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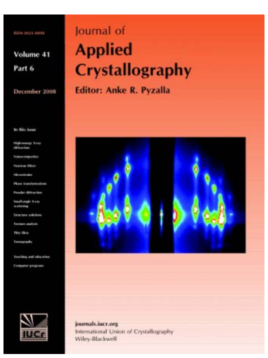

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From space to superspace and back: Superspace Group Finder

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The symmetry of a commensurately modulated crystal structure can be described in two different ways: in terms of a conventional three-dimensional space group or using the superspace concept in (3 + d) dimensions. The three-dimensional space group is obtained as a real-space section of the (3 + d) superspace group. A complete network was constructed linking (3 + 1) superspace groups and the corresponding three-dimensional space groups derived from rational sections. A database has been established and is available at http://superspace.epfl.ch/finder/. It is particularly useful for finding common superspace groups for various series of modular ('composition-flexible') structures and phase transitions. The use of the database is illustrated with examples from various fields of crystal chemistry.

1. Introduction

Superspace groups classify the symmetry of modulated crystals by describing their structure in higher-dimensional periodic space (Janssen *et al.*, 2007; van Smaalen, 2007). If the modulation is incommensurate, the crystal lacks three-dimensional periodicity and its symmetry can be described solely with a (3 + d)-dimensional superspace group. On the other hand, the symmetry of a commensurately modulated crystal structure may be described in two different ways: in terms of a conventional three-dimensional space group or in superspace using a (3 + d)-dimensional group. In general, different three-dimensional space groups can be obtained as rational sections of one superspace group (Perez-Mato, 1991; Tamazyan *et al.*, 1996). It has been shown by many researchers that this property allows series of structurally related compounds to be described using a unified model in (3 + d)-dimensional superspace (Arakcheeva & Chapuis, 2006; Schönleber *et al.*, 2006; Boullay *et al.*, 2002). In the traditional three-dimensional approach, each individual phase is characterized by its own space group and cell parameters, while in the superspace approach, the superspace group is invariant and the modulation vector **q** varies for each member of the series.

The advantage of this approach is the unified description of the series using a single structural model, thus emphasizing the structural relationship between the members of the series. In practice, this approach requires an *a priori* identification of a 'parental' superspace group or groups for a set of space groups describing the family members. While the problem of deriving a set of possible three-dimensional space groups from a (3 + 1)-dimensional superspace group is relatively straightforward and has been described in the literature (Perez-Mato, 1991; Tamazyan *et al.*, 1996), the inverse problem, *i.e.* finding a 'parental' superspace group for a set of three-dimensional space groups, requires the compilation of a large amount of information, and presently no tables containing this information are available to our knowledge.

The purpose of this work is to fill this gap and create a database containing the set of all possible three-dimensional space groups for each (3 + 1)-dimensional superspace group as a function of the modulation vector **q** and the phase t_0, which defines the position of the real-space section along the internal space coordinate.

2. The relationship between (3 + 1)-dimensional and three-dimensional symmetry

The relationship between the symmetry operations of the (3 + 1)-dimensional superspace-group operations and the corresponding three-dimensional space-group operations obtained by real-space sections has been discussed in detail, for example, by Tamazyan *et al.* (1996) and Perez-Mato (1991). Here only a brief overview of the most important concepts and conclusions is given.

A symmetry operation g_s of a (3 + 1)-dimensional space group can be expressed in the form $g_s = \{\mathbf{R}|\mathbf{s}+\mathbf{l}\}$, where **s** is the translational part of the symmetry operation, **l** is an integer lattice translation vector and **R** is a rotation matrix that can be decomposed as

$$\begin{pmatrix} \mathbf{R}_{\rm E} & \mathbf{0} \\ \mathbf{R}_{\rm M} & \varepsilon \end{pmatrix}.$$

$\mathbf{R}_{\rm E}$ is a 3 × 3 rotation matrix, **0** is a 3 × 1 matrix of zeroes, $\mathbf{R}_{\rm M}$ is a 1 × 3 matrix that has nonzero elements only if the modulation vector has rational components fixed by the space group, and $\varepsilon = \pm 1$. A general point **r** can be expressed as $\mathbf{r} = (\mathbf{r}_3, t)$, where $\mathbf{r}_3$ is a projection of the vector onto the real-space section and t is the projection on the additional vector $\mathbf{a}_4$. Two points belonging to the same real-space section have the same coordinate t.

