Practical algorithm for identifying subgroups of space groups

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The problem of identifying subgroups G' of a space group G with respect to a conventional listing is considered. The properties of space groups and subgroups are given in terms of an algebraic rather than a geometric description. In this algebraic description, G' is equivalent to one of the standard listings through a similarity transformation consisting of a linear unimodular component and a translation. A general algorithm is presented to determine which standard listing corresponds to subgroup G'. The algorithm is applied to a specific example, a subgroup of D_{3d}^6.

I. INTRODUCTION

Space-group methods are of significant utility both experimentally and theoretically. The use of these methods in studying symmetry subgroups (particularly isotropy subgroups) of a space group G is of interest in the description of phase transitions as well as in crystallography. (An isotropy subgroup is the largest subgroup of G, which leaves a vector in the representation carrier space unchanged.) The *computer implementation* of these space-group methods allows one to apply them systematically to a large number of situations. For considerations involving subgroups, the identification of the subgroup in a standard form is a necessary and usually nontrivial part of the process.

For example, group-theoretical methods in the Landau theory of phase transitions[1] and its renormalization-group extension[2] have been used to find allowed group-subgroup phase transitions.[3,4] Isotropy subgroups are first obtained and then attention is restricted to those isotropy subgroups which satisfy the Landau and Lifshitz criteria and correspond to the minima of the Landau free energy. We have considered the direct group-theoretical conditions[5] characterizing isotropy subgroups and implemented these conditions on a computer. All of the isotropy subgroups for **k** points of symmetry have been generated for each of the 230 three-dimensional space groups[6] and the 17 two-dimensional space groups.[7]

In generating isotropy subgroups, it was necessary to identify each as one of the space groups by putting them into standard form. Many papers have necessarily gone through this process of subgroup identification. This is often the most difficult part of the general process of subgroup selection. When considering transitions or subgroups of a given space group, nonmaximal subgroups are often considered, as well as inequivalent selections of the same type subgroup, and the associated relative relationships of subgroup to parent group. Such relationships are important for any detailed microscopics associated with x-ray, NMR, EPR, low-energy electron-diffraction (LEED), Auger-electron spectroscopy (AES), etc., analysis. Such information has not been comprehensively given in any existing publication. Of crucial importance, then, is the identification of the subgroup *and* its relative origin and orientation with respect to the parent group.

The identification of the subgroup is actually a rather general problem. Given a subgroup G' of some space group G, which space group is G'? What is the choice of basis vectors for G' which yields its standard form? How are the space-group origins of G' and G related to each other? To be of use, both the basis vectors and origins of space groups must follow some convention, such as that given in Ref. 8 or 9.

The determination of subgroups or isotropy subgroups is simplified if the algebraic description of the space group is exploited.[10] In this paper we indicate an algorithm based upon this algebraic description of space groups which allows the identification of subgroups of space groups. The algorithm is presented here for the first time and has been implemented on computer and used in a larger algorithm[6,7] for obtaining isotropy subgroups. In Sec. II we indicate the distinction between the geometrical and algebraic descriptions of space groups. In Sec. III we briefly describe the characterization of a space subgroup G' based upon a recent discussion by Senechal.[11] In Sec. IV we give a general outline of our algorithm consistent with the algebraic properties of space groups. In Sec. V we apply the algorithm to a specific example, a subgroup of D_{3d}^6.

II. SPACE GROUPS

When the symmetry of a crystalline solid[12] is considered, it is natural to define this geometrical object in three-dimensional Euclidian space E^3. Associated with E^3 is a real vector space $T(3)$ which consists of all translations of E^3. With respect to an arbitrary (but fixed) origin in E^3, there is a one-to-one correspondence between the vectors of $T(3)$ and the points of E^3. E^3 can then be taken as a three-dimensional real vector space.

