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Generation of (3 + *d*)-dimensional superspace groups for describing the symmetry of modulated crystalline structures

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A complete table of (3 + 1)D, (3 + 2)D and (3 + 3)D superspace groups (SSGs) has been enumerated that corrects omissions and duplicate entries in previous tables of superspace groups and Bravais classes. The theoretical methods employed are not new, though the implementation is both novel and robust. The paper also describes conventions for assigning a unique one-line symbol for each group in the table. Finally, a new online data repository is introduced that delivers more complete information about each SSG than has been presented previously.

1. Introduction

As CCD X-ray detectors have made it much easier to detect the presence of incommensurate modulations, crystallographic data-collection software packages have responded with excellent tools for indexing and integrating incommensurate satellite reflections. User-friendly tools for phase determination and structure refinement have also been extended to include modulated structures so that non-specialists can now deal effectively with incommensurate modulations. The result has been a steady increase in the number of modulated structures published each year.

The superspace formalism of de Wolff (1974) and Janner & Janssen (1977) has become the accepted standard for describing incommensurate structures involving displacive and compositional waves. Within this formalism, the translational symmetry lost by an otherwise periodic three-dimensional structure that experiences d integrally independent incommensurate modulation waves is restored upon embedding the structure in a higher $(3+d)$-dimensional [(3 + d)D] space. The symmetry groups that describe modulated structures within this space are restricted by, amongst other things, the requirement that their point operators not mix the three external dimensions with the d internal dimensions of the space, and are called superspace groups (SSGs) to distinguish them from the general higher-dimensional space groups. Because a modulated structure is periodic in superspace, its superspace symmetry can be classified according to $(3+d)$D Bravais classes. The same formalism and the same SSGs can also be used to describe structures of composite crystals.

The $(3+d)$D superspace Bravais classes for $d=1$, $d=2$ and $d=3$ were determined and classified by Janner *et al.* (1983), a work that we abbreviate here as JJdW, and are now tabulated in *International Tables of Crystallography*, Vol. C (Janssen *et al.*, 2004), which we abbreviate here as ITC-C. The $d=1$ SSGs were first determined by de Wolff *et al.* (1981) and corrected by Yamamoto *et al.* (1985). They are also tabulated in ITC-C, which includes the symbol, Bravais class, point group and reflection conditions of each group. The one-line SSG symbols in ITC-C are derived from the basic space-group symbols taken from *International Tables of Crystallography* Vol. A (2002), which we abbreviate here as ITC-A. The online database of Orlov & Chapuis (2005) further presents explicit symmetry operators for each of the $d=1$ SSGs. While not published in the scientific literature, the online database of Yamamoto (1996, 2005) is the most extensive to date, and includes tables of $d=1$, $d=2$ and $d=3$ SSGs. These tables include reflection conditions and group operators for each entry.

The present work is motivated by the need to correct errors discovered in earlier tables and to provide more complete information about the $d=2$ and $d=3$ SSGs. But in doing so, we aim to build upon the content and format of previous work. We have added entries to the tables which were omitted in previous work, and also eliminated many duplicate entries. Furthermore, we have explored the competing factors that influence the assignment of a unique one-line symbol to each $(3+d)$D SSG and established conventions for accomplishing this. These conventions govern the selection of a canonical generating set of SSG operators from which a unique symbol can be computed. Based on these results, we introduce a new online data repository of $d=1$, $d=2$ and $d=3$ SSG information (Stokes *et al.*, 2010).

For the reader's convenience, a list of abbreviations used in this paper is given in the Appendix.

2. Generation of superspace groups

The external three-dimensional part of each $(3+d)$D SSG G is called the basic space group (BSG) G_{3D} and corresponds to one of the 230 three-dimensional crystallographic space groups. Each SSG is also associated with d integrally independent modulations, each characterized by a modulation vector (q vector) in reciprocal space. The q vectors are specified by the Bravais class of the SSG. We begin by specifying the BSG G_{3D}. We then try each superspace Bravais class which is consistent with our choice of G_{3D}. For example, if G_{3D} = 55 *Pbam*, then we would try every superspace Bravais class where the three-dimensional part is P orthorhombic.

For orthorhombic groups, the permutations of the three principal axes often result in additional settings of the BSG relative to the modulation vectors (q vectors), which sometimes produce inequivalent SSGs. For example, we find that $Pbam(0,0,\gamma)000$ and $Pmcb(0,0,\gamma)000$ are distinct SSGs with Bravais class $Pmmm(0,0,\gamma)$ and BSG No. 55 *Pbam*. *Pmcb* turns out to be one of six possible permuted settings of *Pbam*. In the first case, the q vector is perpendicular to a mirror plane, and in the second case the q vector is perpendicular to a glide plane. For orthorhombic groups, all possible permutations of the axes of the BSG must be tried.

Each operator $g \in G$ can be written as an augmented $(4+d)\times(4+d)$ matrix:

$$A(g) = \begin{pmatrix} R & 0 & v \\ M & \varepsilon & \delta \\ 0 & 0 & 1 \end{pmatrix}. \qquad (1)$$

R is a 3×3 matrix and v is a three-dimensional column vector from the operator $\{R|v\} \in G_{3D}$. ε is an integer $d\times d$ matrix and M is an integer $d\times 3$ matrix which obeys the relation (ITC-C)

$$\sum_{i=1}^{3} q_{mi} R_{ij} = \sum_{n=1}^{d} \varepsilon_{mn} q_{nj} + M_{mj}, \qquad (2)$$

where q_{mi} is the ith component of the mth q vector in the Bravais class. δ is a d-dimensional column vector containing internal phase shifts associated with each of the q vectors, *i.e.* it represents the translations along the internal superspace dimensions. The values of R and v come from G_{3D} and are known. The values of M and ε are determined from equation (2) and by the choice of the relative orientation of G_{3D} and the Bravais class, and are therefore also known. Only the values of δ remain to be determined. Each self-consistent choice for the values of δ gives rise to an SSG.

We find it helpful to refer to a set of SSGs that differ only in the values of their δs (*i.e.* in their internal translations) as a variable internal translation (VIT) class. After preparing a list of the unique VIT classes, we solved the problem of determining the δ values for the different SSGs within each VIT class separately.

The possible choices for the values of δ are constrained by the group multiplication properties of G. Let us consider a set of 'representative' operators $\{g_1, g_2 \ldots g_n\}$ in G, where n is the order of the point group of G. In group-theoretical terms, these operators are the coset representatives with respect to the translation group of G. The product of two representative operators, g_a and g_b, is given by

$$\begin{pmatrix} R_a & 0 & v_a \\ M_a & \varepsilon_a & \delta_a \\ 0 & 0 & 1 \end{pmatrix}\begin{pmatrix} R_b & 0 & v_b \\ M_b & \varepsilon_b & \delta_b \\ 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} R_aR_b & 0 & R_av_b + v_a \\ M_aR_b + \varepsilon_a M_b & \varepsilon_a\varepsilon_b & M_av_b + \varepsilon_a\delta_b + \delta_a \\ 0 & 0 & 1 \end{pmatrix}. \qquad (3)$$

There must be some representative operator g_c such that

$$R_c = R_aR_b, \qquad (4)$$

$$\varepsilon_c = \varepsilon_a\varepsilon_b, \qquad (5)$$

$$M_c = M_aR_b + \varepsilon_a M_b, \qquad (6)$$

$$v_c = R_av_b + v_a \,(\mathrm{mod}\,1), \qquad (7)$$

$$\delta_c = M_av_b + \varepsilon_a\delta_b + \delta_a \,(\mathrm{mod}\,1). \qquad (8)$$

Equations (4)–(7) are automatically satisfied because of the group multiplication properties of G_{3D} and the use of equation (2) in constructing the representative operators. It is equation (8) that gives us constraints on the values allowed for each δ. Because there are n^2 pairs of operators, and each δ has d components, equation (8) provides n^2d linear equations containing nd unknowns.

Note that we must use a primitive setting of the SSG in this procedure, where all lattice translations are represented by integers, even those which are centering translations in the conventional BSG setting. The primitive setting is necessary so that the 'mod 1' in equations (7) and (8) includes all possible lattice translations.

Because of the potentially large number of unknowns, simultaneously solving equation (8) for the values of δ for all of the representative operators can be resource intensive in practice. In order to improve the efficiency to a practical level, we must first reduce the number of unknowns. Let us identify n_{gen} of the operators as generators, so that each of the operators can be obtained by various products of these generators. This implies that the δ of each representative operator can be written as a linear combination of the δs of the generators:

$$\delta_{ij} = B_{ij} + \sum_{k=1}^{n_{\mathrm{gen}}} \sum_{m=1}^{d} A_{ijkm}\delta_{km}, \qquad (9)$$

where δ_{ij} is the jth component of the δ of the ith operator. Note that we have ordered the representative operators so that the first n_{gen} operators are the generators. The sum is therefore over the components of δ in the generators.

