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Double antisymmetry and the rotation-reversal space groups

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Rotation-reversal symmetry was recently introduced to generalize the symmetry classification of rigid static rotations in crystals such as tilted octahedra in perovskite structures and tilted tetrahedra in silica structures. This operation has important implications for crystallographic group theory, namely that new symmetry groups are necessary to properly describe observations of rotation-reversal symmetry in crystals. When both rotation-reversal symmetry and time-reversal symmetry are considered in conjunction with space-group symmetry, it is found that there are 17 803 types of symmetry which a crystal structure can exhibit. These symmetry groups have the potential to advance understanding of polyhedral rotations in crystals, the magnetic structure of crystals and the coupling thereof. The full listing of the double antisymmetry space groups can be found in the supplementary materials of the present work and at http://sites.psu.edu/gopalan/research/symmetry/.

1. Introduction

Rotation-reversal symmetry (Gopalan & Litvin, 2011) was introduced to generalize the symmetry classification of tilted octahedra perovskite structures (Glazer, 2011). The rotation-reversal operation, represented by 1* (previously represented by 1^{Φ}) was compared by analogy to the well known time-reversal operation, represented by $1'$ (see Fig. 1). Although reversing time in a crystal is not something that can be performed experimentally, it is nonetheless useful for describing the magnetic symmetry of a crystal structure and this magnetic symmetry description has important consequences which can be observed by experiment (Opechowski, 1986). Likewise, rotation-reversal symmetry is useful in describing the symmetry of a crystal structure composed of molecules or polyhedral units. For example, the structure conventionally described in Glazer notation (Glazer, 1972) as $a_o^+a_o^+c_o^+$ and classified with the group $Immm1'$ is now classified with the rotation-reversal group $I4^*/mmm^*1'$ (No. 4206). An $a_o^+a_o^+c_o^+$ structure with a spin along the z direction in each octahedron was formerly classified with the group $Im'm'm$ and is now classified with the group $I4^*/mm'm'^*$ (No. 16490). The rotation-reversal space groups used in this new classification of tilted octahedra perovskites are isomorphic to, *i.e.* have the same abstract mathematical structure, as *double antisymmetry space groups* (Zamorzaev & Sokolov, 1957*a*,*b*; Zamorzaev, 1976). As rotation-reversal space groups are isomorphic to double antisymmetry space groups, in the present work we will use the terminology and notation associated with double antisymmetry space groups.

	Does not reverse time	Reverses time
Does not reverse rotation	1	1′
Reverses rotation	1*	1′*

Figure 1
Identity (1) and anti-identities (1′, 1* and 1′*) of the rotation-reversal and time-reversal space groups.

Double antisymmetry space groups are among the generalizations of the crystallographic groups which began with Heesch (1930) and Shubnikov (1951) and continued to include a myriad of generalizations under various names as anti-symmetry groups, cryptosymmetry groups, quasisymmetry groups, color groups and metacrystallographic groups (see reviews by Koptsik, 1967, 1968; Zamorzaev & Palistrant, 1980; Opechowski, 1986; Zamorzaev, 1988). Only some of these groups have been explicitly listed, *e.g.* the black-and-white space groups (Belov *et al.*, 1955, 1957*a*,*b*) and various multiple antisymmetry (Zamorzaev, 1976) and color groups (Zamorzaev *et al.*, 1978). While no explicit listing of the double anti-symmetry space groups has been given, the number of these groups, and other generalizations of the crystallographic groups, have been calculated (see Zamorzaev, 1976, 1988; Zamorzaev & Palistrant, 1980; Jablan, 1987, 1990, 1992, 1993*a*,*b*, 2002; Palistrant & Jablan, 1991; Radovic & Jablan, 2005).

In §2, we shall define double antisymmetry space groups and specify which of these groups we shall explicitly tabulate. This is followed by the details of the procedure used in their tabulation. In §3, we set out the format of the tables listing these groups. §4 describes example diagrams of double antisymmetry space groups (Fig. 4*a*: No. 8543 $C2'/m^*$, Fig. 4*b*: No. 16490 $I4^*/mm'm'^*$, Fig. 4*c*: No. 13461 $Ib'^*c'a'$). §5 gives the computational details of how the types were derived.