Each element in the set of affine mappings $A(3)$ of E^3 is uniquely broken down into a nonsingular linear component R which leaves the origin fixed (point operation) and a translation component $\mathbf{x}$. Thus each mapping of $A(3)$ can be written $\alpha=\{\mathbf{x}\,|\,R\}$ with successive mappings (the group binary product) given as $\alpha_1\alpha_2=\{\mathbf{x}_1+R_1\mathbf{x}_2\,|\,R_1R_2\}$. (We have used a reversed Seitz notation to emphasize that the linear component acts first, followed by the translation.) This set of elements forms a group called the affine group of E^3. $T(3)$ is an invariant subgroup of $A(3)$, and the group of nonsingular linear transformations on E^3, $GL(3,R)$, is also a subgroup of $A(3)$. If we define the distance between two points of E^3 to be $d(\mathbf{x},\mathbf{y})=(\mathbf{x}-\mathbf{y},\mathbf{x}-\mathbf{y})^{1/2}$, the Euclidean group $E(3)$ is the subgroup of $A(3)$ whose elements leave the distance between any two points invariant, i.e., they are rigid transformations. $E(3)$ contains $T(3)$ as an invariant subgroup and also contains the group of linear isometric (orthogonal) transformations $O(3)$ which keep the origin fixed. The set of all transformations in $E(3)$ which map a geometrical object onto itself constitutes its symmetry group.

A crystal structure is distinguished by the property that among its symmetry transformations is a discrete translation group T_G generated by three independent vectors of $T(3)$.[3] Thus T_G is the set of all *integral* linear combinations $\mathbf{t}$ of three vectors, $\mathbf{a}_1,\mathbf{a}_2,\mathbf{a}_3$. The set of all symmetry transformations of a crystal structure is the space group G of the structure.

An element of the space group G is of the general form $\{\mathbf{t}+\mathbf{v}_i \mid R_i\}$, where $\mathbf{t}$ is any translation in T_G, $\mathbf{v}_i$ is a fractional translation [i.e., if nonzero, it is in $T(3)$ but is not in T_G] associated with R_i, and R_i is the linear component of g and is in $O(3)$. The set of elements R_i form a subgroup P_G of $O(3)$ (P_G is called the isogonal point group of G) and is isomorphic to the factor group G/T_G. Any two elements g_1,g_2 of G will belong to the same co-set of T_G in G if and only if $R_1=R_2$. Since T_G is an invariant subgroup, the elements of P_G transform the lattice back into itself, i.e., for all $\mathbf{t}\in T_G, R_i\mathbf{t}\in T_G$. Notice that if we select an orthonormal basis for $T(3)$, i.e., $\hat{i},\hat{j},\hat{k}$, then the lattice T_G and the lattice basis, $\mathbf{a}_1,\mathbf{a}_2,\mathbf{a}_3$, are expressed in terms of this orthonormal basis. For example, the basis vectors for space group D_{3d}^6 can be written in the form of Eq. (14). With respect to an orthonormal basis, the representation of each $R_i\in P_G$ is an orthogonal matrix. Any questions about consistency of group products, selection of subgroups, orientation of alternative lattice bases, etc., would be determined with respect to this orthogonal basis selection. This constitutes the geometrical view.

It is often helpful to take an algebraic approach in the above description. In this approach we use a particular *lattice basis* as the basis for $T(3)$. Then T_G can be identified with Z^3, the additive group of triples of integers. In the algebraic formulation, we easily see that the following is true:

(1) A change of lattice basis to one of the infinitely many other choices is obtained through a similarity transformation by a 3×3 matrix whose entries are integral and whose determinant is ±1. Such a matrix is called a unimodular matrix.

(2) The linear component R of a symmetry transformation with respect to the lattice basis is also a unimodular matrix. Furthermore, it can be shown[13] that two three-dimensional space groups, G' and G'', are of the same type if and only if there is a proper affine mapping $\alpha\in A(3)$ that transforms the first space group into the second, i.e., $\alpha G'\alpha^{-1}=G''$. In the *algebraic formulation,* this statement can be written as follows: G' and G'' are space groups of the same type if and only if there is a proper ($\det S=+1$) unimodular matrix S and a real column coordinate vector $\boldsymbol{\tau}$ such that the representation $\{\{\mathbf{t}'+\mathbf{v}_i' \mid R_i'\}\}$ of G' transforms into the representation $\{\{\mathbf{t}''+\mathbf{v}_i'' \mid R_i''\}\}$ of G'' under $\{\boldsymbol{\tau} \mid S\}$. Thus,

(3) G' and G'' are of the same type if and only if there exists a transformation $\{\mathbf{t} \mid S\}$ (S proper, unimodular) such that

$$\{\boldsymbol{\tau} \mid S\}\{\{\mathbf{t}'+\mathbf{v}_i' \mid R_i'\}\}\{\boldsymbol{\tau} \mid S\}^{-1}=\{\{\mathbf{t}''+\mathbf{v}_i'' \mid R_i''\}\}\ ,$$

i.e.,

(a) $S\mathbf{t}'\in T_{G''}$,

(b) $R_i''=SR_i'S^{-1}$,

(c) $\mathbf{v}_i''-\boldsymbol{\tau}-S\mathbf{v}_i'+SR_i'S^{-1}\boldsymbol{\tau}\in T_{G''}$.