One of the operators will be the identity. The components of its δ vector are zero, and the values of each of the A and B coefficients are also zero. The values of A, B are also trivially known for each of the generators. For $i \le n_{\mathrm{gen}}$, we have

$$B_{ij} = 0 \qquad (10)$$

and

$$A_{ijkm} = \begin{cases} 1 & \text{if } i = k \text{ and } j = m, \\ 0 & \text{otherwise.} \end{cases} \qquad (11)$$

Knowing the values of A and B for the generators and for the identity operator, we can then use group multiplication to obtain numeric values of A and B for each of the other operators. The order in which we generate the operators is not important. But once the operators have been generated, several facts become apparent. First, each operator gets generated n times within the group multiplication table, appearing once in each row and once in each column. Second, the combination of generators used to produce a given operator may be different for each of its instances within the multiplication table. This implies that there are n copies of equation (8) associated with a given operator (one for each column of the table), each of which may yield different values for A and B when that operator is expressed in terms of the generators. Equivalently, we can say that the multiplication table provides n distinct copies of equation (9), where the yth copy can be indicated by a superscript. Finally, though any two distinct copies of equation (9) may have different values of the A and B coefficients, they will have the same δ values, so that all of the constraints on the representative δs can be summarized as

$$\left[B_{ij}^{(y)} - B_{ij}^{(y+1)}\right] + \sum_{k=1}^{n_{\rm gen}} \sum_{m=1}^{d} \left[A_{ijkm}^{(y)} - A_{ijkm}^{(y+1)}\right] \delta_{km} = 0 \,(\mathrm{mod}\, 1) \qquad (12)$$

for $1 \le i \le n$, $1 \le j \le d$, $1 \le y \le n-1$.

This constitutes $n(n-1)d$ equations with $n_{\rm gen}d$ unknowns. Linear equations that involve (mod 1) equality can be solved in a straightforward manner using Smith normal forms (Grosse-Kunstleve, 1999). We obtain a finite number of solutions. From each solution, we then generate the representative operators of an SSG.

The solutions to these equations are generated to produce every possible SSG of a given VIT class at least once, but they also tend to produce multiple appearances of many SSGs. For this reason, it is necessary to have an effective means of testing two sets of SSG operators to determine whether they correspond to distinct SSGs or to different settings of the same group, in which case they are equivalent.

Two SSGs are equivalent if there exists an affine transformation matrix S of a specified form such that for every operator g in the first group, SgS^{-1} is an operator in the second group. For $(3+d)$D SSGs in a primitive setting, the transformation matrix must have the form

$$S = \begin{pmatrix} S_R & 0 & S_v \\ S_M & S_\varepsilon & S_\delta \\ 0 & 0 & 1 \end{pmatrix}, \qquad (13)$$

where S_R is a 3×3 matrix of integers, S_ε is a $d\times d$ matrix of integers, S_M is a $d\times 3$ matrix of integers, S_v is a three-dimensional column matrix of rational numbers, S_δ is a d-dimensional column matrix of rational numbers, $\det S_R = 1$ and $\det S_\varepsilon = 1$. If no such transformation exists, then the two SSGs are not equivalent. This required form of S is discussed in §3.5.2 of van Smaalen (2007) and is consistent with the definition of equivalence used by de Wolff *et al.* (1981).

We implemented a robust and efficient algorithm that searches for such a transformation between two $(3+d)$D SSGs. The details of our algorithm will be described elsewhere.

3. Tabulated superspace-group information

Upon tabulating all of the $(3+d)$D SSGs for $d = 1, 2, 3$, we found 775 groups for $d = 1$, 3338 groups for $d = 2$ and 12 584 groups for $d = 3$. Our $d = 1$ list agrees well with the comparable table in ITC-C.

We assigned a numerical identifier to each SSG, which consists of four numbers: (1) the BSG (1–230), (2) the value of d (1, 2, 3), (3) the Bravais class (1–24 for $d = 1$, 1–83 for $d = 2$ and 1–215 for $d = 3$), and (4) a number that enumerates the groups associated with each BSG. For $d = 1$, we number the SSGs in the same order as in ITC-C. For $d = 2, 3$, the SSGs are ordered by Bravais class within each BSG. Within each Bravais class the order is arbitrary. For example, 51.3.122.769 is the 769th $(3+3)$D SSG with BSG No. 51. Its Bravais class is 3.122.

The SSG symbol that we used consists of (1) a standard symbol for the BSG, (2) d q vectors, each within their own parentheses, and (3) symbols $(0, s = \frac{1}{2}, t = \frac{1}{3}, q = \frac{1}{4}, h = \frac{1}{6})$ following each q vector indicating the intrinsic (*i.e.* origin-independent) translations belonging to the internal coordinates of each generator. We elected to use the simple symbols $0, s, t, q, h$ found in ITC-C rather than the more complicated symbols m, g, d, a, b, c, n used by Yamamoto (1996, 2005) to denote specific operations in d-dimensional internal space. We also use $(\bar{t} = -\frac{1}{3}, \bar{q} = -\frac{1}{4}, \bar{h} = -\frac{1}{6})$ to denote negative translations (van Smaalen, 2007).

As an example, consider

$$54.2.29.32 \quad Pbcb(0, \beta_1, 0)000(0, 0, \gamma_2)s00.$$

The BSG is No. 54 *Pbcb* with its axes permuted from the usual *Pcca* setting. The two q vectors are $(0, \beta_1, 0)$ and $(0, 0, \gamma_2)$ and are associated with the internal coordinates t and u, respectively. The three generators denoted by the BSG symbol *Pbcb* are $(\bar{x}, y+\frac{1}{2}, z)$, $(x, \bar{y}, z+\frac{1}{2})$ and $(x, y+\frac{1}{2}, \bar{z}+\frac{1}{2})$. The corresponding generators of the SSG are $(\bar{x}, y+\frac{1}{2}, z, t, u+\frac{1}{2})$, $(x, \bar{y}, z+\frac{1}{2}, \bar{t}, u)$ and $(x, y+\frac{1}{2}, \bar{z}+\frac{1}{2}, t, \bar{u}+\frac{1}{2})$. All of the intrinsic translations associated with the t and u coordinates of these three generators are zero except for that of the u coordinate of the first generator, which is $\frac{1}{2}$, as denoted by the 's'.

Because the sheer number of unique $d = 1$, $d = 2$ and $d = 3$ SSGs is very large, and the data to be presented for each group are quite extensive, it is impractical to attempt to include these data as supplemental information, or even to archive them for

Table 1
Detailed information for SSG 44.3.128.51.

Superspace group	44.3.128.51 $I2mm(\alpha_1, \beta_1, 0)000(\overline{\alpha}_1, \beta_1, 0)000(0, 0, \gamma_2)0s0$ [Y: 3.3821]
Bravais class	3.128 $Immm(\alpha_1, \beta_1, 0)(\overline{\alpha}_1, \beta_1, 0)(0, 0, \gamma_2)$ [JJdW: 3.130]
Transformation to supercentered setting	$A_1 = a_1, A_2 = a_2, A_3 = a_3, A_4 = a_4 - a_5, A_5 = a_4 + a_5, A_6 = a_6$
Basic space-group setting	
Modulation vectors	$q_1 = (\alpha_1, \beta_1, 0), q_2 = (\overline{\alpha}_1, \beta_1, 0), q_3 = (0, 0, \gamma_2)$
Centering	$(0, 0, 0, 0, 0, 0), (\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, 0, 0, 0)$
Non-lattice generators	$(x, \overline{y}, \overline{z}, \overline{u}, \bar{t}, \overline{v}); (x, \overline{y}, z, \overline{u}, \bar{t}, v + \frac{1}{2}); (x, y, \overline{z}, t, u, \overline{v} + \frac{1}{2})$
Non-lattice operators	$(x, y, z, t, u, v); (x, \overline{y}, \overline{z}, \overline{u}, \bar{t}, \overline{v}); (x, \overline{y}, z, \overline{u}, \bar{t}, v + \frac{1}{2}); (x, y, \overline{z}, t, u, \overline{v} + \frac{1}{2})$
Supercentered setting	
Modulation vectors	$Q_1 = (A_1, 0, 0), Q_2 = (0, B_1, 0), Q_3 = (0, 0, \Gamma_2)$, where $A_1 = \alpha_1, B_1 = \beta_1, \Gamma_2 = \gamma_2$
Centering	$(0, 0, 0, 0, 0, 0), (\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, 0, 0, 0), (0, 0, 0, \frac{1}{2}, \frac{1}{2}, 0), (\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, 0)$
Non-lattice generators	$(X, \overline{Y}, \overline{Z}, T, \overline{U}, \overline{V}); (X, \overline{Y}, Z, T, \overline{U}, V + \frac{1}{2}); (X, Y, \overline{Z}, T, U, \overline{V} + \frac{1}{2})$
Non-lattice operators	$(X, Y, Z, T, U, V); (X, \overline{Y}, \overline{Z}, T, \overline{U}, \overline{V}); (X, \overline{Y}, Z, T, \overline{U}, V + \frac{1}{2}); (X, Y, \overline{Z}, T, U, \overline{V} + \frac{1}{2})$
Reflection conditions	$HKLMNP : M + N = 2n; HKLMNP : H + K + L = 2n; H0LM0P : P = 2n$

internet download. Instead, our approach has been to create an online software utility that accesses a minimal database of essential data, and then generates a more extensive set of information for a given group on demand. We also make the essential data for each group available online in ASCII (American standard code for information interchange) text form. We collectively refer to the essential data and the data-on-demand utility as the SSG(3 + d)D superspace-group tables (Stokes *et al.*, 2010).

