Algorithms for deriving crystallographic space-group information II: Treatment of special positions

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Synopsis

Algorithms for the treatment of special positions in 3-dimensional crystallographic space groups are presented.

Abstract

Algorithms for the treatment of special positions in 3-dimensional crystallographic space groups are presented. These include an algorithm for the determination of the site-symmetry group given the coordinates of a point, an algorithm for the determination of the exact location of the nearest special position, an algorithm for the assignment of a Wyckoff letter given the site-symmetry group, and an alternative algorithm for the assignment of a Wyckoff letter given the coordinates of a point directly. All algorithms are implemented in ISO C++ and are integrated into the Computational Crystallography Toolbox. The source code is freely available.

Note to the printer:

Please replace $\underline{Z}$, $\underline{Q}$ and $\underline{R}$ by the standard symbols for integer and rational numbers, respectively.

1. Introduction

When space group symmetry is used in the description of crystal structures, the problem of how to treat atomic sites in special positions arises. By definition (Hahn, 1983, section 2.11), a point in a special position is one that is mapped onto itself by symmetry. This leads to the notion of the *multiplicity* of a point, which is defined as the number of distinct equivalent points per unit cell. If a point is not mapped onto itself by any of the symmetry operations of the given space group, the point is said to be in a *general position*, and the multiplicity is equal to the order of the space group. For a point in a special position, the multiplicity is a factor of the order of the space group. This follows from Lagrange's theorem because the symmetry operations that map a point onto itself form a point group, the *site-symmetry group*, which is a sub-group of the space group.

To determine the multiplicity of a point, the symmetry operations are applied to the coordinates of the point. For each symmetrically equivalent point, the distance to the original point is computed. Since the atomic coordinates are real numbers, these calculations are universally implemented with floating-point arithmetic. To compensate for the rounding errors that are inevitably associated with floating-point arithmetic, a tolerance has to be admitted when determining if a point is mapped onto itself by a given symmetry operation. Necessarily, this tolerance must be very small. Otherwise the results of subsequent calculations, such as structure factor calculations, would significantly violate the space group symmetry.

If the determination of the multiplicity of a point is exclusively based on floating-point distance calculations, it is unfortunately impossible to devise a numerically stable algorithm. Due to the inevitable rounding errors, it may happen that one symmetrically equivalent point is just within the chosen tolerance, and another one just outside. Consequently, the multiplicity of the point will not be computed correctly, and results of subsequent calculations will be incorrect.

A simple method for ruling out incorrectly determined multiplicities is to define an exclusion radius, and to raise an exception if a symmetrically equivalent point is within this radius around the original point, but not within the tolerance. At least, this approach does not silently lead to incorrect results, but manual intervention is required if a problem is detected.

If a point is close to a special position but outside a meaningful tolerance, in some contexts (e.g. Grosse-Kunstleve et al., 1997) it is necessary to determine the exact location of the nearest special position. An obvious approach is to determine this location by averaging all symmetrically equivalent points that are within a given radius around the original point. However, the rounding errors associated with floating point arithmetic pose the same problem as discussed above: one equivalent point may just be inside and another one just outside the chosen radius. This may lead to an incomplete group of symmetrically equivalent points (corresponding to an incorrectly determined multiplicity), and the average of the coordinates of such an incomplete group will result in incorrect coordinates for the exact location of the nearest special position.

The address these problems, in this paper we present numerically robust algorithms for the determination of the multiplicity of a point. Explicitly (section 3) or implicitly (section 6), these algorithms involve the determination of the site-symmetry group, which can then be used also for other purposes, such as deriving a point group symbol, or moving a site to the exact location of the nearest special position. We also present two alternative algorithms for the assignment of Wyckoff letters. One of these algorithms (section 6) is probably similar to the algorithm used by Le Page & Raymond (2001), but has the additional advantage of facilitating the determination of the exact location of the nearest special position.