Here, $SR_i'S^{-1}$, $S\mathbf{v}_i'$, and $S\mathbf{t}'$ are the linear component, its fractional, and the translation expressed in the new basis of $T_{G''}$. Since G' and G'' are conjugate in $GL(3,Z)$, the isogonal point-group representations, $P_{G'}$ and $P_{G''}$, will be also. The groups G' and G'' are said to belong to the same arithmetic class.

In the following we will be interested in identifying a subgroup G' of a given space group. The discrete translation group is then the same for G' and G'' (the standard form). The conditions in (3) for equality of space-group type in the algebraic formulation then become conditions for the proper *equivalence* of the space groups and correspond to the freedom in choosing the basis for $T_{G'}$ and the origin for G'. This algebraic formulation will be of importance in Sec. IV as we describe the computer algorithm for identifying space groups. There we will refer back to results (1)–(3) as listed in this section.

III. SUBGROUPS OF SPACE GROUPS

Recently, Senechal[11] described a simple characterization of subgroups of space groups. Owing to a version of Hermann's theorem and a subgroup theorem due to Frobenius, each subgroup G' of G is determined by a lattice $T_{G'}\in T_G$, an isogonal point group $P_{G'}\in P_G$, and two compatibility conditions. The *first condition,* (A), requires that the lattice $T_{G'}$ be invariant under the isogonal point group $P_{G'}$, i.e., each $R_i'\in P_{G'}$ transforms the lattice back onto itself. The co-set representatives $\{\mathbf{v}_i' \mid R_i'\}$ (representatives of $T_{G'}$ in G') have the form $\{\mathbf{v}_i+\mathbf{t}_i \mid R_i\}$. This means that the new fractional associated with each R_i in G' is equal to the old fractional $\mathbf{v}_i$ associated with R_i in G plus some lattice vector $\mathbf{t}_i$ of G ($\mathbf{t}_i\in T_G$) which, if nonzero, is not a lattice vector of G'. The vectors $\mathbf{t}_i$ associated with the R_i must then satisfy the *second condition,* (B). Namely, for each product $R_k=R_iR_j$, we must have

$$\mathbf{v}_i+R_i\mathbf{v}_j-\mathbf{v}_k+\mathbf{t}_i+R_i\mathbf{t}_j-\mathbf{t}_k\in T_{G'}\ .$$

Note that if any one of the vectors $\mathbf{t}_i$ is replaced by $\mathbf{t}_i+\mathbf{t}'$ ($\mathbf{t}'$ any translation in $T_{G'}$), the above condition (B) is again satisfied. Only subgroups with distinct vector sets $\{\mathbf{t}_i\}$ within the primitive cell of G' correspond to distinct subgroups. In the following we assume subgroups G' of G are specified by co-set representatives $\{\mathbf{v}_i' \mid R_i'\}$, where

R_i',$\mathbf{v}_i'$ are taken as known (each $\mathbf{v}_i'$ is a combination of known vectors, $\mathbf{v}_i$ and $\mathbf{t}_i$). Additionally we assume that *conditions* (A) and (B) are expressed with respect to the lattice basis, i.e., within the algebraic view. Our algorithm for identification of space groups applies to subgroups specified in other forms but the above specification is used here as an important example.

