and in SR the z-coordinate of Eu(1) is misprinted as 0.8151 instead of 0.0815.
^{f}In the abstract the cell parameters given for Pr_2ReC_2 actually refer to Y_2ReC_2.
^{g}On top of p. 336 of the original work the c-parameter is misprinted as 3.78 instead of 3.378 Å. In SR the z-coordinate of the first Ge site is misprinted as 0.075 instead of -0.075.
^{h}Antitype.
^{i}The hydrogen atoms in the ammonium group are not considered.
^{j}Ternary substitution variant of Cr_3C_2 antitype.
^{k}In SR the second refined coordinate of S(1) is misprinted as y instead of z.

no other conditions for "standardization" were applied. Thus it was not possible to recognize isotypic structures described with different unit cells and/or different Wyckoff sequences. Table 6 presents a few examples of compound pairs which were reported in the data compilation [11] to have different structures, but which, after applying the standardization procedure, are readily shown to be isotypic. The last column indicates the main differences in the data which prevented the recognition of isotypism. In contrast, Table 7 lists some compound pairs which were reported to have the same structure in ref. 11, but which according to our analysis are only isopointal. A first indication for a difference in structure was seen in the difference of the Γ and/or CG values of the standardized structure data, and this was further confirmed by a detailed comparison of the structures involved.

6. The same or similar Wyckoff sequence as an indication of possible structural relationships

The classification code based on the Wyckoff sequence can also be useful for the recognition of simple structural relationships. In a list of structure types, ordered according to space group and Wyckoff sequence, the substitution derivatives of a base type which have the same space group and Wyckoff sequence are found near each other. As mentioned above for isopointal structures with the same stoichiometry, identical classification codes do not necessarily indicate a geometrical relationship, and the cell parameters together with the atom coordinations must be compared in order to corroborate the indications. However, the list is of great help in limiting the number of structures which need to be examined.

TABLE 6. List of compound pairs which were reported in ref. 11 to have different structure types but which after applying the standardization procedure are found to be isotypic; in many cases the isotypism was recognized by the authors of the original works; in the last column are pointed out the main difference between the data given for the two compounds in ref. 11, *i.e.* non-comparable cell parameters (C) and/or different Wyckoff sites (W), which did not allow the isotypism to be recognized