All the algorithms presented in this paper lend themselves to a fully automatic treatment of atomic coordinates, and are therefore suitable for integration in highly automated software systems, such as multi-solution systems for structure determination (e.g. Grosse-Kunstleve, 1997, Falcioni & Deem, 1999, Weeks & Miller, 1999, Cerny & Favre-

Nicolin, 2000), or the automatic processing and validation of large databases where the need for human intervention is prohibitive.

2. Notation

IT83: International Tables for Crystallography, Volume A (Hahn, 1983).

Space-group type: See definition in chapter 8.2.1 of IT83 (Wondratschek, 1983). Two space groups belong to the same space-group type if they correspond to the same entry in IT83.

Space-group representation: A particular group of symmetry operations is a representation of the corresponding space-group type. For example, the space-group representations denoted by the Hermann-Mauguin symbols *Pmna*, *Pnmb*, *Pbmn*, *Pcnm*, *Pncm*, and *Pman* all correspond to the same space-group type (space group no. 53 in IT83). In general each space-group type has an infinite number of representations.

Matrices are enclosed by square brackets. However, matrices shown in *Jones-Faithful* notation (for example *x,y,z*) are not enclosed by brackets. For convenience, column vectors are shown transposed and are enclosed by parentheses to distinguish them from matrices (for example (0.1, 0.2, 0.3)).

The (R, T) formalism similar to that of IT83 is used. R is the (3 x 3) rotation part or rotation matrix and T the (3 x 1) translation part or translation vector of the operation.

Sets are enclosed in curly braces (for example {−1,0,1}).

Half-open intervals are denoted as]*x, y*] (*x* is not included, *y* is included) or [*x, y*[(*x* is included, *y* is not included).

A square matrix A is called unimodular if the absolute value of the determinant of A is equal to one ($|\det(A)| = 1$).

$\underline{Z}$ = set of integer numbers, $\underline{Q}$ = set of rational numbers, $\underline{R}$ = set of real numbers.

3. Algorithm for the determination of the site-symmetry group

The input parameters of the algorithm for the determination of the site-symmetry group G_X of a point X are:

- Unit cell parameters (for distance calculations)
- Symmetry operations of the space group G
- Coordinates X of a point
- Minimum distance Δ_{equiv_min} between symmetrically equivalent points of X (tolerance)

The symmetry operations of the space group G are represented by matrices of the form (R, T), where R is the rotation part, and the translation part T is given modulo $\underline{Z}$.

The algorithm for the determination of the site-symmetry group consists of the following steps:

1. Determination of the symmetry operations $S = (R, T)$ that have a translation part T without an intrinsic (screw or glide) component and that lead to close contacts between X and the symmetrically equivalent point SX. Pairs of S and squared distances $(X - SX)^2$ are stored in a list of candidate symmetry operations.

   Details: The trial symmetry operations S are generated by a loop over all symmetry operations $S_i \in G$. The symmetrically equivalent point $X_S = S_iX$ is computed, followed by the determination of the difference $\Delta X_S = X_S - X$. The unit translations of the space group are applied to ΔX_S in the form of the modulus operation to yield a vector $\Delta_{short} X_S$ with all elements in the range $]-\frac{1}{2} , \frac{1}{2}]$. The symmetry operation that corresponds to the mapping of X to $\Delta_{short} X_S$ is defined as $S_{short} = S_iX + nearest\_int(X - \Delta_{short} X_S)$, where $nearest\_int(Y)$ is a function that determines the vector $J \in \underline{Z}^3$ that is closest to $Y \in \underline{R}^3$.

In most cases S_{short} will correspond to the final S, but in the general case it is necessary to loop over 27 additional combinations of unit translations U (this is a 3-deep loop, each over the three integers $\{-1,0,1\}$) because the translation part of S_{short} could have an intrinsic component. The trial symmetry operations S are determined as $S = S_{short} + U$. The intrinsic part of the trial S is determined with the algorithms in section 4 of Grosse-Kunstleve (1999). If the squared distance $(X - SX)^2$ is less than $(\Delta_{equiv\_min})^2$, S is stored in the list of candidate operations for the site-symmetry group.