IV. ALGORITHM

Consider a space group G^α. Let the vector $\mathbf{t}^\alpha$ be a general translation vector of the Bravais lattice of G^α, written as

$$\mathbf{t}^\alpha=\sum_{j=1}^{3} n_j \mathbf{a}_j^\alpha , \tag{1}$$

where n_1,n_2,n_3 are integers and $\mathbf{a}_1^\alpha,\mathbf{a}_2^\alpha,\mathbf{a}_3^\alpha$ are basis vectors for the lattice. The basis vectors $\mathbf{a}_j^\alpha$ transform under a point operation R_i in the following way:

$$R_i^\alpha \mathbf{a}_j^\alpha=\sum_{k=1}^{3} \mathbf{a}_k^\alpha D_{kj}^\alpha(R_i^\alpha) , \tag{2}$$

where $D^\alpha(R_i^\alpha)$ is a unimodular matrix [see property (2) of Sec. II]. (For each Bravais lattice in our computer algorithm, we have defined the connection between conventional basis vectors and the selection of primitive vectors in the same way as in Ref. 9. We develop the algorithm with respect to this primitive basis[14] and assume such a choice through the remainder of this development.)

Let G' be a subgroup of G^α. Thus, as described in Sec. III, we assume that the basis vectors $\mathbf{a}_j'$ of G' are already defined and given by

$$\mathbf{a}_j'=\sum_{k=1}^{3} \mathbf{a}_k^\alpha A_{kj} , \tag{3}$$

where A is a 3×3 matrix containing only integers. The set $\{\mathbf{a}_j'\}$ is chosen such that $\det A$ is positive. Each co-set rep of G' must have the form $\{\mathbf{v}_i' \,|\, R_i'\}=\{\mathbf{v}_i^\alpha+\mathbf{t}_i^\alpha \,|\, R_i^\alpha\}$, that is, each point operation R_i' in G' must be one of the point operations R_i^α in G^α, and the associated fractional $\mathbf{v}_i'$ must be equal to the former fractional $\mathbf{v}_i^\alpha$ in G^α plus a possibly nonzero translation vector $\mathbf{t}_i^\alpha$ of G^α.

The subgroup G' must be properly equivalent to one of the 230 space groups in standard form. Our algorithm finds which one by systematically comparing it to each of them. When one is found, we can stop the process, since no others will be equivalent to G'. The comparison is made by looking for a proper unimodular matrix S and a real coordinate column vector $\boldsymbol{\tau}$ which transforms G' to the standard form. Consider the space group G^β. If G' is equivalent to G^β, their isogonal point groups must be isomorphic and have the same geometric meaning. This is easily checked by simply examining the representation of point operators with respect to the lattice basis, i.e., comparing their determinant and trace. If the isogonal point group of G' and G^β are the same, then we make a one-to-one correspondence $R_i' \leftrightarrow R_i^\beta$ between the point operators R_i' of G' and those R_i^β of G^β. By this we mean that (1) the point operators are of the same type (C_2, σ, I, etc.), and (2) that they have the same multiplication table (if $R_i' R_j' = R_k'$, then $R_i^\beta R_j^\beta = R_k^\beta$). There may be more than one way to make this correspondence.

We next look for an expression for the basis vectors $\mathbf{a}_j^\beta$ in terms of $\mathbf{a}_k'$ by means of a proper unimodular transformation S [property (3) of Sec. II], i.e.,

$$\mathbf{a}_j^\beta=\sum_{k=1}^{3} \mathbf{a}_k' S_{kj} . \tag{4}$$

As written, S will take coordinates of $\mathbf{t}'\in G'$ and transform to coordinates with respect to G^β. This is consistent with definitions in property (3) of Sec. II. Similar to Eq. (2), the transformation of the lattice basis vectors $\mathbf{a}_j^\beta$ transform under a point operation as

$$R_i^\beta \mathbf{a}_j^\beta=\sum_{k=1}^{3} \mathbf{a}_k^\beta D_{kj}^\beta(R_i^\beta) . \tag{5}$$

Using Eqs. (2)–(5) we thus obtain

$$D^\beta(R_i^\beta)=S^{-1}A^{-1}D^\alpha(R_i^\alpha)AS \tag{6}$$

as a condition on S since we assume everything else given.

We solve for the elements S_{kj} of S which satisfy this equation. If we multiply each side by S,

$$SD^\beta(R_i^\beta)=A^{-1}D^\alpha(R_i^\alpha)AS , \tag{7}$$

we obtain equations linear in the elements S_{kj}. There are nine such equations for each point operator R_i^α. Not all of these equations are independent though, since we need only consider the generators of $P_{G'}$ and even these equations are not all independent. Usually, there are less than nine *independent* equations and thus an infinite number of solutions. Remember, however, that we are looking for solutions such that all S_{kj} are integers and $\det S=1$. These requirements severely restrict the solutions to Eq. (7). On the computer we solve Eq. (7) by trial and error. We first find those equations in Eq. (7) which are linearly independent. Suppose there are m such equations. Since there are nine variables S_{kj}, then $9-m$ of them are independent. We are free to choose any values for the independent S_{kj}, from which the values of the remaining S_{kj} can be uniquely determined. We thus only need to try assigning various sets of integers to the independent S_{kj}, and then determine the remaining S_{kj}. If the latter are also integers and if $\det S=1$, then we have found a solution.