A symmetry operation g_s gives rise to a symmetry operation g_r of the real-space section only if it maps a point $\mathbf{r} = (\mathbf{r}_3, t)$ to another point $\mathbf{r}' = (\mathbf{r}'_3, t')$ that lies on the same real-space section, *i.e.* such that $t' = t$. It can be shown (Tamazyan *et al.*, 1996) that this is fulfilled only if

$$s_4 + l_4 - (\mathbf{s}_3 + \mathbf{l}_3)\mathbf{q} + (\varepsilon - 1)t = 0. \qquad (1)$$

Here $\mathbf{s}_3$ and $\mathbf{l}_3$ are the vectors of the first three components of **s** and **l**, respectively, s_4 and l_4 are the fourth components of **s** and **l**, and **q** is the modulation vector $\mathbf{q} = q_1\mathbf{a}^* + q_2\mathbf{b}^* + q_3\mathbf{c}^*$. If a structure is commensurately modulated, the components of the modulation vector are rational numbers and can be expressed as fractions: $\mathbf{q} = (K/$

N_1, L/N_2, M/N_3). The resulting three-dimensional symmetry operation g_r will have the form $g_r = \{\mathbf{R}_E|\mathbf{T}(\mathbf{s}_3 + \mathbf{l}_3)\}$, where $\mathbf{T}$ is the transformation matrix that transforms the unit cell of the basic structure to the unit cell of the superstructure. $\mathbf{T}$ can be written in the form

$$\mathbf{T} = \begin{pmatrix} 1/N_1 & 0 & 0 \\ 0 & 1/N_2 & 0 \\ 0 & 0 & 1/N_3 \end{pmatrix}, \quad (2)$$

where $N_i = 1$ if the corresponding component of the modulation vector is zero. The three-dimensional symmetry operations derived from all the (3 + 1)-dimensional symmetry operations of a superspace group G_s for a given modulation vector and for a constant value of t form a three-dimensional space group. This space group is a possible space group of a commensurately modulated structure with modulation vector $\mathbf{q}$ and superspace symmetry G_s. The specific value of t leading to the three-dimensional space group will be hereafter denoted as t_0. The number of different space groups that can be derived from a single superspace group for different values of t and different modulation vectors is limited. The set of such space groups is designated a 'family of sectional real-space groups' and the corresponding superspace group a 'parental superspace group' (compare with *International Tables for Crystallography*, 2002, Vol. E, ch. 5.2, pp. 393–416).

The basic observations following from equations (1) and (2) are as follows:

(i) If $\varepsilon = 1$, then equation (1) is independent of t, and the three-dimensional symmetry operation either exists for all values of t or does not exist at all. If $\varepsilon = -1$, it is always possible to find a value of t so that equation (1) is fulfilled, giving rise to a nontrivial three-dimensional symmetry operation.

(ii) For $\varepsilon = 1$, the exact form of the operation g_r depends not only on t and $\mathbf{q}$, but also on the form of $\mathbf{l}_3$ that is necessary to fulfil equation (1). Thus, depending on $\mathbf{q}$, a superspace mirror plane can lead to a three-dimensional glide plane, and a superspace rotation axis can result in a three-dimensional screw axis. On the other hand, if $\varepsilon = -1$, the intrinsic translational part of the three-dimensional operation is numerically equal to the first three components of the intrinsic translational part of $\mathbf{s}$, and the type of operation does not change.

Tables 1 and 2 present examples of families of sectional real-space groups for the parental superspace groups $Pbnm(00\gamma)s00$ and $B2/b(\alpha\beta0)$, depending on the parity of the numerators and denominators of the $\mathbf{q}$-vector components and the value of t_0.

3. The construction of the database

The core of the database is a table of sectional real-space groups for each superspace group as a function of the $\mathbf{q}$-vector class and values of t_0. A brief analysis of equation (1) shows that, despite its seeming simplicity, it is a complex equation involving many variables. It would be almost impossible to analyse all the possible cases manually and very difficult to handle the equation with a computer program in its symbolic form.