Zamorzaev & Palistrant (1980) have calculated not only the total number of types of double antisymmetry space groups, but they have also specified the number in sub-categories. We have found errors in these numbers. Consequently, the total number of types of groups is different than that calculated by Zamorzaev & Palistrant (1980). This is discussed in §6.

2. Double antisymmetry space groups

Space groups, in the present work, will be limited to the conventional three-dimensional crystallographic space groups as defined in Volume A of *International Tables for Crystallography* (Hahn, 2006). An *antisymmetry space group* is similar to a space group, but some of the symmetry elements may also 'flip' space between two possible states, *e.g.* $(\mathbf{r}, t)$ and $(\mathbf{r}, -t)$. A *double antisymmetry space group* extends this concept to allow symmetry elements to flip space in two independent ways between four possible states, *e.g.* $(\mathbf{r}, t, \varphi)$, $(\mathbf{r}, -t, \varphi)$, $(\mathbf{r}, t, -\varphi)$ and $(\mathbf{r}, -t, -\varphi)$. A more precise definition will be given below.

To precisely define antisymmetry space groups, we will start by defining an anti-identity. An operation, *e.g.* $1'$, is an anti-identity if it has the following properties:

(*a*) Self-inverse: $1'\cdot1' = 1$ where 1 is identity.

(*b*) Commutivity: $1'\cdot g = g\cdot1'$ for all elements g of $\mathbf{E}(3)$.

(*c*) $1'$ is not an element of $\mathbf{E}(3)$.

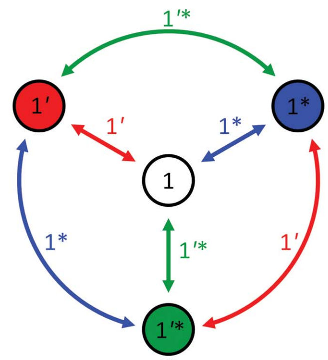
$\mathbf{E}(3)$ is the three-dimensional Euclidean group, *i.e.* the group of all distance-preserving transformations of three-dimensional Euclidean space. A *space group* can be defined as a group $\mathbf{G} \subset \mathbf{E}(3)$ such that the subgroup composed of all translations in $\mathbf{G}$ is minimally generated by a set of three translations with linearly independent translation vectors. We can extend this to define antisymmetry space groups as follows:

Let an *n-tuple antisymmetry space group* be defined as a group $\mathbf{G} \subset \mathbf{E}(3) \times \mathbf{P}$ such that the subgroup composed of all translations in $\mathbf{G}$ is minimally generated by a set of three translations with linearly independent translation vectors and $\mathbf{P}$ is minimally generated by a set of n anti-identities and is isomorphic to $\mathbb{Z}_2{}^n$.

Thus, for single antisymmetry space groups, $\mathbf{P}$ is minimally generated by just one anti-identity, for double, two, for triple, three, and so forth. It should be noted that the above definition could be generalized to arbitrary spaces and coloring schemes by changing $\mathbf{E}(3)$ and $\mathbf{P}$, respectively, but that is beyond the scope of the present work.

	1	1′	1*	1′*
1	1	1′	1*	1′*
1′	1′	1	1′*	1*
1*	1*	1′*	1	1′
1′*	1′*	1*	1′	1

(*a*)



(*b*)

Figure 2
(*a*) Multiplication table of $\mathbf{1'1^*}$. To evaluate the product of two elements, we find the row associated with the first element and the column associated with the second element, *e.g.* for $1'\cdot1^*$, go to the second row, third column to find $1'^*$. (*b*) Cayley graph generated by $1'$, 1^* and $1'^*$. To evaluate the product of two elements, we start from the circle representing the first element and follow the arrow representing the second, *e.g.* for $1'\cdot1^*$, we start on the red circle ($1'$) and take the blue path (1^*) to the green circle ($1'^*$).