Pearson code	Space group and Wyckoff sequence	Structure type	Reference	Γ	CG	Isotypic compound	Reference	Γ	CG	Difference in the data
$mP16$	(14) $P2_1/c$-e^4	$LaCuS_2$	SR 48A,45	2.16	0.460	$SmCuS_2$	SR 51A,41	2.26	0.542	C[a]
$mS60$	(15) $C2/c$-f^6e^2a	$Na_6Sn_2S_7$	SR 44A,31	3.82	0.411	$Na_6Ge_2Se_7$	[21]	3.83	0.417	C
$mS92$	(12) $C2/m$-$i^{22}ca$	$Ca_{3.1}In_{6.6}S_{13}$[b]	SR 38A,59	11.99	0.970	$Sn_{2.5}In_7S_{13}$[c]	SR 55A,51	11.97	0.972	C[a]
$oP48$	(55) $Pbam$-$i^3h^2g^3e$	$ZrCrSi_2$	SR 49A,24	3.75	0.348	$TiMnSi_2$	SR 49A,46	3.76	0.350	C
$oP60$	(55) $Pbam$-h^7g^7da	$In_9Pb_4S_{17}$	SR 44A,70	7.63	0.603	$In_9Sn_{3.5}S_{17}$[d]	SR 54A,51	6.91	0.550	C
$oF48$	(70) $Fddd$-g^2f	Mg_2Cu	SR 8,64	1.20	0.480	Mn_2B	SR 48A,35	1.09	0.463	C, W
$oI12$	(74) $Imma$-he	KHg_2	SR 19,231	0.78	0.469	$CeCu_2$	SR 26,107	0.77	0.459	C, W
$oI20$	(72) $Ibam$-j^2a	K_2ZnO_2	SR 33A,325	0.84	0.247	K_2SiP_2	SR 51A,77	0.83	0.262	C, W
$oI22$	(71) $Immm$-$ljiha$	$Gd_3Cu_4Ge_4$	SR 35A,54	1.83	0.551	$Li_4Sr_3Sb_4$	SR 35A,9	1.81	0.543	C, W
$tP4$	(131) $P4_2/mmc$-ec	PtS	SR 24,210	0.75	0.276	PdO	SR 17,383	0.75	0.276	W
$tP6$	(129) $P4/nmm$-c^2a	$PbFCl$[e]	SB 3,369	1.94	0.580	$TiCuH_{0.9}$[f]	SR 44A,55	1.88	0.576	W
$tP14$	(136) $P4_2/mnm$-ifa	$ZrFe_4Si_2$	SR 41A,82	1.01	0.400	$CaCu_4P_2$	SR 54A,35	1.01	0.402	W
$tI12$	(141) $I4_1/amd$-ea	β-Mo_2N[g]	[22]	0.73	0.429	α-Ti_2N[h]	SR 34A,115	0.74	0.468	W
$hP4$	(187) $P\bar6m2$-hba	$TaTl_{0.33}Se_2$[i]	SR 40A,94	1.27	0.465	$TaIn_{0.67}S_2$[j]	SR 55A,52	1.27	0.461	W
						$NbInS_2$	[12]	1.27	0.457	W
$hR18$	(166) $R\bar3m$-dca	Mg_2Ni_3Si	SR 52A,64	1.09	0.539	Y_2Rh_3Ge	SR 54A,20	1.08	0.522	W
$cF36$	(225) $Fm\bar3m$-eca	Sr_2RuH_6[k]	SR 37A,83	0.66	0.197	Gd_2MnGa_6	SR 53A,12	0.71	0.213	W

[a]Transformed from setting with *c*-axis unique.

[b]Refined composition $Ca_3In_7S_{13}$. In the original work the *x*-coordinate of In(4) was misprinted as 0.2670 instead of 0.1670, in SR the Wyckoff sites are misprinted as $4(i)$ for all sites and the *a*-parameter as 36.630 instead of 37.630 Å.

[c]$mS92$-2.

[d]$oP60$-1.

[e]Ternary variant of Cu_2Sb (SB 3,33,288).

[f]$tP6$-0.2.

[g]$tI12$-0.96.

[h]An additional, partly occupied site was reported in SR 52A,71.

[i]$hP4$-0.672; the Ta and Se sites with refined occupancy 0.99 and 0.97 respectively, are considered to be fully occupied.

[j]$hP4$-0.33.

[k]K_2PtCl_6 structure type (SR 51A,145).

TABLE 7. List of compound pairs which were reported to be isotypic in ref. 11 but which are only isopointal

Pearson code	Space group and Wyckoff sequence	Structure type	Reference	Γ	CG	Isopointal compound	Reference	Γ	CG
$mP44$	(14) $P2_1/c$-e^{11}	P_4O_7	SR 51A,184	5.68	0.464	α-P_4S_7	SR 30A,353	5.61	0.565
$mS20$	(9) Cc-a^5	α'-Ga_2S_3[a]	SR 42A,86	2.04	0.339	β-Ga_2Se_3	SR 50A,35	1.94	0.368
$oP36$	(33) $Pna2_1$-a^9	P_4Se_5	SR 37A,121	4.25	0.399	$Sn_2Ga_2S_5$	SR 50A,36	4.68	0.484
$oS12$	(63) $Cmcm$-c^2a	$AgCuS$ LT[b]	SR 19,412	0.92	0.352	$KAuS$	SR 54A,45	1.00	0.356
$oS24$	(63) $Cmcm$-fc^3a	$YNiAl_4$	SR 38A,8	2.03	0.778	$LaNiH_{3.7}$[c]	SR 49A,38	1.54	0.494
$oI10$	(71) $Immm$-jha	W_2CoB_2	SR 31A,27(I.)	1.12	0.421	K_2PtS_2	SR 38A,139	1.16	0.432
$hP36$	(194) $P6_3/mmc$-khf^3ea	Ce_2Ni_7	SR 23,108	3.68	0.851	$Mg(Cu,Ni)_2$ 6H	SR 38A,85	3.79	0.838
$hR12$	(160) $R3m$-a^4	$Na_{0.55}TiS_2$[d]	SR 37A,135	1.16	1.016	$CuAsSe_2$ II	SR 33A,30	1.24	0.932
$cP12$	(205) $Pa\bar3$-ca	FeS_2 pyrite	SR 34A,97	0.67	0.333	CO_2	SR 46A,228	0.21	0.103
$cP24$	(213) $P4_132$-dca	Mo_3Al_2C	[24]	1.27	0.411	$Mg_{28.4}Cu_{57.9}Si_{13.7}$	SR 51A,40	1.08	0.348