Therefore, we took advantage of the existing code of the computer program *JANA2000* (Petříček *et al.*, 2000), which allows one to derive sectional real-space groups as a function of t_0 for a given superspace group and a given modulation vector. We have modified the program so that it can scan through an externally supplied list of superspace groups and modulation vectors. We devised the list of modulation vectors to include all possibly distinct combinations of parities of the nominators/denominators of the $\mathbf{q}$-vector components. To avoid ambiguities, the list contained three or four different modulation vectors for each tested parity class. The program output contains a list of three-dimensional groups for each superspace group and modulation vector, making it possible to merge modulation vectors producing an identical sequence of sectional space groups into one record with generic symbolic representation of the $\mathbf{q}$-vector class (as in Tables 1 and 2).

Table 1
Space groups for commensurate structures with superspace group $Pbnm(00\gamma)s00$ depending on the parity of the numerator M and denominator N_3 of the component γ of the modulation vector (the generic symbol N is used in the case of only one nonzero component).

The three-dimensional derivatives inherit the basis of the parental (3 + 1)-dimensional group; n denotes any integer.

q-vector components K/N_1, L/N_2, M/N_3	t_0: General	n/N	$1/4N + n/N$	$1/2N + n/N$	$3/4N + n/N$
0, 0, $2n + 1/2n + 1$	$P2_1$	$P2_1/m$	$P2_12_12_1$	$P2_1/m$	$P2_12_12_1$
0, 0, $2n/2n + 1$	Pn	$P2_1/n$	$P2_1nm$	$P2_1/n$	$P2_1nm$
0, 0, $2n + 1/2n$	Pn	$P2_1/n$	$Pn2_1m$	$P2_1/n$	$Pn2_1m$

For many superspace groups the results of the scanning could be directly processed and the table produced. However, particular cases occurred for some space groups that required closer attention. These cases will be described in the following subsections.

3.1. Nonconventional space-group settings

Frequently, the sectional three-dimensional space groups are not in the standard setting as they are derived from the basic structure by application of the matrix $\mathbf{T}$. *JANA2000* can handle the common nonstandard settings, but in extreme cases it is not able to derive the space-group symbol. In such cases, the list of three-dimensional symmetry operations generated by *JANA2000* was inspected and the corresponding space-group symbol was derived manually. This problem was particularly frequent in some monoclinic superspace groups, where a diagonal glide plane occurs with the glide vector equal to one-half of a nonstandard centring vector (see Table 2), and in tetragonal superspace groups, where sometimes the axial symmetry operations are lost in the section and the three-dimensional sectional group is formed only by the diagonal symmetry operations. In cases where an explanation is needed, a note about the meaning of the space-group symbol is added in the database.

3.2. Nonconventional centring

If the modulation vector has more than one component, it can occur that the denominators of the components have a common divisor. In this case the space group will contain nonconventional centring vectors if it is described in a unit cell obtained from the basic unit cell by application of matrix $\mathbf{T}$ [see equation (2)]. For example, a modulation vector $(\frac{1}{3}, \frac{1}{3}, 0)$ will imply centring vectors $(\frac{1}{3}, \frac{2}{3}, 0)$ and $(\frac{2}{3}, \frac{1}{3}, 0)$ in the supercell. In these cases, the database contains always the space group obtained with the modulation vector without the special relationship between the components, and a note is added to the database explaining the problem.

Sometimes, however, a nonconventional centring occurs owing to a combination of the modulation vector with the lattice centring of the superspace group. In these cases the nonconventional centring is independent of the particular value of the modulation vector $\mathbf{q}$ within a given $\mathbf{q}$-vector class, and therefore the nonstandard centring is retained in the database and denoted by the letter X in the space-group symbol.

Table 2
Space groups for commensurate structures derived from superspace group $B2/b(\alpha\beta0)$ depending on the numerators (K, L) and denominators (N_1, N_2) of the **q**-vector components.