Let the two anti-identities which generate $\mathbf{P}$ for double antisymmetry space groups be labeled as $1'$ and 1^*. The product of $1'$ and 1^* is also an anti-identity which will be labeled $1'^*$. The coloring of $1'$, 1^* and $1'^*$ is intended to assist the reader and has no special meaning beyond that. Double antisymmetry has a total of three anti-identities: $1'$, 1^* and $1'^*$. Note that these three anti-identities are not independent because each can be generated from the product of the other two. So although we have three anti-identities, only two are independent and thus we call it 'double antisymmetry' (more generally n-antisymmetry has $2^n - 1$ anti-identities). $1'$ generates the group $\mathbf{1'} = \{1,1'\}$, 1^* generates the group $\mathbf{1^*} = \{1,1^*\}$, and together $1'$ and 1^* generate the group $\mathbf{1'1^*} = \{1,1',1^*,1'^*\}$. For double antisymmetry space groups, $\mathbf{P} = \mathbf{1'1^*}$.

Fig. 2 shows how the elements of $\mathbf{1'1^*}$ multiply. To evaluate the product of two elements of $\mathbf{1'1^*}$ with the multiplication table given in Fig. 2(*a*), we find the row associated with the first element and the column associated with the second element, *e.g.* for $1'\cdot1^*$, go to the second row, third column to find $1'^*$. To evaluate the product of two elements of $\mathbf{1'1^*}$ with the Cayley graph given in Fig. 2(*b*), we start from the circle representing the first element and follow the arrow representing the second, *e.g.* for $1'\cdot1^*$, we start on the red circle ($1'$) and take the blue path (1^*) to the green circle ($1'^*$).

2.1. The structure of double antisymmetry groups

When a spatial transformation is coupled with an anti-identity, we shall say it is *colored* with that anti-identity. This is represented by adding $'$, * or $'^*$ to the end of the symbol representing the spatial transformation, *e.g.* a fourfold rotation coupled with time-reversal (*i.e.* the product of 4 and $1'$) is $4'$.

We shall say that all double antisymmetry groups can be constructed by coloring the elements of a *colorblind parent group*. In the case of a double antisymmetry space group, the colorblind parent group, **Q**, is one of the crystallographic space groups. There are four different ways of coloring an element of **Q**, namely coloring with 1, $1'$, 1^* or $1'^*$ which we shall then refer to as being *colorless*, *primed*, *starred* or *prime–starred*, respectively. Let $\mathbf{Q1'1^*}$ be the group formed by including all possible colorings of the elements of **Q**, *i.e.* the direct product of **Q** and $\mathbf{1'1^*}$. Since $\mathbf{Q1'1^*}$ contains all possible colorings of the elements of **Q**, every double antisymmetry space group whose colorblind parent is **Q** must be a subgroup of $\mathbf{Q1'1^*}$.

Every subgroup of $\mathbf{Q1'1^*}$ whose colorblind parent is **Q** is of the form of one of the 12 categories of double antisymmetry groups listed in Table 1. The formulae of Table 1 are represented visually in Appendix *A* using Venn diagrams.

Table 1
Double antisymmetry group categories and group structure.

The minus sign, '−', indicates the set-theoretic difference, also known as the relative complement. The plus sign, '+', indicates union. **H** and **K** are unique index-2 subgroups of **Q** (an index-2 subgroup has half as many elements as the group, or equivalently: $|\mathbf{Q/H}| = 2$). These category symbols were introduced by Litvin *et al.* (1994, 1995).