It should be noted that the determination of the squared distance $(X - SX)^2$ involves the unit cell parameters, for example in the form of the metrical matrix, or alternatively an orthogonalization matrix (see, e.g. chapter 2 of Giacovazzo, 1992).

2. Sorting of the list of candidate symmetry operations by squared distance, smallest distance first.

3. Generation of the site-symmetry group G_X starting with the symmetry operation that has the smallest distance. The symmetry operations are added to the group in the order in which they appear in the sorted list, and group multiplication is carried out. If the group multiplication leads to a symmetry operation with a pure translation, the operation that was added last is discarded.

The group multiplication in step 3 ensures that the algorithm is not negatively affected by rounding errors in the distance calculations. The elimination of operations that lead to pure translations ensures that the site-symmetry group is a point group. If Δ_{equiv_min} is large compared to the unit cell parameters, it can happen that X is close enough to more than one distinct special position, and that the whole set of candidate operations therefore generates a space group.

Given the operations of the site-symmetry group, the point-group type can easily be determined with the algorithm described in section 5.2 of Grosse-Kunstleve (1999). This gives immediate access to a point group symbol for the site-symmetry group. Using the

algorithms for the characterization of symmetry operations as described in section 4 of Grosse-Kunstleve (1999), it is straightforward to also derive an oriented site-symmetry symbol from the knowledge of the point group type and the operations of the site-symmetry group.

4. Algorithm for the determination of the exact location of the nearest special position

The main steps of the algorithm for the determination of the exact location of the nearest special position are:

1. Determination of the site-symmetry group G_X according to the algorithm in section 3.
2. Determination of the special position operator.

    The special position operator P_X is the average of the symmetry operations S of the site-symmetry group G_X:

    $$P_X = \frac{1}{O(G_X)} \sum_i S_i \, , \qquad (1)$$

    where $O(G_X)$ is the or order of the site-symmetry group, and the S_i are the $O(G_X)$ symmetry operations.

    Example:

    Space group: $P6$

    Unit cell parameters: $a = b = 10$ Å, $c = 13$ Å, $\alpha = \beta = 90$, $\gamma = 120$

    Using a tolerance of 0.5 Å, the symmetry operations of the site-symmetry group G_X of $X = (0.35, 0.65, 0.1234)$ are:

    x,y,z; $-y+1,x-y+1,z$; $-x+y,-x+1,z$

    The sum of these operations is $(1, 2, 3z)$, corresponding to the special position operator $P_X = (1/3, 2/3, z)$.

3. Determination of the exact location of the nearest special position.

    The exact location X_P of the special position nearest to X is defined by the average of all symmetrically equivalent points of X in the site-symmetry group G_X:

$$X_P = \frac{1}{O(G_X)} \sum_i S_i X \qquad (2)$$

From this it follows that X_P can be obtained as the product:

$$X_P = P_X X \qquad\qquad (3)$$

Example:

$$P_X X = (1/3,\ 2/3,\ z)(0.35,\ 0.65,\ 0.1234)$$

$$= \left(\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1/3 \\ 2/3 \\ 0 \end{bmatrix} \right) \begin{bmatrix} 0.35 \\ 0.65 \\ 0.1234 \end{bmatrix} = (1/3,\ 2/3,\ 0.1234)$$

The distance between X and X_P is 0.29 Å.

5. Algorithm for the determination of the Wyckoff letter for a given special position operator

In general the assignment of Wyckoff letters is ambiguous. This is discussed in detail by Fischer & Koch (1983a). When two assignments of Wyckoff positions are compared, operations of the affine normalizer (Fischer & Koch, 1983b) have to be taken into account. The algorithm presented here will produce one possible assignment of Wyckoff letters that is determined by (1) the assignments for a reference setting and (2) the selection of a "canonical" change-of-basis matrix for the transformation of symmetry operations from that reference setting to a given space group representation.

The *International Tables for Crystallography* (Hahn, 1983) (IT83) define a Wyckoff position W_G as the set of all points X for which the site-symmetry groups X_G are conjugate subgroups of G.