When considering isotropy groups of all 230 space groups corresponding to $\mathbf{k}$ points of symmetry, we have found that, for all cases, $|S_{kj}|\le 2$. For $9-m$ independent variables S_{kj}, we would need to try 5^{9-m} sets of integers. It is conceivable that for other subgroup considerations a solution may exist only for some $|S_{kj}|>2$. In this case our computer solution may become impractical.

Once we have found an appropriate solution S to Eq. (7), we need to express $\mathbf{v}_i'$ with respect to this new basis, which we denote $S\mathbf{v}_i'$ [see property (3) of Sec. II] and then compare the fractionals $S\mathbf{v}_i'$ and $\mathbf{v}_i^\beta$. Although the fractionals $S\mathbf{v}_i'$ and $\mathbf{v}_i^\beta$ may not appear to be the same, they may still differ through a translation of space-group origins. If we translate the origin (of G') by an amount $\boldsymbol{\tau}$, then the new fractionals become

$$S\mathbf{v}_i' \to S\mathbf{v}_i' - \boldsymbol{\tau} + R_i^\beta \boldsymbol{\tau} . \tag{8}$$

We thus look for a translation $\boldsymbol{\tau}$ such that the new fractionals are equal to $\mathbf{v}_i^\beta$ modulo a lattice vector $\mathbf{t}^\beta$. This means that

$$S\mathbf{v}^{i'}-\boldsymbol{\tau}+R_i^\beta\boldsymbol{\tau}=\mathbf{v}_i^\beta+\mathbf{t}^\beta \tag{9}$$

for each R_i. [This is equivalent to expression (c) of property (3) in Sec. II.] The lattice vector $\mathbf{t}^\beta$ may be different for each R_i. If we write all the vectors in terms of $\mathbf{a}_j^\beta$,

$$S\mathbf{v}_1'=\sum_{j=1}^{3}v_{ij}'\mathbf{a}_j^\beta\ , \tag{10}$$

$$\boldsymbol{\tau}=\sum_{j=1}^{3}\tau_j\mathbf{a}_j^\beta\ , \tag{11}$$

$$\mathbf{v}_i^\beta=\sum_{j=1}^{3}v_{ij}^\beta\mathbf{a}_j^\beta\ , \tag{12}$$

then Eq. (9) becomes

$$v_{ij}'-\tau_j+\sum_{k=1}^{3}D_{jk}^\beta\tau_k=v_{ij}^\beta+n_{ij}\ , \tag{13}$$

where n_{ij} are integers. This gives us three equations ($j=1,2,3$) for each R_i^β.

Note that although we began with only three unknowns τ_j we now have all of the n_{ij} also as unknowns, since they can each be *any* integer. Thus, there are three more variables than equations. We solve these equations in a similar way to Eq. (7) except that here, the three variables τ_j are not restricted to integer values. We expect simple fractions for τ_j. If we find an appropriate solution to Eq. (13), we then know that $G'=G^\beta$ and our search is ended. If we do not find a solution, we must return to Eq. (7) and see if there is yet another way to choose S which may allow us to find a solution to Eq. (13). If all attempts here also fail, then we must try a different set of one-to-one correspondences $R_i'\leftrightarrow R_i^\beta$. If this also fails, then $G'\neq G^\beta$ and we should examine another space group G^β as a possibility.

In summary, the algorithm consists of the following steps, assuming that a subgroup G' is given in terms of group transformations of G.

Step 1: Choose one of the 230 space groups G^β with an isogonal point group isomorphic to $P_{G'}$.

Step 2: Choose an isomorphic mapping between the isogonal point groups of G' and G^β such that each linear component has the same geometric meaning.