Category	Symbol and structure			Number of double antisymmetry space-group types
(1)	$\mathbf{Q}$	=	$\mathbf{Q}$	230
(2)	$\mathbf{Q1'}$	=	$\mathbf{Q} + \mathbf{Q}1'$	230
(3)	$\mathbf{Q(H)}$	=	$\mathbf{H} + (\mathbf{Q} - \mathbf{H})1'$	1191
(4)	$\mathbf{Q1^*}$	=	$\mathbf{Q} + \mathbf{Q}1^*$	230
(5)	$\mathbf{Q1'1^*}$	=	$\mathbf{Q} + \mathbf{Q}1' + \mathbf{Q}1^* + \mathbf{Q}1'^*$	230
(6)	$\mathbf{Q(H)1^*}$	=	$\mathbf{H} + (\mathbf{Q} - \mathbf{H})1' + \mathbf{H}1^* + (\mathbf{Q} - \mathbf{H})1'^*$	1191
(7)	$\mathbf{Q\{H\}}$	=	$\mathbf{H} + (\mathbf{Q} - \mathbf{H})1^*$	1191
(8)	$\mathbf{Q1'^*}$	=	$\mathbf{Q} + \mathbf{Q}1'^*$	230
(9)	$\mathbf{Q\{H\}1'}$	=	$\mathbf{H} + (\mathbf{Q} - \mathbf{H})1^* + \mathbf{H}1' + (\mathbf{Q} - \mathbf{H})1'^*$	1191
(10)	$\mathbf{Q(H)1'^*}$	=	$\mathbf{H} + (\mathbf{Q} - \mathbf{H})1' + \mathbf{H}1'^* + (\mathbf{Q} - \mathbf{H})1^*$	1191
(11)	$\mathbf{Q(H)\{H\}}$	=	$\mathbf{H} + (\mathbf{Q} - \mathbf{H})1'^*$	1191
(12)	$\mathbf{Q(H)\{K\}}$	=	$\mathbf{H} \cap \mathbf{K} + (\mathbf{H} - \mathbf{K})1^* + (\mathbf{K} - \mathbf{H})1' + (\mathbf{Q} - (\mathbf{H} + \mathbf{K}))1'^*$	9507
				Total: 17803

2.2. Example of generating double antisymmetry groups

As an example, consider applying the formulae in Table 1 to point group **222**. **222** has four elements: $\{1,2_x,2_y,2_z\}$. **222** has three index-2 subgroups: $\{1,2_x\}$, $\{1,2_y\}$ and $\{1,2_z\}$ which will be denoted by $\mathbf{2_x}$, $\mathbf{2_y}$ and $\mathbf{2_z}$, respectively. The subscripts indicate the axes of rotation. Applying the formulae in Table 1 yields the following:

Category (1): **Q**
1. $\mathbf{Q} = \mathbf{222} \rightarrow \mathbf{Q} = \{1,2_x,2_y,2_z\}$

Category (2): $\mathbf{Q} + \mathbf{Q}1'$
2. $\mathbf{Q} = \mathbf{222} \rightarrow \mathbf{Q1'} = \{1,2_x,2_y,2_z,1',2_x',2_y',2_z'\}$

Category (3): $\mathbf{H} + (\mathbf{Q} - \mathbf{H})1'$
3. $\mathbf{Q} = \mathbf{222}, \mathbf{H} = \mathbf{2_x} \rightarrow \mathbf{Q(H)} = \{1,2_x,2_y',2_z'\}$
4. $\mathbf{Q} = \mathbf{222}, \mathbf{H} = \mathbf{2_y} \rightarrow \mathbf{Q(H)} = \{1,2_x',2_y,2_z'\}$
5. $\mathbf{Q} = \mathbf{222}, \mathbf{H} = \mathbf{2_z} \rightarrow \mathbf{Q(H)} = \{1,2_x',2_y',2_z\}$

Category (4): $\mathbf{Q} + \mathbf{Q}1^*$
6. $\mathbf{Q} = \mathbf{222} \rightarrow \mathbf{Q1^*} = \{1,2_x,2_y,2_z,1^*,2_x^*,2_y^*,2_z^*\}$

Category (5): $\mathbf{Q} + \mathbf{Q}1' + \mathbf{Q}1^* + \mathbf{Q}1'^*$
7. $\mathbf{Q} = \mathbf{222} \rightarrow \mathbf{Q1'1^*} = \{1,2_x,2_y,2_z,1',2_x',2_y',2_z',1^*,2_x^*,2_y^*,2_z^*, 1'^*,2_x'^*,2_y'^*,2_z'^*\}$

Category (6): $\mathbf{H} + (\mathbf{Q} - \mathbf{H})1' + \mathbf{H}1^* + (\mathbf{Q} - \mathbf{H})1'^*$
8. $\mathbf{Q} = \mathbf{222}, \mathbf{H} = \mathbf{2_x} \rightarrow \mathbf{Q(H)1^*} = \{1,2_x,2_y',2_z',1^*,2_x^*,2_y'^*,2_z'^*\}$
9. $\mathbf{Q} = \mathbf{222}, \mathbf{H} = \mathbf{2_y} \rightarrow \mathbf{Q(H)1^*} = \{1,2_x',2_y,2_z',1^*,2_x'^*,2_y^*,2_z'^*\}$
10. $\mathbf{Q} = \mathbf{222}, \mathbf{H} = \mathbf{2_z} \rightarrow \mathbf{Q(H)1^*} = \{1,2_x',2_y',2_z,1^*,2_x'^*,2_y'^*,2_z^*\}$