At present, the SSG(3 + d)D tables can only be accessed *via* the internet using a web browser. The web interface allows one to download the complete database of essential SSG data. It also provides three ways to obtain detailed information about an SSG. (1) First, there is a page containing a long list of hyperlinks, one for each $d = 1$, $d = 2$ and $d = 3$ SSG. Following one of these links calls the data-on-demand utility and returns detailed information for the group selected. (2) One can also select a specific SSG by entering its identification number into a web form. (3) Finally, one can enter a list of the SSG operators (either the complete set or just the generators), which are then equivalence tested against any potential matching groups in the SSG(3 + d)D tables. If the operators obey a group multiplication table, they will match exactly one group in the tables. Detailed information is then presented for the matching group, along with the affine transformation matrix T that takes the group operators from the user-specified setting (*i.e.* the setting implied by the form of the operators provided) to the reference setting used in the tables. Thus, if g_u is an operator entered by the user, then the corresponding operator in the reference setting is $g_r = T \times g_u \times T^{-1}$.

While additional information may be added to the output of the data-on-demand utility in the future, it currently displays the following information for each SSG: (1*a*) the SSG number, (1*b*) the SSG label, (1*c*) a cross-reference to Yamamoto's tables when possible, (2*a*) the corresponding Bravais class symbol, (2*b*) a cross-reference to the JJdW Bravais-class tables when possible, (3) the number and label of the enantiomorphic SSG when applicable and (4) the transformation from the BSG setting to the conventional supercentered group (SCG) setting. It then presents (5*a*) the modulation vectors, (5*b*) the centering vectors, (5*c*) the group generators and (5*d*) the complete list of group operators in the BSG setting, followed by (6*a*) the modulation vectors, (6*b*) the centering vectors, (6*c*) the group generators, (6*d*) the complete list of group operators and (6*e*) a minimal but complete set of reflection conditions in the SCG setting.

Let us consider SSG 44.3.128.51 as an example. The detailed information is given in Table 1. The SSG number and symbol are followed by a cross-reference to group #3821 in Yamamoto's $d = 3$ SSG tables. When multiple entries in Yamamoto's tables turn out to be equivalent, we cross-reference all of them. In similar fashion, the Bravais-class number and symbol are followed by a cross-reference to the JJdW tables. Because our Bravais-class numberings only differ from those of JJdW for $d = 3$ classes, we only cross-reference the JJdW tables for $d = 3$ classes. When an SSG is missing from the cross-referenced table, the cross-reference is displayed as 'none'.

The BSG setting is the setting in which the external part of each operator has a form that matches the corresponding entry for the three-dimensional BSG in ITC-A, and where none of the centering translations include components along the internal coordinates. The SCG setting, on the other hand, eliminates any rational components in the q vectors and otherwise simplifies the forms of the q vectors, often giving rise to centering translations that include non-zero internal-coordinate components. SSG(3 + d)D uses lower-case letters for the BSG setting and upper-case letters for the SCG setting, as seen in Table 1. In the example in Table 1, observe that the supercentering transformation preserves the identities of a_1, a_2, a_3 and a_6, while mixing a_4 and a_5. This also simplifies the form of the modulation vectors, relative to their appearance in the SSG symbol, doubles the cell volume, and provides two new centering translations with non-zero internal-space components.

The SSG operators associated with the general Wyckoff orbit are presented in both the BSG setting and the SCG setting. The SSG generators in the BSG setting are selected so as to correspond precisely to the non-lattice generators of the BSG symbol as they appear in ITC-A. The lattice-translation generators are not listed here because they are obvious and trivial to obtain. In Table 1, *I*2*mm* denotes three generators:

(2) a twofold rotation about the *a* axis, (*m*) a reflection through the *ac* plane and (*m*) a reflection through the *ab* plane. The detailed form of the generators is useful when attempting to interpret the SSG symbol, and will be discussed in more detail below. Note that the ordering of the operator and generator lists is identical in both settings, so that applying the supercentering transformation to the *n*th operator or generator in the BSG setting produces the *n*th operator or generator in the SCG setting.

The list of reflection conditions includes both the centering translations of the Bravais class and any non-lattice translations associated with non-symmorphic group operators. The list of conditions displayed is always minimal, which means each condition listed will result in some extinctions that are not produced by any of the other conditions. The list is always complete too, in the sense that any additional reflection conditions that can be defined will fail to add new extinctions to the set of extinctions already produced by the conditions in the list. The list is not, however, unique, in the sense that one can usually find other distinct lists of reflection conditions that are both minimal and complete and which describe the same set of extinctions. The SSG(3 + *d*)D tables typically only express reflection conditions in the SCG setting. When the BSG and SCG settings are identical, however, no SCG data are presented in the SSG(3 + *d*)D tables. In such a case, the reflection conditions are described in the BSG setting.

4. Comparison with other tables

4.1. Bravais classes

Because our method of generating SSGs uses Bravais-class data as input, it was important to have a table of Bravais classes that was both accurate and complete. JJdW (Janner *et al.*, 1983) described and implemented a method for generating all Bravais classes of a $(3+d)$-dimensional superspace. When we implemented their method on computer, using our own algorithm for testing equivalence, we found the following errors in their tables.

(1) Two $d = 3$ Bravais classes were omitted by JJdW:
$P2/m(\alpha\beta 0, \frac{1}{2}0\nu, 0\frac{1}{2}\theta)$ (our 3.23)
$P2/m(\alpha\beta\frac{1}{2}, \frac{1}{2}0\nu, 0\frac{1}{2}\theta)$ (our 3.24).

(2) Four of the $d = 3$ Bravais classes presented by JJdW are equivalent to another class in their table. The equivalent pairs are as follows:
7 $P2/m(\frac{1}{2}0\gamma, 0\frac{1}{2}\nu, 00\theta)$ and 8 $P2/m(\frac{1}{2}0\gamma, 0\frac{1}{2}\nu, \frac{1}{2}0\theta)$
79 $Pmmm(\frac{1}{2}0\gamma, 0\mu\nu)$ and 83 $Pmmm(\frac{1}{2}0\gamma, \frac{1}{2}\mu\nu)$
82 $Pmmm(\frac{1}{2}\frac{1}{2}\gamma, 0\mu\nu)$ and 85 $Pmmm(\frac{1}{2}\frac{1}{2}\gamma, \frac{1}{2}\mu\nu)$
92 $Ammm(\frac{1}{2}0\gamma, 0\mu\nu)$ and 94 $Ammm(\frac{1}{2}0\gamma, \frac{1}{2}\mu\nu)$.

For each pair, the operators g_1 of the group on the left can be transformed into the operators g_2 of the group on the right by a similarity transform involving a $(3+d+1)$-dimensional affine transformation matrix S: $g_2 = S \times g_1 \times S^{-1}$. The affine transformations that relate these four class pairs are, respectively,

$$\begin{pmatrix} 1&0&0&0&0&0&0\\ 0&1&0&0&0&0&0\\ 0&0&1&0&0&0&0\\ 0&0&0&1&0&0&0\\ 0&0&0&0&1&0&0\\ -1&0&0&1&0&1&0\\ 0&0&0&0&0&0&1 \end{pmatrix}, \begin{pmatrix} 1&0&0&0&0&0&0\\ 0&1&0&0&0&0&0\\ 0&0&1&0&0&0&0\\ 0&0&0&1&0&0&0\\ -1&0&0&1&0&1&0\\ -1&0&0&1&1&0&0\\ 0&0&0&0&0&0&1 \end{pmatrix},$$

$$\begin{pmatrix} 1&0&0&0&0&0&0\\ 0&1&0&0&0&0&0\\ 0&0&1&0&0&0&0\\ 0&0&0&1&0&0&0\\ -1&-1&0&1&0&1&0\\ -1&0&0&1&1&0&0\\ 0&0&0&0&0&0&1 \end{pmatrix} \text{and} \begin{pmatrix} 1&0&0&0&0&0&0\\ 0&1&0&0&0&0&0\\ 0&0&1&0&0&0&0\\ 0&0&0&1&0&0&0\\ -1&0&0&1&0&1&0\\ -1&0&0&1&1&0&0\\ 0&0&0&0&0&0&1 \end{pmatrix}.$$

Because adding two new classes and removing four duplicate classes force a renumbering of the $d = 3$ table, we took this opportunity to further modify the class numbering so that classes with the same Q vectors in the SCG setting are grouped together in the table. In contrast, JJdW tended to group classes according to the appearance of their q vectors in the setting of the BSG. While neither Q-centric nor q-centric orderings conflict for any of the $d = 1$ or $d = 2$ classes, they do occasionally conflict for $d = 3$. For example, the Q vectors for JJdW class 162 $P4/mmm(\alpha 00, 00\gamma)$ are $(A, 0, 0)(0, 0, \Gamma)$, while the Q vectors for JJdW class 166 $P4/mmm(\alpha 00, \frac{1}{2}\frac{1}{2}\gamma)$ are $(A, A, 0)(0, 0, \Gamma)$. The q vectors of these groups appear to have the same form, but the Q vectors do not. JJdW's classes 162–165, 167, 169–170, 173–174, 177–179 share the form $(A, 0, 0)(0, 0, \Gamma)$, and classes 166, 168, 171–172, 175–176, 180–181 share the form $(A, A, 0)(0, 0, \Gamma)$, so that these two forms effectively get intermingled. We reordered these classes so that those with the first form of Q are consecutive followed by those with the second form of Q.