If a potentially nonzero **q**-vector component has a zero value, the combination of even/odd applies (0 = 0/1). N' denotes the least common multiple of N_1 and N_2. The basis of the three-dimensional space group is obtained from the basis of the parental (3 + 1)-dimensional group by application of the transformation matrix **T** [equation (2)]. To obtain a conventional three-dimensional space-group setting and the space-group symbol, a basis transformation might be necessary. X in the space-group symbol indicates nonstandard centring, discussed in §3.2.

	t_0				
q-vector components K/N_1, L/N_2, M/N_3	General	n/N'	$1/4N' + n/N'$	$1/2N' + n/N'$	$3/4N' + n/N'$
$2n/2n + 1$, $2n + 1/\text{any}$, 0	$B1$	$B\bar{1}$	$B2$	$B\bar{1}$	$B2$
$2n + 1/2n + 1$, $2n + 1/2n$, 0	$I1$	$I\bar{1}$	$I2$	$I\bar{1}$	$I2$
$2n +1 /2n + 1$, $2n + 1/2n + 1$, 0	Pn	$P2_1/n$	$P2/n$	$P2_1/n$	$P2/n$
$2n + 1/\text{any}$, $2n/2n + 1$, 0	Pb	$P2/b$	$P2_1/b$	$P2/b$	$P2_1/b$
$2n + 1/2n$, $2n + 1/2n + 1$, 0					
If N_1 and N_2 do not have common divisor	Pn	$P2/n$	$P2_1/n$	$P2/n$	$P2_1/n$
If N_1 and N_2 have common divisor	Xd'	$X2/d$	$X2_1/d'$	$X2/d'$	$X2_1/d'$
$2n/2n + 1$, $2n/2n + 1$, 0	Bb	$B2/b$	–	$B2/b$	–
$2n + 1/2n$, $2n + 1/2n$, 0					
If N_1 and N_2 contain equal powers of 2 (*e.g.* $N_1 = 4 = 2 \times 2$, $N_2 = 12 = 2 \times 2 \times 3$)	Xd'	$X2_1/d'$	$X2/d'$	$X2_1/d'$	$X2/d'$
If N_1 contains larger powers of 2 than N_2 (*e.g.* $N_1 = 8 = 2 \times 2 \times 2$, $N_2 = 6 = 2 \times 3$)	Xd'	$X2/d'$	$X2_1/d'$	$X2/d'$	$X2_1/d'$
If N_1 contains smaller power of 2 than N_2 (*e.g.* $N_1 = 6 = 2 \times 3$, $N_2 = 8 = 2 \times 2 \times 2$)	$X1$	$X\bar{1}$	$X2$	$X\bar{1}$	$X2$

3.3. Nonconventional q-vector classes

In one family of sectional groups, the **q**-vector classes usually differ only in the moduli of the numerators and denominators of the components. Most often only modulo 2 has to be considered, but sometimes modulo 3, 4 or 6 is needed. However, in some planar monoclinic superspace groups modulo n is not sufficient to decide which sectional real-space groups are possible for a given modulation vector. In these groups the modulation vector has two free components, and if both components have an even denominator, then the **q**-vector class must be determined from the difference in the powers of two contained in the two denominators (see Table 2 for an example).

4. Guide to the use of the database

On the basis of the results described above, the Superspace Group Finder database was created in order to provide online access to the data. The application is available *via* a World Wide Web front-end, http://superspace.epfl.ch/finder/, written in HTML/CGI, and uses MySQL for processing the queries. As such, it can run on a wide variety of platforms and browsers. It has been tested on Safari 3.0 (Mac and PC), Internet Explorer (PC) and FireFox (PC). The client-side code is relatively light-weight and does not require any special hardware. Standard crystallographic conventions are used for space group and superspace group notations.

The main functions of the front-end are described in the following subsections.

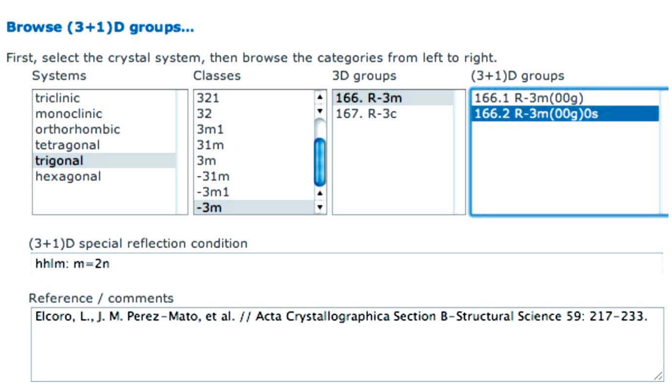

Figure 1
Superspace Group Finder interface. Browsing the list of superspace groups.