Category (7): $\mathbf{H} + (\mathbf{Q} - \mathbf{H})1^*$
11. $\mathbf{Q} = \mathbf{222}, \mathbf{H} = \mathbf{2_x} \rightarrow \mathbf{Q\{H\}} = \{1,2_x,2_y^*,2_z^*\}$
12. $\mathbf{Q} = \mathbf{222}, \mathbf{H} = \mathbf{2_y} \rightarrow \mathbf{Q\{H\}} = \{1,2_x^*,2_y,2_z^*\}$
13. $\mathbf{Q} = \mathbf{222}, \mathbf{H} = \mathbf{2_z} \rightarrow \mathbf{Q\{H\}} = \{1,2_x^*,2_y^*,2_z\}$

Category (8): $\mathbf{Q} + \mathbf{Q}1'^*$
14. $\mathbf{Q} = \mathbf{222} \rightarrow \mathbf{Q1'^*} = \{1,2_x,2_y,2_z,1'^*,2_x'^*,2_y'^*,2_z'^*\}$

Category (9): $\mathbf{H} + (\mathbf{Q} - \mathbf{H})1^* + \mathbf{H}1' + (\mathbf{Q} - \mathbf{H})1'^*$
15. $\mathbf{Q} = \mathbf{222}, \mathbf{H} = \mathbf{2_x} \rightarrow \mathbf{Q\{H\}1'} = \{1,2_x,2_y^*,2_z^*,1',2_x',2_y'^*,2_z'^*\}$
16. $\mathbf{Q} = \mathbf{222}, \mathbf{H} = \mathbf{2_y} \rightarrow \mathbf{Q\{H\}1'} = \{1,2_x^*,2_y,2_z^*,1',2_x'^*,2_y',2_z'^*\}$
17. $\mathbf{Q} = \mathbf{222}, \mathbf{H} = \mathbf{2_z} \rightarrow \mathbf{Q\{H\}1'} = \{1,2_x^*,2_y^*,2_z,1',2_x'^*,2_y'^*,2_z'\}$

Category (10): $\mathbf{H} + (\mathbf{Q} - \mathbf{H})1' + \mathbf{H}1'^* + (\mathbf{Q} - \mathbf{H})1^*$
18. $\mathbf{Q} = \mathbf{222}, \mathbf{H} = \mathbf{2_x} \rightarrow \mathbf{Q(H)1'^*} = \{1,2_x,2_y',2_z',1'^*,2_x'^*,2_y^*,2_z^*\}$
19. $\mathbf{Q} = \mathbf{222}, \mathbf{H} = \mathbf{2_y} \rightarrow \mathbf{Q(H)1'^*} = \{1,2_x',2_y,2_z',1'^*,2_x^*,2_y'^*,2_z^*\}$
20. $\mathbf{Q} = \mathbf{222}, \mathbf{H} = \mathbf{2_z} \rightarrow \mathbf{Q(H)1'^*} = \{1,2_x',2_y',2_z,1'^*,2_x^*,2_y^*,2_z'^*\}$

Category (11): $\mathbf{H} + (\mathbf{Q} - \mathbf{H})1'^*$
21. $\mathbf{Q} = \mathbf{222}, \mathbf{H} = \mathbf{2_x} \rightarrow \mathbf{Q(H)\{H\}} = \{1,2_x,2_y'^*,2_z'^*\}$
22. $\mathbf{Q} = \mathbf{222}, \mathbf{H} = \mathbf{2_y} \rightarrow \mathbf{Q(H)\{H\}} = \{1,2_x'^*,2_y,2_z'^*\}$
23. $\mathbf{Q} = \mathbf{222}, \mathbf{H} = \mathbf{2_z} \rightarrow \mathbf{Q(H)\{H\}} = \{1,2_x'^*,2_y'^*,2_z\}$