[a]In the original work the *y*-coordinate of Ga(2) is misprinted as 0.0097 instead of -0.0097.

[b]Most recent refinement [23] indicated space group $Cmc2_1$.

[c]$oS24$-1.2.

[d]$hR12$-1.35. The original description in space group $R3$ does not consider all symmetry elements (see ref. 10).

A list of selected examples of substitution derivatives, found in such a way, is given in Table 8. This list is limited to completely ordered ternary variants of binary base structures. Well known examples, such as the Fe_2P type ordering variants, have not been mentioned. The three binary structures with Pearson code $oP12$ may be considered as branches of the $PbCl_2$ structure type (SR 42A, 184). For all three there are known ternary

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TABLE 8. Examples of ternary substitution variants of binary base structure types; some of the relationships had already been observed by the authors of the original works

Pearson code	Space group and Wyckoff sequence	Binary type	Reference	Γ	CG	Ternary variant	Reference	Γ	CG
$mS12$	(12) $C2/m$-i^3	α-$PdBi_2$	SR 21,52	1.43	0.528	CeCoAl	SR 50A,6	1.45	0.528
$mS18$	(12) $C2/m$-i^4a	K_5Sb_4[a]	[25]	2.22	0.532	Y_4Co_4Ga	SR 51A,34	2.22	0.556
$oP12$	(62) $Pnma$-c^3	Co_2P	SR 24,128	1.52	0.534	TiNiSi	SR 30A,75	1.54	0.538
$oP12$	(62) $Pnma$-c^3	Co_2Si	SR 19,124	1.58	0.591	HoNiGa	SR 45A,50	1.63	0.549
$oP12$	(62) $Pnma$-c^3	$SnBr_2$	[26]	1.67	0.676	BiSCl	SR 46A,217	1.66	0.671
$oP16$	(62) $Pnma$-c^4	YZn_3	SR 33A,100	2.30	0.682	$ScRhSi_2$	SR 48A,86	2.31	0.684
$oP36$	(62) $Pnma$-d^3c^3	Sm_5Ge_4[b]	SR 32A,87	2.99	0.417	$Zr_2Nb_3Ge_4$	SR 51A,51	2.88	0.408
$oP36$	(62) $Pnma$-d^3c^3	Gd_5Si_4	SR 38A,91	3.31	0.516	$Sc_3Ce_2Si_4$	SR 45A,52	3.33	0.518
$oS12$	(63) $Cmcm$-c^2a	UPt_2[c]	SR 23,210	1.08	0.528	YAlGe	[27]	1.05	0.533
$oS12$	(65) $Cmmm$-$jica$	$ZrGa_2$	SR 27,203	1.55	0.320	Ag_3TlTe_2[d]	SR 38A,146	1.54	0.310
$oS16$	(63) $Cmcm$-gca	CeAl	SR 32A,9	0.82	0.242	Na_2CuAs	SR 42A,16	0.80	0.235
$oS20$	(36) $Cmc2_1$-b^2a	B_2O_3 II	SR 33A,259	0.97	0.272	Si_2N_2O	SR 46A,136	0.92	0.265
$oS24$	(63) $Cmcm$-gec^2	$BaZn_5$	SR 20,44	1.59	0.330	$CaNi_2Ga_3$	[28]	1.60	0.330
$oS28$	(63) $Cmcm$-f^2c^2a	K_4P_3	[29]	1.96	0.457	W_3CoB_3	SR 34A,39	1.73	0.471
						Y_3Co_3Ga	SR 44A,50	1.87	0.445
$oS32$	(63) $Cmcm$-f^3c^2	Ca_3Ga_5	SR 53A,3	2.32	0.586	$Hf_3Ni_2Si_3$	SR 43A,68	2.31	0.592