4.1. Inspecting sectional real-space groups of a superspace group

This option allows one to view the complete family of sectional real-space groups for a particular superspace group (Fig. 1). In the query, the user selects first the crystal system and then browses a tree of crystal classes, basic three-dimensional groups and (3 + 1)-dimensional groups. For each selected (3 + 1)-dimensional superspace group, the special reflection conditions are listed according to the *International Tables for Crystallography* (2004, Vol. C, ch. 9.8, pp. 921–934). The second field, ‘Reference / comments’ is used for two purposes. Firstly, it indicates warnings on nonconventional settings and symmetry elements appearing in the query output (see §3). Secondly, if the selected superspace group has been applied for a structure description, it displays the literature reference.

The main output window (not shown in the figures) displays the family of sectional real-space groups for the selected parental superspace group, listing conditions for modulation vector (**q**-vector) components and t_0 values, similar to Tables 1 and 2.

4.2. Search for parental superspace groups for a given set of three-dimensional space groups

This option allows one to search for parental superspace groups for a given set of three-dimensional groups observed, for example, in a sequence of phase transitions or in a series of modular structures. For the query, the user types the set of space groups separated by a space or a comma in the query line. The matching superspace groups are presented in order of completeness, starting from those containing all required three-dimensional space groups. In the example shown in Fig. 2, each of the superspace groups $P6/mmc(00\gamma)s00s$, $P6_3/mcm(00\gamma)00ss$ and $P6_3/mmc(00\gamma)00ss$ listed under the title ‘Complete match’ involves all three space groups $P\bar{3}1c$, $P3c1$ and $P6_3$

Table 3
Space groups for the commensurate structures derived from superspace group *Amam*(00γ)*s*00 depending on the parity of the numerator *M* and denominator N_3 of component γ of the **q** vector (the generic symbol *N* is used in the database in the case of only one nonzero component).

n denotes any integer.

q-vector components K/N_1, L/N_2, M/N_3	t_0 General	*n*/*N*	1/4*N* + *n*/*N*	1/2*N* + *n*/*N*	3/4*N* + *n*/*N*
0, 0, 2*n*/2*n* + 1	*Aa*	*A*2/*a*	$A2_1am$	*A*2/*a*	$A2_1am$
0, 0, 2*n* + 1/2*n*	$Pca2_1$	*Pcam*	*Pcab*	*Pcam*	*Pcab*
0, 0, 2*n* + 1/2*n* + 1	$Pna2_1$	*Pnab*	*Pnam*	*Pnab*	*Pnam*

enumerated in the query. Each of the superspace groups indicated under the next item involves only two out of the three required space groups, *etc*. The family of sectional real-space groups can be obtained by selecting the superspace group from the list as described in §4.1.

5. Examples of application

Two representative examples of the application of the Superspace Group Finder are presented: the unified description of the $(TS)_nT$ subfamily of hexagonal ferrites and the solid solution $NiGe_{1-x}P_x$

5.1. Hexagonal ferrites

The $(TS)_nT$ subfamily of hexagonal ferrites is closely related to the Y ferrite with chemical composition $Ba_2M_2Fe_{12}O_{22}$ (*M* = Zn, Fe, Co, Mg and Mn) and space group $R\bar{3}m$. Its unit cell with *c* = 43.56 Å includes 18 oxygen layers and can be divided into three parts symmetrically related by the *R* centring. Each part can be described in terms of rigid T and S units extending over four and two oxygen layers, respectively. Experimentally observed structures involve extra T blocks on a periodic basis. Starting with an ideal (TS) stacking along the (001) direction, the extra T blocks can be seen as a stacking fault between two successive TS units. These TT faults occur in the reference sequence when one of the T blocks is not directly followed by an S block, but by an identical T block, which is then followed by the 'expected' S block. Electron microscopy and direct lattice imaging of known periodic ferrites show that these faults are distributed along the stacking sequence in the most uniform way, forming a uniform sequence (Pollert, 1985).

Symmetry considerations show that the superspace group for the $(TS)_nT$ subfamily should generate the space groups $R\bar{3}m$ in obverse and reverse setting and $P\bar{3}m1$ depending on the parity of the numerator and denominator of γ (Orlov *et al.*, 2007). The Superspace Group Finder database yields the superspace group $R\bar{3}m(00\gamma)$ as the only superspace group meeting this criterion. This superspace group leads to the reflection condition *hklm*: $h - k + l = 3m$, which – with the appropriate choice of the basic unit – enables the (3 + 1)-dimensional indexing of the observed diffraction pattern of each compound. The resulting superspace model takes into account the essential structural units, which also carry the magnetic properties, thus making a step toward embedding the physical properties of ferrites into the superspace.