Category (12): $\mathbf{H} \cap \mathbf{K} + (\mathbf{H} - \mathbf{K})1^* + (\mathbf{K} - \mathbf{H})1' + (\mathbf{Q} - (\mathbf{H} + \mathbf{K}))1'^*$
24. $\mathbf{Q} = \mathbf{222}, \mathbf{H} = \mathbf{2_y}, \mathbf{K} = \mathbf{2_z} \rightarrow \mathbf{Q(H)\{K\}} = \{1,2_x'^*,2_y^*,2_z'\}$
25. $\mathbf{Q} = \mathbf{222}, \mathbf{H} = \mathbf{2_x}, \mathbf{K} = \mathbf{2_z} \rightarrow \mathbf{Q(H)\{K\}} = \{1,2_x^*,2_y'^*,2_z'\}$
26. $\mathbf{Q} = \mathbf{222}, \mathbf{H} = \mathbf{2_x}, \mathbf{K} = \mathbf{2_y} \rightarrow \mathbf{Q(H)\{K\}} = \{1,2_x^*,2_y',2_z'^*\}$
27. $\mathbf{Q} = \mathbf{222}, \mathbf{H} = \mathbf{2_z}, \mathbf{K} = \mathbf{2_y} \rightarrow \mathbf{Q(H)\{K\}} = \{1,2_x'^*,2_y',2_z^*\}$
28. $\mathbf{Q} = \mathbf{222}, \mathbf{H} = \mathbf{2_z}, \mathbf{K} = \mathbf{2_x} \rightarrow \mathbf{Q(H)\{K\}} = \{1,2_x',2_y'^*,2_z^*\}$
29. $\mathbf{Q} = \mathbf{222}, \mathbf{H} = \mathbf{2_y}, \mathbf{K} = \mathbf{2_x} \rightarrow \mathbf{Q(H)\{K\}} = \{1,2_x',2_y^*,2_z'^*\}$.

Note that although 29 double antisymmetry point groups are generated from using **222** as a colorblind parent group, they are not all of distinct antisymmetry point-group types, as is explained in §2.3. In the above example, there are only 12 unique types of groups, as discussed further on. Two additional examples, using point group ***2/m*** and space group *Cc*, are given in Appendix *B*.

Since the index-2 subgroups of the crystallographic space groups are already known and available in *International Tables for Crystallography* Volume A, applying this set of formulae is straightforward. If applied to a representative group of each of the 230 crystallographic space-group types, 38 290 double antisymmetry space groups are generated. These 38 290 generated groups can be sorted into 17 803 equivalence classes, *i.e.* *double antisymmetry space-group types*, by applying an equivalence relation.

2.3. Double antisymmetry space-group types and the proper affine equivalence relation

The well known 230 *crystallographic space-group types* given in *International Tables for Crystallography* Volume A (Hahn, 2006) are the *proper affine classes of space groups* ('types' is used instead of 'classes' to avoid confusion with 'crystal classes'). The equivalence relation of proper affine classes is as follows: two space groups are equivalent if and only if they can be bijectively mapped by a proper affine transformation (*proper* means *chirality-preserving*) (Opechowski, 1986). In the literature, the '*space-group types*' are often referred to as simply '*space groups*' when the distinction is unnecessary.

For the present work, we will use 'double antisymmetry space-group types' to refer to the proper affine classes of double antisymmetry space groups. This is consistent with Zamorzaev's works on generalized antisymmetry (Zamorzaev & Sokolov, 1957*a*,*b*; Zamorzaev, 1976, 1988; Zamorzaev *et al.*, 1978; Zamorzaev & Palistrant, 1980).