Our notation is similar to that of JJdW except that we specifically present all of the d q vectors and not just the generating q vectors. Also, we use subscripts on α, β, γ rather than employing additional symbols (*e.g.* $\lambda, \mu, \nu, \zeta, \eta, \theta$). For example, JJdW's 2.50 $Pmmm(0\beta\gamma)$ becomes $Pmmm(0, \beta, \gamma)(0, \overline{\beta}, \gamma)$, and JJdW's 2.18 $Pmmm(00\gamma, 00\nu)$ becomes $Pmmm(0, 0, \gamma_1)(0, 0, \gamma_2)$.

Our table of Bravais classes for $d = 1, 2, 3$ is provided in the SSG(3 + *d*)D tables. We list 24 classes for $d = 1$, 83 classes for $d = 2$ and 215 classes for $d = 3$. In addition to the class symbol, this table includes the transformation to the SCG setting, as well as the q vectors and centering translations in both the SCG and BSG settings.

4.2. Superspace groups

Comparison against the $(3+d)$D SSG tables $(d = 1, 2, 3)$ prepared by Yamamoto (1996, 2005) provided an opportunity to test the validity of our tables and the robustness of the tools that we used to generate them. Using our algorithm for determining whether two SSGs are equivalent, which uses the group operators as input, we attempted to identify each of the groups in Yamamoto's tables with groups in our table. This comparison showed good agreement with his $d = 1$ table which also matches the corresponding tables of Orlov & Chapuis (2005) and of ITC-C. However, we found that Yamamoto's $d = 2$ table is missing six SSGs:

6.2.3.4 $Pm(\alpha_1, \beta_1, \frac{1}{2})0(\alpha_2, \beta_2, 0)s$
13.2.5.4 $P2/a(0, 0, \gamma_1)s0(0, 0, \gamma_2)00$
14.2.5.2 $P2_1/a(0, 0, \gamma_1)00(0, 0, \gamma_2)00$
15.2.8.3 $B2/b(0, 0, \gamma_1)s0(0, 0, \gamma_2)00$
20.2.40.6 $C222_1(0, \beta_1, 0)0s0(0, 0, \gamma_2)000$
98.2.71.8 $I4_122(\alpha, \alpha, 1)000(\overline{\alpha}, \alpha, 1)00s$.

We also found that his table contains 59 pairs of SSGs that are equivalent, *e.g.* 299 $Pmm2(00p, 0\frac{1}{2}q).s0.s0.0$ and 300 $Pmm2(00p, 0\frac{1}{2}q).ss.s0.0s$.

For $d = 3$, we found that 2806 of the SSG entries in Yamamoto's table have operators listed that do not obey a multiplication table, *e.g.* 2351 $Pba2(\frac{1}{2}r + \frac{1}{2}p, q\frac{1}{2}p, q + \frac{1}{2}r0)d?s$. We could not identify those groups. For entries with valid operators, however, we were able to match each one to an SSG in our table. This allowed us to identify 611 pairs of group entries in Yamamoto's $d = 3$ table that proved to be equivalent. We do not list them here, though our SSG(3 + 1)D tables do cross-reference each group entry to all equivalent groups in Yamamoto's tables.

5. Superspace-group symbol

The intrinsic translation of a space-group (or superspace-group) operator is the origin-invariant part of the translational component of that operator. Let $\{R, v\}$ denote an operator which consists of a point operation R followed by a translation v. From §8.1.5 of ITC-A, or equation (9.8.3.5) of ITC-C, the intrinsic translation v_I of that operator is calculated as

$$v_I = \frac{1}{n}\left(\sum_{m=1}^{n} R^m\right)v, \qquad (14)$$

where n is the order of R, *i.e.* $R^n = 1$.

The traditional three-dimensional space-group symbols display the intrinsic translations for each of the non-lattice generators of a space group in order to distinguish among groups that correspond to the same symmorphic space group. Both screw axes and glide planes have non-zero intrinsic translations (mod 1). Screw axes are represented by adding a subscript to a rotation-axis generator symbol, and glide planes are represented by replacing a mirror-plane symbol ('*m*') with the corresponding glide symbol ('*a*', '*b*', '*c*', '*n*' or '*d*'). For space group No. 26 ($Pmc2_1$), the symbol contains three generators: a mirror reflection through (100), a *c* glide through (010) with an intrinsic translation along [001], and a 2_1 screw rotation about [001] also with an intrinsic translation along [001].

It is important to realize that the part of the space-group symbol corresponding to a given generator does not uniquely identify a specific symmetry operator of the space group, but rather identifies a class of operators (*e.g.* all of the *c*-glide planes perpendicular to the *b* axis). This many-to-one correspondence between generators and their symbols becomes problematic when generators of the same class fail to share the same intrinsic translation, a situation that causes a space group's identifying symbol to vary as a function of the generators selected, even while holding the space-group setting constant.

For this reason, a system of space-group symbols based on intrinsic translations does not generally deliver a unique symbol for each group. By exploring all of the possible sets of generators consistent with a given space-group symbol, one often obtains a variety of other symbols that can represent the same space group, a situation that we refer to as symbol 'ambiguity'. In some cases, one even encounters a single symbol or set of symbols that can correctly represent more than one space group, a situation that we refer to as symbol 'degeneracy'.

Space-group symbol ambiguity and degeneracy are most commonly observed in centered groups because a given generator can be combined with any centering translation to obtain an equivalent generator that may have a different intrinsic translation. As a classic example, consider the combination of the $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ body-centering translation with the three twofold rotation generators of space group No. 23 $I222$. One can either add or not add this translation to each of the three generators, resulting in $2^3 = 8$ possible combinations, eight different sets of intrinsic translations, and eight possible symbols for the group: $I222$, $I222_1$, $I22_12$, $I22_12_1$, $I2_122$, $I2_122_1$, $I2_12_12$, $I2_12_12_1$. Surprisingly, the same procedure applied to space group No. 24 $I2_12_12_1$ produces the same eight symbols. Thus, the traditional choice of $I222$ as the symbol for space group No. 23 and $I2_12_12_1$ as the symbol for space group No. 24 is not grounded purely on the intrinsic translations of their generators, but rather on other considerations. The only other pair of three-dimensional space groups which exhibits symbol degeneracy is $I23$ and $I2_13$.

Lattice translations can also contribute to symbol ambiguity. For example, space group No. 100 $P4bm$ has both mirror and glide planes parallel to the [110] directions. In the symbol, the third generator is a mirror reflection, though the symmetry operator listed in ITC-A is $(y + \frac{1}{2}, x + \frac{1}{2}, z)$, which has an intrinsic translation of $(\frac{1}{2}, \frac{1}{2}, 0)$ and is therefore actually a glide reflection. The operator $(y + \frac{1}{2}, x - \frac{1}{2}, z)$, on the other hand, has an intrinsic transition of (0, 0, 0), and is therefore a true mirror reflection. Because both operators generate the same group, $P4bm$ and $P4bg$ are both appropriate symbols. The use of $P4bm$ is simply a convention. Also recall that a generator symbol does not always uniquely specify the orientation of the associated generator. Depending on the lattice translation employed, the first '*m*' in No. 129 $P4/nmm$ indicates a class of operations that includes mirror planes normal to both the [100] and [010] directions, while the second '*m*' indicates a class of operations that includes both mirror planes and glide planes normal to both the [110] and $[1\overline{1}0]$ directions.

The (3 + 1)D SSG symbols in ITC-C, and their generalization in the SSG(3 + *d*)D tables, also rely on intrinsic translations in order to provide distinct symbols for distinct SSGs. For the 230 crystallographic space groups, symbol

Table 2
Choice of generators for crystallographic point-group symbols.