$oF32$	(69) $Fmmm$-$ihgf$	U_3Si orth.[e]	SR 46A,117	1.18	0.216	$NiPt_2Ge$ orth.	SR 45A,74	1.17	0.215
$oI14$	(71) $Immm$-j^2ia	Ta_3B_4	SR 12,31	1.60	0.683	$Ba_3Al_2Ge_2$	SR 42A,4	1.59	0.657
$oI44$	(72) $Ibam$-j^4ga	V_6Si_5	SR 38A,101	2.16	0.429	$Nb_4Cr_2Si_5$	SR 43A,47	2.16	0.426
						$Nb_2Cr_4Si_5$	SR 33A,64	2.17	0.457
$tP32$	(130) $P4/ncc$-$gfcb$	Pu_5Rh_3	SR 43A,67	2.31	0.622	Ce_5NiGe_2	SR 54A,10	2.29	0.619
$tI12$	(139) $I4/mmm$-e^2c	La_2Sb	SR 46A,13	0.96	0.393	ScCeSi	SR 45A,52	0.95	0.373
$tI16$	(139) $I4/mmm$-e^2dc	$ZrAl_3$	SB 7,14,100	1.54	0.510	$SrZnBi_2$	SR 42A,17	1.51	0.514
$tI16$	(140) $I4/mcm$-hba	TlSe	SB 7,6,77	1.51	0.443	$NaInTe_2$	SR 39A,100	1.51	0.443
$tI26$	(87) $I4/m$-h^3a	Sm_9Ga_4	SR 52A,45	1.15	0.360	$Nb_5Cu_4Si_4$	SR 33A,77	1.17	0.378
$tI32$	(140) $I4/mcm$-$khba$	W_5Si_3	SR 19,277	1.74	0.448	Nb_5Sn_2Si	SR 35A,84	1.72	0.452
$tI32$	(140) $I4/mcm$-$lhca$	Cr_5B_3	SR 42A,54	1.58	0.270	Mo_5SiB_2	SR 22,60(II.)	1.59	0.271
$tI84$	(139) $I4/mmm$-$n^2mjh^2e^2d$	$Ho_{11}Ge_{10}$	SR 32A, 77	3.34	0.306	$Sc_{11}Al_2Ge_8$	[30]	3.36	0.306
$hP5$	(164) $P\bar3m1$-d^2a	La_2O_3 A	SR 45A,220	1.77	0.582	Ce_2SO_2[f]	SR 12,174	1.78	0.606
$hP6$	(194) $P6_3/mmc$-dca	Ni_2In	SR 9,90(II.)	1.84	0.592	ZrBeSi	SR 17,50	1.84	0.660
$hP18$	(193) $P6_3/mcm$-g^2db	Ti_5Ga_4	SR 27,203	1.80	0.407	$Gd_5SiCuBi_3$[g]	SR 34A,34	1.77	0.397
$hP24$	(194) $P6_3/mmc$-$kfdcba$	$CeNi_3$	SR 23,112	3.41	0.801	YRh_2Si	SR 52A,83	3.41	0.725
						$Dy_3Ni_7B_2$	[32]	3.40	0.738
						Ce_3Co_8Si	[33]	3.41	0.800
$hP28$	(194) $P6_3/mmc$-kh^2ca	Co_2Al_5	SB 6,175	2.99	0.553	Hf_9Mo_4B	SR 39A,37	3.05	0.564
$hP30$	(169) $P6_1$-a^5	α-Al_2S_3	[34]	2.03	0.330	$GaInSe_3$	SR 54A,50	2.02	0.390
$hP30$	(169) $P6_1$-a^5	γ-In_2Se_3	SR 44A,73	2.18	0.507	$GaInS_3$	SR 54A,50	2.20	0.517
$hR36$	(166) $R\bar3m$-hc^2ba	$PuNi_3$	SR 23,111	1.69	0.641	$Ca_3Cu_2Al_7$	SR 51A,8	1.69	0.616
$hR42$	(148) $R\bar3$-f^2c	Mo_3Se_4	SR 39A,85	0.88	0.245	Mo_3Se_3Br	SR 45A,205	0.89	0.247
$cP39$	(200) $Pm\bar3$-$jihgfa$	Mg_2Zn_{11}	SR 12,8	2.67	0.392	$Mg_2Cu_6Al_5$	SR 12,8	2.69	0.396
$cF96$	(227) $Fd\bar3m$-fec	Ti_2Ni	SR 28,20	0.84	0.269	Mn_3Ni_2Si	SR 28,28	0.84	0.268
$cF116$	(225) $Fm\bar3m$-f^2eda	Th_6Mn_{23}	SR 16,113	1.42	0.246	$Mg_6Cu_{16}Si_7$	SR 20,95	1.46	0.252
$cF184$	(227) $Fd\bar3m$-$gfdca$	$ZrZn_{22}$	SR 26,277	1.93	0.356	$Mg_3Cr_2Al_{18}$[h]	SR 22,8	1.93	0.356
$cI44$	(229) $Im\bar3m$-hec	Ca_3Ag_8	SR 29,33	1.18	0.328	$Ce_3Ni_6Si_2$	SR 31A,35	1.18	0.326