Step 3: Look for elements of the matrix S satisfying Eq. (7). This corresponds to a change of lattice basis, so S must be a unimodular matrix of determinant 1. S defines the change of basis from G' to G^β. If this is unsuccessful, return to step 2.

Step 4: Look for solutions of Eq. (13), which corresponds to a translation of origin. The translation $\boldsymbol{\tau}$ may not be integral in the basis $\mathbf{a}_i^\beta$. If this step is successful, the subgroup is in standard form with $\boldsymbol{\tau}$ the position of the origin of G^β with respect to G'. If unsuccessful, return to step 3.

V. EXAMPLE

Consider the space group $G^\alpha=D_{3d}^6$.[15] (We use the notation and conventions of Bradley and Cracknell[9] throughout this section.) The lattice is trigonal with

$$\begin{aligned}&\mathbf{a}_1^\alpha=(0,-a,c)\ ,\\&\mathbf{a}_2^\alpha=(\tfrac12\sqrt{3}a,\tfrac12 a,c)\ ,\\&\mathbf{a}_3^\alpha=(-\tfrac12\sqrt{3}a,\tfrac12 a,c)\ ,\end{aligned}\tag{14}$$

where the vectors are given in terms of the Cartesian coordinates. The co-set reps of D_{3d}^6 are

$$\begin{aligned}&\{000\,|\,E\},\ \ \{000\,|\,C_3^+\},\ \ \{000\,|\,C_3^-\}\ ,\\&\{000\,|\,I\},\ \ \{000\,|\,S_3^-\},\ \ \{000\,|\,S_3^+\}\ ,\\&\{\tfrac12\tfrac12\tfrac12\,|\,C_{21}'\},\ \ \{\tfrac12\tfrac12\tfrac12\,|\,C_{22}'\},\ \ \{\tfrac12\tfrac12\tfrac12\,|\,C_{23}'\}\ ,\\&\{\tfrac12\tfrac12\tfrac12\,|\,\sigma_{d1}\},\ \ \{\tfrac12\tfrac12\tfrac12\,|\,\sigma_{d2}\},\ \ \{\tfrac12\tfrac12\tfrac12\,|\,\sigma_{d3}\}\ ,\end{aligned}\tag{15}$$

where the fractionals are the components of $\mathbf{v}_i^\alpha$ in terms of $\mathbf{a}_j^\alpha$.

Consider the subgroup G' with the lattice,

$$\begin{aligned}&\mathbf{a}_1'=\mathbf{a}_1^\alpha\ ,\\&\mathbf{a}_2'=\mathbf{a}_2^\alpha-\mathbf{a}_3^\alpha\ ,\\&\mathbf{a}_3'=\mathbf{a}_2^\alpha+\mathbf{a}_3^\alpha\ ,\end{aligned}\tag{16}$$

and co-set reps,

$$\{000\,|\,E\},\ \ \{000\,|\,I\},\ \ \{\tfrac12\tfrac32\tfrac12\,|\,C_{21}'\},\ \ \{\tfrac12\tfrac32\tfrac12\,|\,\sigma_{d1}\}\ . \tag{17}$$

(The fractionals here are still given in terms of $\mathbf{a}_j^\alpha$.) The matrix A is thus

$$A=\begin{bmatrix}1&0&0\\0&1&1\\0&-1&1\end{bmatrix}. \tag{18}$$

The matrices of the point operators are given by

$$\begin{aligned}&D_{ij}^\alpha(E)=\delta_{ij}\ ,\\&D_{ij}^\alpha(I)=-\delta_{ij}\ ,\\&D^\alpha(C_{21}')=\begin{bmatrix}-1&0&0\\0&0&-1\\0&-1&0\end{bmatrix},\\&D_{ij}^\alpha(\sigma_{d1})=-D_{ij}^\alpha(C_{21}')\ .\end{aligned}\tag{19}$$

To this point, we have just given the specification of the subgroup consistent with Eqs. (1)–(3). We now compare G' with the standard listing of space groups. The isogonal point group of G' is C_{2h}. There are six space groups (C_{2h}^{1-6}) with this isogonal point group. In each of these space groups the point operators are E, I, C_{2z}, and σ_z. There is only one possible way to make a one-to-one correspondence between R_i' and R_i^β in this case:

$$\begin{aligned}&E\leftrightarrow E\ ,\\&I\leftrightarrow I\ ,\\&C_{21}'\leftrightarrow C_{2z}\ ,\\&\sigma_{d1}\leftrightarrow\sigma_z\ .\end{aligned}\tag{20}$$