Symbol	Generators
422	$(\bar{y}, x, z), (x, \bar{y}, \bar{z}), (\bar{y}, \bar{x}, \bar{z})$
$4mm$	$(\bar{y}, x, z), (\bar{x}, y, z), (y, x, z)$
$\bar{4}2m$	$(y, \bar{x}, \bar{z}), (x, \bar{y}, \bar{z}), (y, x, z)$
$\bar{4}m2$	$(y, \bar{x}, \bar{z}), (\bar{x}, y, z), (\bar{y}, \bar{x}, \bar{z})$
$4/mmm$	$(\bar{y}, x, z), (x, y, \bar{z}), (\bar{x}, y, z), (y, x, z)$
312	$(\bar{y}, x-y, z), (x, y, z), (\bar{y}, \bar{x}, \bar{z})$
321	$(\bar{y}, x-y, z), (\bar{x}, \bar{x}+y, \bar{z}), (x, y, z)$
$3m1$	$(\bar{y}, x-y, z), (x, x-y, z), (x, y, z)$
$31m$	$(\bar{y}, x-y, z), (x, y, z), (y, x, z)$
622	$(x-y, x, z), (\bar{x}, \bar{x}+y, \bar{z}), (\bar{y}, \bar{x}, \bar{z})$
$6mm$	$(x-y, x, z), (x, x-y, z), (y, x, z)$
$\bar{6}m2$	$(\bar{x}+y, \bar{x}, \bar{z}), (x, x-y, z), (\bar{y}, \bar{x}, \bar{z})$
$\bar{6}2m$	$(\bar{x}+y, \bar{x}, \bar{z}), (\bar{x}, \bar{x}+y, \bar{z}), (y, x, z)$
$6/mmm$	$(x-y, x, z), (x, y, \bar{z}), (x, x-y, z), (y, x, z)$
23	$(\bar{x}, \bar{y}, z), (z, x, y)$
$m\bar{3}$	$(x, y, \bar{z}), (\bar{z}, \bar{x}, \bar{y})$
432	$(\bar{y}, x, z), (z, x, y), (\bar{y}, \bar{x}, \bar{z})$
$\bar{4}3m$	$(y, \bar{x}, \bar{z}), (z, x, y), (y, x, z)$
$m\bar{3}m$	$(x, y, \bar{z}), (\bar{z}, \bar{x}, \bar{y}), (y, x, z)$

ambiguity and degeneracy problems have been managed on a case-by-case basis *via* manually applied conventions. For (3 + d)D SSGs, however, problems of symbol ambiguity and degeneracy are greatly compounded and far too numerous for case-by-case consideration owing to the large number of rather complex lattice centerings available. In order to assign a unique and meaningful SSG symbol to each group in the SSG(3 + d)D tables, we found it necessary to establish strict systematic conventions for selecting the generators of each group. We describe these conventions below.

5.1. Generators of basic space group

(1) Because the intrinsic translation of a crystallographic non-lattice generator can be influenced by its orientation, we need a convention for choosing the orientation whenever the generator symbol permits more than one orientation. Table 2 lists all of the crystallographic point-group symbols that have orientational ambiguities, together with the generators that we have selected for each one. The generators listed for a given point group are listed in the same order as the generator symbols within the point-group symbol, so that the second '2' in 422 corresponds to $(\bar{y}, \bar{x}, \bar{z})$. While $(y, x, \bar{z})$ would also have been an appropriate generator for this symbol, we simply choose one orientation and apply it uniformly. In the case of SSG 90.1.19.1 $P42_12(0, 0, \gamma)000$, the generators in the SSG(3 + d)D tables are $(\bar{y}+\frac{1}{2}, x+\frac{1}{2}, z, t)$, $(x+\frac{1}{2}, \bar{y}+\frac{1}{2}, \bar{z}, \bar{t})$ and $(\bar{y}, \bar{x}, \bar{z}, \bar{t})$. Observe that the external non-translational part of each generator is taken directly from Table 2.

(2) In cases where ITC-A presents more than one setting for a BSG, the SSG(3 + d)D tables use the following setting conventions: monoclinic cell choice 1, hexagonal axes for trigonal groups and origin choice 2.

(3) The translational components of the external parts of the generators of an SSG must be selected so that the corresponding external intrinsic translations strictly match the BSG symbol in ITC-A. (This choice sometimes differs from the generators explicitly listed in ITC-A.) While these external translational components are usually chosen to be positive and less than 1, we often find it necessary to use equivalent translational components (*i.e.* related by a lattice translation) that lie outside this range in order to ensure that the generators operate in a way that exactly matches the BSG symbol. As mentioned above, the last generator of space-group symbol No. 100 $P4bm$ could either be the $(y+\frac{1}{2}, x+\frac{1}{2}, z)$ g glide or the $(y+\frac{1}{2}, x-\frac{1}{2}, z)$ mirror operation. Despite the fact that it includes a negative translational component, SSG(3 + d)D uses the mirror operation because its intrinsic translation strictly matches the 'm' in the space-group symbol. And though $(y+\frac{5}{2}, x+\frac{3}{2}, z)$ is an equivalent generating mirror plane, we chose $(y+\frac{1}{2}, x-\frac{1}{2}, z)$ so as to keep the absolute values of the translational components as small as possible while still matching the space-group symbol. As an example involving a centered lattice, the third generator of space-group No. 67 $Cmma$ is listed as $(x, y+\frac{1}{2}, \bar{z})$ in ITC-A, which is actually a b-glide operation. In order to strictly represent the symbol $Cmma$, we add centering translation $(\frac{1}{2}, \frac{1}{2}, 0)$ to $(x, y+\frac{1}{2}, \bar{z})$ to obtain $(x+\frac{1}{2}, y, \bar{z})$.

(4) The SSG(3 + d)D tables specify the transformation of the SSG from the BSG setting to the SCG setting for each Bravais class, and use this same transformation for every SSG that belongs to the same Bravais class.

5.2. Choice of internal intrinsic translations

While ITC-A is not generally concerned with the level of detail described above for three-dimensional space groups, these restrictions (or conventions) are needed for SSGs in order to reduce symbol ambiguity and degeneracy to a manageable level. However, even these BSG conventions still allow multiple lattice translations (conventional or centering translations) to be combined with a given generator, so that additional conventions involving the internal translations are required. The procedure that we followed has four steps.

Step 1. For the generators of a given SSG, identify every combination of lattice translations with those generators that produce a distinct set of internal intrinsic translations (IITs) in the SCG setting and create the corresponding SSG symbol for each one. While the set of lattice translations to be explored is infinite, the finite set of translations that actually needs to be tested on a generator $\{R|v\}$ is limited by the fact that adding the cyclic order n of R to any component of v does not affect v_I.

Step 2. Discard generator sets whose external intrinsic translations (EITs) in the BSG setting do not strictly match (mod 1) the symbol of the BSG. This step reduces both symbol ambiguity and symbol degeneracy.

Step 3. In cases where symbol degeneracy persists (*i.e.* a set of SSGs share the same candidate symbols), assign the 'nicest' symbol (see step 4 below) to the first SSG in the degenerate set. Then further restrict the lattice translations that can be combined with the generators of subsequent SSGs in the degenerate set by requiring that their EITs in the BSG setting be *exactly* identical (not just equivalent mod 1) to those of the

Table 3
Possible internal intrinsic translations for generators in 48.2.51.12 $Pnnn(\frac{1}{2}, \beta, \gamma)q0q(\frac{1}{2}, \overline{\beta}, \gamma)qq0$.