[a]The coordinates of K(3) should be 1/2 1/2 1/2 instead of 0.475 1/2 0.483 (private communication from the authors).
[b]In SR the Wyckoff site of Ge(3) is misprinted as $4(d)$ instead of $8(d)$.
[c]Description by the authors in space group $Ama2$ does not consider all symmetry elements (see ref. 27).
[d]Description by the authors in space group $Pmna$ does not consider all symmetry elements (see ref. 10).
[e]In Table 1 of the original work the space group is misprinted as $Pmmm$ instead of $Fmmm$.
[f]In SR the position for S is misprinted as 2S in (b) instead of 1S in (a).
[g]Hf_5CuSn_3 structure type [31], atom coordinates are not refined for the stannide.
[h]In SR the origin was erroneously assumed to be at a centre of symmetry.

substitution variants. Some of the substitution variants in Table 8 can be explained with known crystal chemical concepts, as for example B_2O_3 II and Si_2N_2O, both with VEC = 4.80 and $VEC_A = 8$, where structural features and the available number of valence electrons correspond to the adamantane structure equation (see ref. 2). The majority of the examples in Table 8 is, however, unexpected and provides sufficient material for further crystal chemical studies.

Also vacancy and filled-in structure variants with the same space group might be identified by similarities in their Wyckoff sequences. For example, the $Sc_{57}Rh_{13}$

structure type (SR 52A, 82), Pearson code $cP140$ and classification code (200) $Pm\bar{3}$-$l^2k^3j^3hfeba$, and the $Sc_{29}Fe_6$ structure type (SR 53A, 5), same codes, both turn out to be filled-in substitution variants of the $Al_9Mn_2Si_{1.8}$ or α-AlMnSi type (SR 31A, 8) with Pearson code $cP138$ and classification code (200) $Pm\bar{3}$-$l^2k^3j^3hfe$.

In conclusion, the standardization procedure is found to be useful for recognizing isotypic crystal structures. This has led to the correction of lists of structure types which were based on non-standardized structure data. The use of the Wyckoff sequence allows a much finer classification of structure types and in addition offers suggestions for possible structural relationships such as substitution, vacancy or filled-in structure variants.

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