Two subgroups X_G and Y_G of G are conjugate subgroups if there exists a symmetry operation $M \in G$ such that:

$$Y_G = M^1 X_G M \qquad\qquad (4)$$

Equation (1) defines the special position operator P as the average of the symmetry operations of a site-symmetry group. From this it follows that if two subgroups of G are conjugate subgroups, the condition

$$P_Y = M^{-1} P_X M \qquad (5)$$

must hold, where P_X is the average of the operations of X_G, and P_Y is the average of the operations of Y_G.

To find the Wyckoff letter for a given special position operator P_X, a table is needed for each of the 230 space group types. These tables correspond to the tables labeled *Positions* in chapter 7 of IT83. However, there are two important differences between the tables needed for the algorithm that is described here, and the tables in chapter 7 of IT83:

- Only one *representative* operator per Wyckoff position is needed from the *Coordinates* column of chapter 7. The other operators are simply products of the symmetry operations and the representative operator. (The idea of representative operators is also found in Altermatt & Brown, 1987.)

- The entries in the *Coordinates* columns of chapter 7 are re-parameterized special position operators. For example, the first entry for Wyckoff position f of space group $P42_12$ (No. 90) is listed as $(x, x, ½)$ (see also Table 1). However, the operations of the site-symmetry group of, e.g., $(0.1, 0.1, ½)$ are:
    $x,y,z; \; y,x,-z+1$
  This leads to the special position operator $(½x+½y, ½x+½y, ½)$. Comparison with the entry in IT83 shows that x in chapter 7 corresponds to $½x+½y$ in the special position operator.

The parameterization of the special position operators in chapter 7 is convenient for a human reader, but not in general useful for the purposes of the algorithm presented in this section. Therefore new two-column tables were derived from the tables as found in chapter 7. As an example, the table for space group $P42_12$ (No. 90) is shown in Table 1.

The first column of each table lists the Wyckoff letters along with the position multiplicities as listed in chapter 7. The second column lists the corresponding representative special position operators P_W that are the strict averages of the symmetry operations of the corresponding site-symmetry groups.

A table of representative special position operators P_W is provided for a reference setting for each of the 230 space group types. To obtain the P_W for an arbitrary space group representation, the P_W are transformed using a change-of-basis matrix that transforms the given symmetry operations to the setting for which the reference table was computed. This transformation property follows immediately from the fact that the P_W are averages of symmetry operations. The change-of-basis matrices are determined with the algorithm for the determination of the space group type that is described in section 5 of Grosse-Kunstleve (1999) and then combined with the operations of the affine normalizer. Each product of a given change-of-basis matrix and an operation of the affine normalizer is an alternative change-of-basis matrix. Since the assignment of Wyckoff letters is in general ambiguous and depends on the exact choice of the change-of-basis matrix, a "canonical" change-of-basis matrix is selected. The selection is based on a set of rules which ensure that the selected matrix is independent of the order in which the alternative matrices are generated. This ensures a reproducible assignment of Wyckoff letters for any given space group representation.

To determine the Wyckoff letter for a given special position operator P_X, and given a table of representative P_W for the given space group representation G, the $M \in G$ has to be found that solves the equation:

$$P_X = M^{-1} P_W M \qquad (6)$$

Since both the multiplicity of X and the multiplicity corresponding to each P_W are known, comparing these is used as a pre-selection.

For the remaining P_W in the table, the solution of equation (6) is implemented as a trial-and-error algorithm with a predictably finite number of trials that is less than or equal to

the order of **G**, per candidate P_W. Trial matrices for **M** are derived from the symmetry operations of **G**. Let **R** be the rotation part of a symmetry operation of **G**, and **T** be the corresponding translation part modulo 1. A trial matrix **M** is defined as **M** = (**R**, **T** + **U**), where **U** is an unknown integer vector of unit translations. Rearrangement of equation (6) and substitution of **M** = (**R**, **T** + **U**), P_X = (R_X, T_X) and P_W = (R_W, T_W) leads to:

$$MP_X = P_W M \Leftrightarrow (R,T+U)(R_X,T_X) = (R_W,T_W)(R,T+U) \qquad (7)$$

U is the only unknown in the equation. Elementary rearrangement leads to:

$$(RR_X, RT_X + T + U) = (R_W R, R_W(T+U) + T_W) \qquad (8)$$

The condition

$$RR_X = R_W R \qquad (9)$$

is used as a second pre-selection for the candidate P_W from the table of Wyckoff letters. For the remaining P_W, the unknown **U** is determined as the solution of

$$RT_X + T + U = R_W(T+U) + T_W \Leftrightarrow (R_W - I)U = RT_X + T - R_W T - T_W, \qquad (10)$$

where **I** is the (3 x 3) unit matrix. Equation (10) is of the general form:

$$Mx = b, x \in Z \qquad (11)$$

Comparison with equation (10) leads to **M** = (R_W - **I**), **x** = **U**, **b** = RT_X + **T** − R_W**T** − T_W. A procedure for solving equation (11) is given by, for example, Domenjoud (1991). Let r be the rank of **M**. There exist then two unimodular matrices **P** and **Q** such that:

$$PMQ = \begin{bmatrix} D & 0 \\ 0 & 0 \end{bmatrix} \qquad (12)$$

D is a (r x r) diagonal matrix and the 0's stand for null matrices of suitable sizes. The determination of **P** and **Q** amounts to computing the *Smith normal form*. A procedure for this is given, for example, in section 5.5 of Grosse-Kunstleve (1999). Any solution of **x** is then of the form **Qx'**, where **x'** is a solution of:

$$\begin{bmatrix} D & 0 \\ 0 & 0 \end{bmatrix} x' = Pb \qquad (13)$$

Checking the satisfiability of equation (13) and computing the solution is straightforward. If equation (13) has a solution for a given P_W, both the Wyckoff letter and the matrix $M = (R, T + U)$ are determined simultaneously.

An M that solves equation (4) is necessarily a solution of equation (5), but it is not immediately clear that the converse is also true. A rigorous proof for this is currently not available. However, we were able to show empirically that equation (5) combined with the condition that the multiplicity of the site-symmetry group of X and the multiplicity of the Wyckoff position must be equal, can be used as a necessary and sufficient condition. This was done by comparing the Wyckoff letters assigned with the algorithm in this section with the letters assigned by the alternative algorithm that is presented in the next section. The two algorithms produce consistent results for a very large number of test cases that include all conventionally used space group representations and an additional large number of unconventional settings.

6. Algorithm for the determination of the Wyckoff letter given the coordinates of a point

The input parameters for the algorithm for the determination of the Wyckoff letter given the coordinates of a point are:

- Unit cell parameters (for distance calculations)
- Symmetry operations of the space group G
- Coordinates X of a point
- Minimum distance Δ_{near} to the nearest special position of X (tolerance)

The algorithm consists of the following steps:

1. Construction of a table of representative special position operators P_W as explained in section 5.

   As before, the P_W are strict averages of a the operations of a site-symmetry group. To facilitate the algorithm presented in this section, the locations X_W to which the P_W apply are chosen such that all elements of the vector X_W are in the range $]-\frac{1}{2}, \frac{1}{2}]$.

2. Application of the unit translations to X:

$$X_0 = mod\_short(X) \qquad (14)$$

   mod_short is a function that applies the unit translations to the elements of X such that the elements are in the range $]-\frac{1}{2}, \frac{1}{2}]$. The unit shifts applied are defined as $U_0 = X_0 - X$.

3. For each P_W, starting with Wyckoff position a and working upwards in the alphabet, the shortest distance squared

$$\Delta P_W = (P_W M' X_0 - M' X_0)^2, \qquad (15)$$

   with $M' = (R, T + U')$, is computed in a loop over all symmetry operations $(R, T) \in G$ and unit shifts U' with vector elements in the set of integers $\{-1,0,1\}$ (i.e., the number of loop iterations is 27 times the order of G, per P_W). The symmetry operations of G are manipulated such that the elements of T are in the range $]-\frac{1}{2}, \frac{1}{2}]$.