Original generator	Lattice translation	New generator	IIT	IIT symbols
$(\overline{X}, Y+\frac{1}{2}, Z+\frac{1}{2}, T+\frac{1}{4}, U+\frac{1}{4})$	$(0, 0, 0, 0, 0)$	$(\overline{X}, Y+\frac{1}{2}, Z+\frac{1}{2}, T+\frac{1}{4}, U+\frac{1}{4})$	$\frac{1}{4}, \frac{1}{4}$	q, q
	$(\frac{1}{2}, 0, 0, 0, \overline{\frac{1}{2}})$	$(\overline{X}+\frac{1}{2}, Y+\frac{1}{2}, Z+\frac{1}{2}, T+\frac{1}{4}, U-\frac{1}{4})$	$\frac{1}{4}, \overline{\frac{1}{4}}$	$q, \overline{q}$
	$(0, 0, 0, \overline{\frac{1}{2}}, \overline{\frac{1}{2}})$	$(\overline{X}, Y+\frac{1}{2}, Z+\frac{1}{2}, T-\frac{1}{4}, U-\frac{1}{4})$	$\overline{\frac{1}{4}}, \overline{\frac{1}{4}}$	$\overline{q}, \overline{q}$
	$(\frac{1}{2}, 0, 0, \overline{\frac{1}{2}}, 0)$	$(\overline{X}+\frac{1}{2}, Y+\frac{1}{2}, Z+\frac{1}{2}, T-\frac{1}{4}, U+\frac{1}{4})$	$\overline{\frac{1}{4}}, \frac{1}{4}$	$\overline{q}, q$
$(X+\frac{1}{4}, \overline{Y}, Z+\frac{1}{2}, \overline{T}, U+\frac{1}{4})$	$(0, 0, 0, 0, 0)$	$(X+\frac{1}{4}, \overline{Y}, Z+\frac{1}{2}, \overline{T}, U+\frac{1}{4})$	$0, \frac{1}{4}$	$0, q$
	$(\overline{\frac{1}{2}}, 0, 0, 0, \overline{\frac{1}{2}})$	$(X-\frac{1}{4}, \overline{Y}, Z+\frac{1}{2}, \overline{T}, U-\frac{1}{4})$	$0, \overline{\frac{1}{4}}$	$0, \overline{q}$
	$(0, 0, 0, \frac{1}{2}, \overline{\frac{1}{2}})$	$(X+\frac{1}{4}, \overline{Y}, Z+\frac{1}{2}, \overline{T}+\frac{1}{2}, U-\frac{1}{4})$	$0, \overline{\frac{1}{4}}$	$0, \overline{q}$
	$(\overline{\frac{1}{2}}, 0, 0, \frac{1}{2}, 0)$	$(X-\frac{1}{4}, \overline{Y}, Z+\frac{1}{2}, \overline{T}+\frac{1}{2}, U+\frac{1}{4})$	$0, \frac{1}{4}$	$0, q$
$(X+\frac{1}{4}, Y+\frac{1}{2}, \overline{Z}, T+\frac{1}{4}, \overline{U})$	$(0, 0, 0, 0, 0)$	$(X+\frac{1}{4}, Y+\frac{1}{2}, \overline{Z}, T+\frac{1}{4}, \overline{U})$	$\frac{1}{4}, 0$	$q, 0$
	$(\overline{\frac{1}{2}}, 0, 0, 0, \frac{1}{2})$	$(X-\frac{1}{4}, Y+\frac{1}{2}, \overline{Z}, T+\frac{1}{4}, \overline{U}+\frac{1}{2})$	$\frac{1}{4}, 0$	$q, 0$
	$(0, 0, 0, \overline{\frac{1}{2}}, \frac{1}{2})$	$(X+\frac{1}{4}, Y+\frac{1}{2}, \overline{Z}, T-\frac{1}{4}, \overline{U}+\frac{1}{2})$	$\overline{\frac{1}{4}}, 0$	$\overline{q}, 0$
	$(\overline{\frac{1}{2}}, 0, 0, \overline{\frac{1}{2}}, 0)$	$(X-\frac{1}{4}, Y+\frac{1}{2}, \overline{Z}, T-\frac{1}{4}, \overline{U})$	$\overline{\frac{1}{4}}, 0$	$\overline{q}, 0$

first SSG. This step usually lifts the degeneracy and further reduces symbol ambiguity.

Step 4. When residual symbol ambiguity exists after the application of the previous steps (*i.e.* an SSG still has more than one candidate symbol), use the symbol that has the 'nicest' appearance. We determine which symbols are nicest in our opinion by applying the following rules to the IITs, which are listed in order of priority: (*a*) minimum number of negative components; (*b*) maximum number of zero components; (*c*) minimum value of the maximum denominator among the components; (*d*) smallest denominators occur first; (*e*) smallest numerators occur first.

Because step 4 resolves symbol ambiguity by selecting the nicest-looking symbol available, a healthy level of residual ambiguity is generally helpful. Symbol ambiguity provides more candidate symbols to choose from and generally results in nicer-looking symbols. Step 3 is more restrictive than step 2, and is only applied where step 2 fails to lift a degeneracy. If we eliminate step 3, we encounter many hundreds of instances of symbol degeneracy, the most severe example being ten SSGs that share identical candidate symbols. If we entirely replace step 2 with the more restrictive step 3, residual symbol ambiguity is so greatly reduced that step 4 produces symbols that are unnecessarily complicated. The use of step 2, followed by the conditional application of step 3, is a practical compromise that comes close to eliminating symbol degeneracy altogether, while also delivering symbols with reasonably simple IITs. The handful of residual degeneracies that survive this process are treated manually in Example 4 below.

An important oddity of these SSG symbols is that the q vectors are displayed in the BSG setting while the internal translations are displayed in the SCG setting. It is important to display the q vectors in the BSG setting because the symbol is based primarily on the BSG symbol itself. If we were to display the Q vectors in the SCG setting instead, we would need to replace the BSG symbol with a unique supercentered lattice-type name (16 types for $d = 1$, 44 types for $d = 2$ and 119 types for $d = 3$), which would be impractical. Furthermore, the intrinsic translations that arise in the BSG setting when a complicated supercentered lattice is present tend to be unintuitive and are subject to additional ambiguities. The IITs in the SCG setting are much more desirable as symbol elements, despite the fact that our conventions for restricting them must be applied in the BSG setting. It is readily apparent that these same issues were carefully considered when the (3 + 1)D one-line symbols in ITC-C were formulated.

5.2.1. Example 1. 48.2.51.12 $Pnnn(\frac{1}{2}, \beta, \gamma)q0q(\frac{1}{2}, \overline{\beta}, \gamma)qq0$. The generators in the SCG setting are $(\overline{X}, Y+\frac{1}{2}, Z+\frac{1}{2}, T+\frac{1}{4}, U+\frac{1}{4})$, $(X+\frac{1}{4}, \overline{Y}, Z+\frac{1}{2}, \overline{T}, U+\frac{1}{4})$ and $(X+\frac{1}{4}, Y+\frac{1}{2}, \overline{Z}, T+\frac{1}{4}, \overline{U})$. There are four centering translations for this Bravais class. In Table 3, we list the possible IITs that we found for each generator. Note that although two of the centering translations change the EITs in the SCG setting of the second and third generators, they do not change the EITs in the BSG setting of those generators and are therefore allowed. Based on four symbol sets for the first generator and two unique symbol sets for the second and third generators, we have 16 possible symbols for this SSG. Of these, the nicest-looking one is the one without any minus signs.

5.2.2. Example 2. 100.2.68.12 $P4bm(\alpha, \alpha, 0)00s(\overline{\alpha}, \alpha, 0)000$. In this case, though there are no centering translations (thus no distinction between the BSG setting and the SCG setting), we can still obtain different symbols by applying integer lattice translations to the generators. Table 4 shows the intrinsic translations associated with the group generators, including multiple outcomes associated with different lattice translations.

In this case, the two distinct intrinsic translations associated with the second generator lead to two possible symbols: $P4bm(\alpha, \alpha, 0)00s(\overline{\alpha}, \alpha, 0)000$ and $P4bm(\alpha, \alpha, 0)0ss(\overline{\alpha}, \alpha, 0)0s0$. We choose the symbol with the greatest number of zeros.

5.2.3. Example 3. 47.2.36.60 $Pmmm(\frac{1}{2}, \beta_1, \frac{1}{2})000(\frac{1}{2}, 0, \gamma_2)000$ is the first of four groups in its VIT class. For the sake of brevity, let us just consider its first generator, which is $(\overline{x}, y, z, \overline{x}+t, \overline{x}+u)$ in the BSG setting and $(\overline{X}, Y, Z, T, U)$ in the SCG setting, where there are four centering translations: $(0, 0, 0, 0, 0)$, $(\frac{1}{2}, 0, 0, \frac{1}{2}, \frac{1}{2})$, $(0, 0, \frac{1}{2}, \frac{1}{2}, 0)$ and $(\frac{1}{2}, 0, \frac{1}{2}, 0, \frac{1}{2})$. Table 5 shows the intrinsic translation of the first group generator in the SCG setting when combined with each of these centering translations.

Note that although the last two centering translations actually change the EITs in the SCG setting, they do not affect

Table 4
Possible intrinsic translations for generators in 100.2.68.12 $P4bm(\alpha, \alpha, 0)00s(\overline{\alpha}, \alpha, 0)000$.

Original generator	Lattice translation	New generator	IIT	IIT symbols
$(\overline{y}, x, z, \overline{u}, t)$	$(0, 0, 0, 0, 0)$	$(\overline{y}, x, z, \overline{u}, t)$	$0, 0$	$0, 0$
$(\overline{x}+\frac{1}{2}, y+\frac{1}{2}, z, u+\frac{1}{2}, t+\frac{1}{2})$	$(0, 0, 0, 0, 0)$	$(\overline{x}+\frac{1}{2}, y+\frac{1}{2}, z, u+\frac{1}{2}, t+\frac{1}{2})$	$\frac{1}{2}, \frac{1}{2}$	s, s
	$(0, 0, 0, 0, \overline{1})$	$(\overline{x}+\frac{1}{2}, y+\frac{1}{2}, z, u+\frac{1}{2}, t-\frac{1}{2})$	$0, 0$	$0, 0$
$(y+\frac{1}{2}, x-\frac{1}{2}, z, t+\frac{1}{2}, \overline{u}+\frac{1}{2})$	$(0, 0, 0, 0, 0)$	$(y+\frac{1}{2}, x-\frac{1}{2}, z, t+\frac{1}{2}, \overline{u}+\frac{1}{2})$	$\frac{1}{2}, 0$	$s, 0$

Table 5
Possible intrinsic translations for the first generator in 47.2.36.60 $Pmmm(\frac{1}{2}, \beta_1, \frac{1}{2})000(\frac{1}{2}, 0, \gamma_2)000$.