5.2. $NiGe_{1-x}P_x$ solid solution: the 'missing' link between the MnP and NiP structure types

The (3 + 1)-dimensional incommensurately modulated structures of four members of the $NiGe_{1-x}P_x$ solid solution have been refined from X-ray powder diffraction data by Larsson *et al.* (2007). The

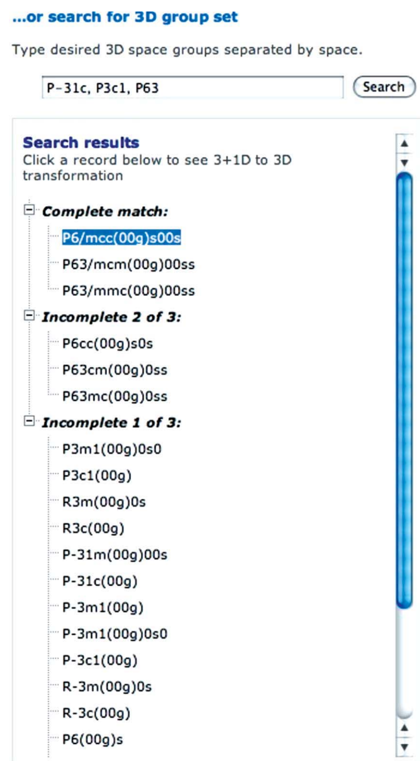

Figure 2
Search result: common superspace denominators for a three-dimensional group set.

underlying average structure is of NiAs type with the wavevector **q** = γ**c*** varying with composition.

Although the authors believe that γ never truly locks into an exact rational fraction M/N_3, the three-dimensional space-group symmetries derived for commensurate conditions are nonetheless important for considering the relationship between the $NiGe_{1-x}P_x$ solid solution and the structures of the end-members NiGe and NiP.

The structure adopts space-group symmetry $Pca2_1$ if *M* is odd and N_3 is even, as in the case of Ni_2GeP (γ = 3/4), $Ni_5Ge_3P_2$ (γ = 7/10) and the hypothetical compound NiP (γ = 1/2). On the other hand, if *M* and N_3 are both odd, as is the case for the other hypothetical end-member NiGe (γ = 1/1), then the reported space group is *Pnam.*

In this case, the Superspace Group Finder yields four possible parental superspace groups: *Pcam*(01/2γ), *Amam*(00γ)*s*00, *Aeam*(00γ)*s*00 and *Ibam*(00γ)*s*00. From this list only *Amam*(00γ)*s*00 (No. 63.6) satisfies the above conditions for the modulation vector (Table 3).

The result indicates that the solid solution, including the end-member NiGe and NiP structures, may be described in the superspace group *Amam*(00γ)*s*00. This result confirms the finding of Larsson *et al.* (2007) and provides a natural link between the two structure types NiGe (of MnP structure type) and NiP by using the commensurate options with γ = 1 and 1/2, respectively.

6. Conclusions

The present study is an extension of the scanning tables listed in Section 6 of the *International Tables for Crystallography* (2002, Vol. E). Whereas the complete listing of the (two-dimensional) sectional layer groups from the 230 space groups occupy roughly a quarter of the volume, the complete listing of the three-dimensional space groups resulting from hyper-sections of the (3 + 1)-dimensional superspace groups can only be presented in electronic form in view of the large amount of data. The relevance and usefulness of these tools for the crystal chemical description of modular or flexible structures has already been demonstrated in many examples of materials with interesting properties, including perovskites, ferrites, scheelites and many others.

The constructed database provides a vast ground for further investigations both in theoretical and in practical fields. We hope that the direct access made possible by the web interface will inspire other scientists to pursue studies on new families and strengthen our knowledge of structure–property relations.

The three-dimensional space groups were derived in the parental superspace group basis. As a result, some three-dimensional space groups appear in nonconventional settings. It is desirable to complete the database with the conventional settings of the space groups. This improvement will be the main direction of the future development of the database.

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