4. The Wyckoff letter for X is determined by the first P_W for which the smallest $\Delta P_W < \Delta_{near}$. The exact location X_P of the special position nearest to X is determined as:

$$X_P = M^{-1} P_W M X \qquad (16)$$

   M is defined as $M = M' + R U_0 = (R, T + U' + R U_0)$, with the M' that corresponds to the smallest $\Delta P_W < \Delta_{near}$.

In this algorithm, the problem of determining U is solved in two steps, instead of one as in the algorithm of section 5. The first step is to bring X within ± 1 unit translations of the space where the P_W are known to apply (equation 14). The remaining unit shifts U' are determined with a trial-and-error approach.

7. Discussion

The central algorithm presented in this paper is that for the determination of the site-symmetry group (section 3). This algorithm determines the multiplicity of a point in a numerically robust way, and at the same time provides the information from which the special position operator can easily be computed (section 4). This special position operator can then be used to move a site to the exact location of the nearest special position.

In section 5 we show that the Wyckoff positions as listed in IT83 are re-parameterized special position operators. We have derived tables of *representative special position operators* for the Wyckoff positions of 230 reference space group representations (one for each of the 230 space group types) where the operations listed in IT83 are replaced by the corresponding special position operators. This table facilitates the determination of a Wyckoff letter for a given point. The Wyckoff letter can then be used in turn to obtain the special position operator P_W from the table. To explain how the special position operator P_W that is produced by either of the alternative algorithms in section 5 or section 6 can be used, we will analyze the combination of equations (3) and (6), which is identical to equation (16):

$$X_P = M^{-1} P_W M X \qquad (17)$$

MX is a symmetrically equivalent point of X for which P_W is a special position operator. M^{-1} is another symmetry operation of G that maps the exact location of the special position as defined by P_W back to the special position that is nearest to X. In applications where it is not important which symmetrically equivalent point of X appears in an symmetry-unique set of sites, X in this set could be replaced by MX, and the Wyckoff letter for this site could be stored. In computing intensive calculations, such as structure factor calculations, the Wyckoff letter could then be used as a reference into a table of lists of non-redundant symmetry operations for each Wyckoff position. This leads to implementations that are both robust and fast.

The alternative algorithms for assigning Wyckoff letters and computing special positions operators are largely interchangeable. The question of which one is best selected has to be answered for each application individually. In most cases it is expected that the combination of the algorithms in section 3 and 5 is slightly faster than the algorithm in section 6, especially if the number of sites in general positions is large. If the operations of the site-symmetry group are needed, for example to derive a symbol for the point-group type, clearly the algorithm in section 3 has to be used. In such a case the special position operator is already known, and it is always best to use the algorithm in section 5 for the assignment of Wyckoff letters.

The algorithms presented in this paper are building blocks that are intended for integration into highly automated software system where a fully automatic and robust treatment of atomic coordinates is essential. The choice of a modern programming language (ISO C++, International Standardization Organization et al., 1998) that supports a modular system design through object-orientation and exception handling ensures both ease of use and a high degree of flexibility.

8. Source code availability

All algorithms that we present in this paper are implemented in ISO C++ and are integrated into the Computational Crystallography Toolbox (cctbx). The cctbx source code is freely available under an Open Source license for both non-profit and commercial use at http://cctbx.sourceforge.net/. The tables of representative special position operators P_W (section 5) are included in the source code. They may also be accessed via an end-user friendly web interface at http://cci.lbl.gov/servers/ ("Explore symmetry" example).

Acknowledgements

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Table 1: Table of representative special position operators for space group $P42_12$ (No. 90). The representative special position operators are the strict averages of the symmetry operations of the corresponding site-symmetry groups. For comparison, the first entry in the *Coordinates* table of IT83 is also shown.

Multiplicity, Wyckoff letter	First entry in IT83	Representative special position operator
8 g	x,y,z	x,y,z
4 f	x,x,½	½ x+½y,½x+½y,½
4 e	x,x,0	½ x+½y,½x+½y,0
4 d	0,0,z	0,0,z
2 c	0,½,z	0,½,z
2 b	0,0,½	0,0,½
2 a	0,0,0	0,0,0