Lattice translation SCG setting	New generator SCG setting	New generator BSG setting	IIT SCG setting	IIT symbol
$(0, 0, 0, 0, 0, 0)$	$(\overline{X}, Y, Z, T, U)$	$(\overline{x}, y, z, \overline{x}+t, \overline{x}+u)$	$0, 0$	$0, 0$
$(\frac{1}{2}, 0, 0, \frac{1}{2}, \frac{1}{2})$	$(\overline{X}+\frac{1}{2}, Y, Z, T+\frac{1}{2}, U+\frac{1}{2})$	$(\overline{x}+1, \overline{y}, z, \overline{x}+t+1, \overline{x}+u+1)$	$\frac{1}{2}, \frac{1}{2}$	s, s
$(0, 0, \frac{1}{2}, \frac{1}{2}, 0)$	$(\overline{X}, Y, Z+\frac{1}{2}, T+\frac{1}{2}, U)$	$(\overline{x}, y, z+1, \overline{x}+t+1, \overline{x}+u)$	$\frac{1}{2}, 0$	$s, 0$
$(\frac{1}{2}, 0, \frac{1}{2}, 0, \frac{1}{2})$	$(\overline{X}+\frac{1}{2}, Y, Z+\frac{1}{2}, T, U+\frac{1}{2})$	$(\overline{x}+1, y, z+1, \overline{x}+t+1, \overline{x}+u+1)$	$0, \frac{1}{2}$	$0, s$

Table 6
Possible intrinsic translations for generators in 16.3.137.108 $P222(0, \beta, \gamma)000(\alpha, 0, \gamma)000(\alpha, \beta, 0)000$.

Original generator	Lattice translation	New generator	IIT	IIT symbols
$(X, \overline{Y}, \overline{Z}, T, \overline{U}, \overline{V})$	$(0, 0, 0, 0, 0, 0)$	$(X, \overline{Y}, \overline{Z}, T, \overline{U}, \overline{V})$	$0, 0, 0$	$0, 0, 0$
	$(0, 0, 0, \frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	$(X, \overline{Y}, \overline{Z}, T+\frac{1}{2}, \overline{U}+\frac{1}{2}, \overline{V}+\frac{1}{2})$	$\frac{1}{2}, 0, 0$	$s, 0, 0$
$(\overline{X}, Y, \overline{Z}, \overline{T}, U, \overline{V})$	$(0, 0, 0, 0, 0, 0)$	$(\overline{X}, Y, \overline{Z}, \overline{T}, U, \overline{V})$	$0, 0, 0$	$0, 0, 0$
	$(0, 0, 0, \frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	$(\overline{X}, Y, \overline{Z}, \overline{T}+\frac{1}{2}, U+\frac{1}{2}, \overline{V}+\frac{1}{2})$	$0, \frac{1}{2}, 0$	$0, s, 0$
$(\overline{X}, \overline{Y}, Z, \overline{T}, \overline{U}, V)$	$(0, 0, 0, 0, 0, 0)$	$(\overline{X}, \overline{Y}, Z, \overline{T}, \overline{U}, V)$	$0, 0, 0$	$0, 0, 0$
	$(0, 0, 0, \frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	$(\overline{X}, \overline{Y}, Z, \overline{T}+\frac{1}{2}, \overline{U}+\frac{1}{2}, V+\frac{1}{2})$	$0, 0, \frac{1}{2}$	$0, 0, s$

Table 7
Possible intrinsic translations for generators in 16.3.137.109 $P222(0, \beta, \gamma)000(\alpha, 0, \gamma)000(\alpha, \beta, 0)00s$.

Original generator	Lattice translation	New generator	IIT	IIT symbols
$(X, \overline{Y}, \overline{Z}, T, \overline{U}+\frac{1}{2}, \overline{V})$	$(0, 0, 0, 0, 0, 0)$	$(X, \overline{Y}, \overline{Z}, T, \overline{U}+\frac{1}{2}, \overline{V})$	$0, 0, 0$	$0, 0, 0$
	$(0, 0, 0, \frac{1}{2}, \frac{\overline{1}}{2}, \frac{1}{2})$	$(X, \overline{Y}, \overline{Z}, T+\frac{1}{2}, \overline{U}, \overline{V}+\frac{1}{2})$	$\frac{1}{2}, 0, 0$	$s, 0, 0$
$(\overline{X}, Y, \overline{Z}, \overline{T}, U, \overline{V}+\frac{1}{2})$	$(0, 0, 0, 0, 0, 0)$	$(\overline{X}, Y, \overline{Z}, \overline{T}, U, \overline{V}+\frac{1}{2})$	$0, 0, 0$	$0, 0, 0$
	$(0, 0, 0, \frac{1}{2}, \frac{1}{2}, \frac{\overline{1}}{2})$	$(\overline{X}, Y, \overline{Z}, \overline{T}+\frac{1}{2}, U+\frac{1}{2}, \overline{V})$	$0, \frac{1}{2}, 0$	$0, s, 0$
$(\overline{X}, \overline{Y}, Z, \overline{T}+\frac{1}{2}, \overline{U}, V)$	$(0, 0, 0, 0, 0, 0)$	$(\overline{X}, \overline{Y}, Z, \overline{T}+\frac{1}{2}, \overline{U}, V)$	$0, 0, 0$	$0, 0, 0$
	$(0, 0, 0, \frac{\overline{1}}{2}, \frac{1}{2}, \frac{1}{2})$	$(\overline{X}, \overline{Y}, Z, \overline{T}, \overline{U}+\frac{1}{2}, V+\frac{1}{2})$	$0, 0, \frac{1}{2}$	$0, 0, s$

the EITs (mod 1) in the BSG setting. So we are allowed to consider them because they still agree with the BSG symbol. While we would like to assign the nicest symbol, which is the one with the greatest number of zeros, the other three members of the VIT class turn out to share the same set of candidate symbols. We refer to these four groups as a symbol-degenerate set. Our procedure requires that we assign the nicest symbol to the first group in the set, and then further restrict the translations that can be combined with the generators of the other groups in the set to include only those translations that have all-zero external components. The only translation that fits this requirement is (0, 0, 0, 0, 0), so that the other three groups now have only one possible symbol. This procedure lifts the symbol degeneracy and results in the following symbols:

47.2.36.60 $Pmmm(\frac{1}{2}, \beta_1, \frac{1}{2})000(\frac{1}{2}, 0, \gamma_2)000$
47.2.36.61 $Pmmm(\frac{1}{2}, \beta_1, \frac{1}{2})000(\frac{1}{2}, 0, \gamma_2)0s0$
47.2.36.62 $Pmmm(\frac{1}{2}, \beta_1, \frac{1}{2})000(\frac{1}{2}, 0, \gamma_2)s00$
47.2.36.63 $Pmmm(\frac{1}{2}, \beta_1, \frac{1}{2})000(\frac{1}{2}, 0, \gamma_2)ss0$.

In general, a single VIT class can contain a combination of multiple non-degenerate groups and symbol-degenerate sets of groups. This case was simple in that the entire VIT class comprised one symbol-degenerate set.

5.2.4. Example 4.

16.3.137.108 $P222(0, \beta, \gamma)000(\alpha, 0, \gamma)000(\alpha, \beta, 0)000$

and

16.3.137.109 $P222(0, \beta, \gamma)000(\alpha, 0, \gamma)000(\alpha, \beta, 0)00s$

belong to a Bravais class with two centering translations: (0, 0, 0, 0, 0, 0) and $(0, 0, 0, \frac{1}{2}, \frac{1}{2}, \frac{1}{2})$. Tables 6 and 7 show the intrinsic translations of the generators of both groups when combined with each of these centering translations.

Table 8
Pairs of SSGs that exhibit residual twofold symbol degeneracy.

16.3.137.108 *P*222(0, *b*, *g*)000(*a*, 0, *g*)000(*a*, *b*, 0)000	16.3.137.109 *P*222(0, *b*, *g*)000(*a*, 0, *g*)000(*a*, *b*, 0)00*s*
21.3.142.105 *C*222(0, *b*, *g*)000(*a*, 0, *g*)000(*a*, *b*, 0)000	21.3.142.106 *C*222(0, *b*, *g*)000(*a*, 0, *g*)000(*a*, *b*, 0)00*s*
22.3.144.37 *F*222(0, *b*, *g*)000(*a*, 0, *g*)000(*a*, *b*, 0)000	22.3.144.38 *F*222(0, *b*, *g*)000(*a*, 0, *g*)000(*a*, *b*, 0)00*s*
23.3.141.15 *I*222(0, *b*, *g*)000(*a*, 0, *g*)000(*a*, *b*, 0)000	23.3.141.16 *I*222(0, *b*, *g*)000(*a*, 0, *g*)000(*a*, *b*, 0)00*s*
195.3.210.7 *P*23(0, *b*, *b*)00(*b*, 0, *b*)00(*b*, *b*, 0)00	195.3.210.8 *P*23(0, *b*, *b*)00(*b*, 0, *b*)00(*b*, *b*, 0)*s*0
196.3.212.5 *F*23(0, *b*, *b*)00(*b*, 0, *b*)00(*b*, *b*, 0)00	196.3.212.6 *F*23(0, *b*, *b*)00(*b*, 0, *b*)00(*b*, *b*, 0)*s*0
197.3.211.3 *I*23(0, *b*, *b*)00(*b*, 0, *b*)00(*b*, *b*, 0)00	197.3.211.4 *I*23(0, *b*, *b*)00(*b*, 0, *b*)00(*b*, *b*, 0)*s*0

Table 9
SSGs for which the symbol that follows from our conventions is different from the corresponding ITC-C symbol.