Let us try a space group G^{β} with a primitive monoclinic lattice (space groups $C_{2h}^{1,2,4,5}$). The basis vectors are given in terms of Cartesian coordinates by

$$\begin{aligned} \mathbf{a}_1^{\beta} &= (0,-b,0)\ , \\ \mathbf{a}_2^{\beta} &= (a\sin\gamma,\ -a\cos\gamma,0)\ , \\ \mathbf{a}_3^{\beta} &= (0,0,c)\ . \end{aligned} \tag{21}$$

The matrices for the point operators in this lattice are given by

$$\begin{aligned} D_{ij}^{\beta}(E) &= \delta_{ij}\ , \\ D_{ij}^{\beta}(I) &= -\delta_{ij}\ , \\ D^{\beta}(C_{2z}) &= \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \\ D_{ij}^{\beta}(\sigma_z) &= -D_{ij}^{\beta}(C_{2z})\ . \end{aligned} \tag{22}$$

Using Eq. (7) we find that $S_{13}=S_{21}=S_{22}=S_{33}=0$. The remaining five variables S_{kj} can take on any value and are thus independent variables. There are many possible choices for these S_{kj} which will give us $\det S=1$. The choice we will use here is

$$S=\begin{bmatrix} -1 & -1 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}. \tag{23}$$

Of course, this is not the only choice of S which will lead to the successful identification of the space group. This choice of S is the one which the computer found. Using this S, we thus find that

$$\begin{aligned} \mathbf{a}_1^{\beta} &= -\mathbf{a}_1^{\alpha}\ , \\ \mathbf{a}_2^{\beta} &= -\mathbf{a}_1^{\alpha}+\mathbf{a}_2^{\alpha}+\mathbf{a}_3^{\alpha}\ , \\ \mathbf{a}_3^{\beta} &= \mathbf{a}_2^{\alpha}-\mathbf{a}_3^{\alpha}\ . \end{aligned} \tag{24}$$

Thus the isogonal point groups of G' and G^{β} are in the same arithmetic class, and the Bravais lattice of G' is primitive monoclinic. We can now limit our search for G^{β} to the four space groups ($C_{2h}^{1,2,4,5}$) with this lattice. The co-set reps of G', when written with the fractionals in terms of $\mathbf{a}_j^{\beta}$, are

$$\{000\,|\,E\},\ \ \{000\,|\,I\},\ \ \{\tfrac{1}{2}0\tfrac{1}{2}\,|\,C_{2z}\},\ \ \{\tfrac{1}{2}0\tfrac{1}{2}\,|\,\sigma_z\}\ . \tag{25}$$

Let us try to identify these co-set reps with those of C_{2h}^{5}. The co-set reps of C_{2h}^{5} are

$$\{000\,|\,E\},\ \ \{\tfrac{1}{2}0\tfrac{1}{2}\,|\,I\},\ \ \{00\tfrac{1}{2}\,|\,C_{2z}\},\ \ \{\tfrac{1}{2}00\,|\,\sigma_z\}\ . \tag{26}$$

Using Eq. (13), we find that

$$\begin{aligned} -2\tau_1 &= \tfrac{1}{2}+n_{21}\ , \\ -2\tau_2 &= n_{22}\ , \\ -2\tau_3 &= \tfrac{1}{2}+n_{23}\ . \end{aligned} \tag{27}$$

An obvious solution is $\tau=(\frac{1}{4}0\frac{1}{4})$, which tells us that indeed $G'=C_{2h}^{5}$.

We note that although we gave the x,y,z coordinates of the basis vectors in Eqs. (14) and (21) for the reader's benefit, we did not use them. Our method only used the transformation properties of these vectors as given by the D matrices in Eqs. (19) and (22), consistent with the algebraic view. In the systematic approach to identifying subgroups, the above algorithm based on the algebraic view is mathematically well justified and is original with our description here.

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[14]Billiet approaches the calculation of subgroups in terms of the conventional basis, and thus the matrices could have noninteger entries. We find it advantageous to describe our algorithm in terms of primitive vectors. Reference to Billiet's work is Y. Billiet, Match **9**, 177 (1980), and references therein.

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