Group	ITC-C symbol	Symbol using our conventions
35.1.14.5	$Cmm2(1, 0, \gamma)s0s$	$Cmm2(1, 0, \gamma)s00$
36.1.14.4	$Cmc2_1(1, 0, \gamma)s0s$	$Cmc2_1(1, 0, \gamma)s00$
37.1.14.4	$Ccc2(1, 0, \gamma)s0s$	$Ccc2(1, 0, \gamma)s00$
42.1.18.5	$Fmm2(1, 0, \gamma)s0s$	$Fmm2(1, 0, \gamma)s00$
99.1.20.6	$P4mm(\frac{1}{2}, \frac{1}{2}, \gamma)0ss$	$P4mm(\frac{1}{2}, \frac{1}{2}, \gamma)00s$
101.1.20.4	$P4_2cm(\frac{1}{2}, \frac{1}{2}, \gamma)0ss$	$P4_2cm(\frac{1}{2}, \frac{1}{2}, \gamma)00s$
104.1.20.3	$P4nc(\frac{1}{2}, \frac{1}{2}, \gamma)qq0$	$P4nc(\frac{1}{2}, \frac{1}{2}, \gamma)qqs$
106.1.20.3	$P4_2bc(\frac{1}{2}, \frac{1}{2}, \gamma)qq0$	$P4_2bc(\frac{1}{2}, \frac{1}{2}, \gamma)qqs$
123.1.20.6	$P4/mmm(\frac{1}{2}, \frac{1}{2}, \gamma)00ss$	$P4/mmm(\frac{1}{2}, \frac{1}{2}, \gamma)000s$
126.1.20.3	$P4/nnc(\frac{1}{2}, \frac{1}{2}, \gamma)q0q0$	$P4/nnc(\frac{1}{2}, \frac{1}{2}, \gamma)q0qs$
132.1.20.4	$P4_2/mcm(\frac{1}{2}, \frac{1}{2}, \gamma)00ss$	$P4_2/mcm(\frac{1}{2}, \frac{1}{2}, \gamma)000s$

Observe that, in this case, both centering translations have all-zero external components, so that we still obtain the same set of candidate symbols for each group. Thus, our conventions do not entirely prevent SSG symbol degeneracy. However, instances of residual degeneracy prove to be very rare and are easily resolved by manually assigning appropriate generators. In this case, the symmorphic group 16.3.137.108 clearly has a greater claim on the symbol with all-zero translations. For 16.3.137.109, we simply choose the next-nicest symbol, which happens to include one '*s*'. In total, there are seven pairs of groups (listed in Table 8) that exhibit residual twofold symbol degeneracy. In each case, one of the groups is symmorphic and receives the symbol with no translational components, while the other group gets the next-nicest symbol available. It is interesting that the three-dimensional internal part of each of these (3 + 3)D SSGs is identical to one of $I222$, $I2_12_12_1$, $I23$ or $I2_13$.

5.2.5. Comparison against (3 + 1)D symbols in ITC-C. There are only 11 SSGs for which the symbol that follows from our conventions as described above is different from the corresponding ITC-C symbol. These cases are listed in Table 9. For eight of these SSGs, our method found a 'nicer' symbol. For the remaining three SSGs, our method could not obtain the symbol in ITC-C without using EITs that did not strictly match the symbol of the BSG.

We do not want to advocate changing the (3 + 1)D symbols established in ITC-C. Therefore, we propose to continue using those symbols, and not the new symbols generated by our method.

5.2.6. Internal-space origin. Because we are concerned about the impact that the detailed form of the generators has on the SSG symbol, the SSG(3 + d)D tables list the generators used to obtain the preferred symbol explicitly. In order to make these generators (and group operators) more meaningful, we have established a procedure for uniquely specifying the origin of each SSG. The origin affects the total translational components of each operator, but not their intrinsic translations. We already set the external-space origin of each SSG to match that of the conventional setting of the corresponding BSG in ITC-A. Only the internal-space origin needs to be addressed here. We set the d-dimensional internal-space origin of a (3 + d)D SSG as follows:

(1) Beginning with group operators that have been defined relative to an arbitrary internal-space origin in the SCG setting, first isolate the internal-space portions of each of the operators in the SCG setting, including the centering translations. For $d = 1$ or $d = 2$ groups, further extend each operator to three dimensions by adding extra rows and columns with unity on diagonal and zeros off diagonal. The resulting group of operators must be equivalent to one of the 230 crystallographic space groups.

(2) Find the affine transformation that takes these operators into the conventional setting of the corresponding three-dimensional group in ITC-A, and decompose this transformation into two sequential operations: an origin shift followed by a point operation. Then extract the d-dimensional part of this three-dimensional origin shift and apply it to the internal-space portions of each of the original SSG operators.

(3) If the BSG is centrosymmetric, apply an additional internal-space origin shift to each of the operators (if necessary) in order to place the inversion at the origin of the internal space. This internal-space convention is analogous to the external-space preference for origin choice 2.

In the future, the crystallographic community may eventually converge on a more elegant way to select the internal-space origin. Our origin-selection procedure is straightforward and meets an immediate need, but cannot be extended to superspace dimensions higher than 3 + 3.

6. Conclusions

Our Bravais-class tables are in agreement with those of JJdW for $d = 1$ and $d = 2$. Our $d = 3$ table of Bravais classes, however, corrects omissions and duplicate classes in the corresponding table in JJdW, which also led us to renumber and partially reorder this table. Our $d = 1$ table of SSGs agrees well with those of Orlov & Chapuis, Yamamoto and ITC-C. We have exhaustively corrected omissions and duplicate entries in Yamamoto's $d = 2$ table, and also corrected many duplicate entries in Yamamoto's $d = 3$ SSG table. The $d = 3$ comparison was limited by the fact the operators of some of Yamamoto's $d = 3$ groups do not obey a multiplication table.

For $d > 1$, we employed SSG symbols that are a direct extension of the $d = 1$ one-line symbols in ITC-C, and therefore include the three-dimensional basic space-group symbol and the modulation vectors in the BSG setting, as well as the IITs of the generators in the SCG setting. If specific labels were assigned to each of the many (3 + d)D supercentered lattice types, one could alternatively define a new type of symbol based only on the SCG setting, analogous to the three-dimensional space-group symbols in ITC-A. But the number of lattice types increases rapidly with internal dimension, making this approach impractical. We felt it best to directly extend the one-line symbols of ITC-C, despite the fact that they must be interpreted using two different settings (BSG and SCG).

Because the IITs in the SSG symbol vary according to the specific form of the group generators used, we applied a system of conventions that algorithmically determines a unique set of canonical generators, and hence a unique symbol, for each group. We resolve symbol ambiguity by choosing the nicest-looking symbol available to a given group (*i.e.* nicest set of SCG IITs). Thus, increased ambiguity provides more candidate symbols to choose from and generally results in a nicer symbol. However, increased ambiguity goes hand in hand with increased symbol degeneracy, which is generally unacceptable. After exploring the consequences of a variety of different approaches, we selected the current conventions because they were easy to apply and also provided a reasonable compromise between the competing need to reduce symbol degeneracy and improve symbol appearance. The restrictions that we imposed on the BSG EITs eliminated symbol degeneracies for all but seven pairs of SSGs, where we then selected the SCG IITs manually.

A new online data repository called SSG(3 + d)D contains a wealth of new information about each of the $d = 1$, $d = 2$ and $d = 3$ groups, including the SSG symbol, cross-references to other SSG tables, an explicit description of the transformation between the BSG and SCG settings, a list of enantiomorphic groups if any, and a minimal list of independent reflection conditions. It also includes lists of canonical generators, complete lists of group operators, and lists of centering translations for both the BSG and SCG settings of each SSG.

APPENDIX *A*

The following is a list of abbreviations used in this paper:

SSG(3 + d)D, online data at http://stokes.byu.edu/ssg.html
BSG, basic space group
BSG setting, basic space-group setting of a superspace group
EIT, external intrinsic translation
IIT, internal intrinsic translation
ITC-A and ITC-C, *International Tables for Crystallography*, Vols. A and C, respectively
JJdW, Janner, Janssen & de Wolf (1983)
SCG setting, supercentered group setting of a superspace group
SSG, superspace group
VIT class, variable internal translation class.

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