As an example, we consider the proper affine equivalence classes of the 29 **Q** = **222** double antisymmetry groups generated using the formulae given in Table 1. Only 12 such classes exist, one in each category. For categories (1), (2), (4), (5) and (8), the reason for this is that there is only one group generated in each to begin with. For categories (3), (6), (7), (9), (10) and (11), there are three groups generated which are related to each other by 120° rotations (*e.g.* $\{1,2_x,2_y',2_z'\} = 3_{xyz}\cdot\{1,2_x',2_y,2_z'\}\cdot 3_{xyz}^{-1} = 3_{xyz}^{-1}\cdot\{1,2_x',2_y',2_z\}\cdot 3_{xyz}$) and therefore they are members of the same equivalence class. For category (12), the six generated groups are all in the same equivalence class because $\{1,2_x'^*,2_y^*,2_z'\} = 3_{xyz}\cdot\{1,2_x^*,2_y',2_z'^*\}\cdot 3_{xyz}^{-1} = 3_{xyz}^{-1}\cdot\{1,2_x',2_y'^*,2_z^*\}\cdot 3_{xyz} = 4_x\cdot\{1,2_x'^*,2_y',2_z^*\}\cdot 4_x^{-1} = 4_x\cdot 3_{xyz}\cdot\{1,2_x',2_y^*,2_z'^*\}\cdot 3_{xyz}^{-1}\cdot 4_x^{-1} = 4_x\cdot 3_{xyz}^{-1}\cdot\{1,2_x^*,2_y'^*,2_z'\}\cdot 3_{xyz}\cdot 4_x^{-1}$. This is demonstrated with point-group diagrams in Fig. 3.

Proper affine equivalence and other definitions of equivalence are discussed in Appendix *C*.

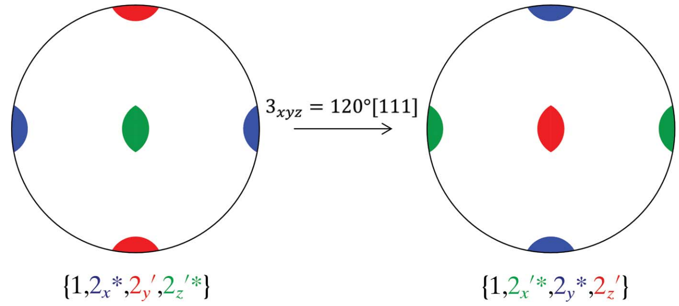


Figure 3
Demonstration of proper affine equivalence of **Q**(**H**){**K**} groups generated for **Q** = **222** using point-group diagrams (stereographic projections).

2.4. Derivation of the double antisymmetry space-group types

Double antisymmetry space-group types of categories (1) through (11) of Table 1 are already known or easily derived. The group types of category (1) are the well known 230 conventional space-group types. The groups of categories (2), (4), (5) and (8) are effectively just products of the groups of category (1) with **1′**, **1***, **1′1*** and **1′***, respectively. The groups of category (3) are the well known black-and-white space groups (Belov *et al.*, 1955, 1957*a*,*b*) [also known as type **M** magnetic space groups (Opechowski, 1986)]. The groups of categories (7) and (11) are derived by substituting starred operations and prime–starred operations, respectively, for the primed operations of category (3) groups. And finally, the groups of categories (6), (9) and (10) are products of the groups of categories (3), (7) and (11), respectively, with **1***, **1′** and **1′***, respectively.

For the groups of category (12) we have used the following four-step procedure:

(i) For one representative group **Q** from each of the 230 types of crystallographic space groups, we list all subgroups of index 2 (Aroyo, Kirov *et al.*, 2006; Aroyo, Perez-Mato *et al.*, 2006; Aroyo *et al.*, 2011).

(ii) We construct and list all double antisymmetry space groups **Q**(**H**){**K**} for each representative group **Q** and pairs of distinct subgroups, **H** and **K**, of index 2. This step results in 26 052 **Q**(**H**){**K**} groups.

(iii) For every pair of groups $\mathbf{Q}_1(\mathbf{H}_1)\{\mathbf{K}_1\}$ and $\mathbf{Q}_2(\mathbf{H}_2)\{\mathbf{K}_2\}$ where $\mathbf{Q}_1$ and $\mathbf{Q}_2$, $\mathbf{H}_1$ and $\mathbf{H}_2$ and $\mathbf{K}_1$ and $\mathbf{K}_2$ are pairwise of the same space-group type, we evaluate the proper affine equivalence relation to determine if $\mathbf{Q}_1(\mathbf{H}_1)\{\mathbf{K}_1\}$ and $\mathbf{Q}_2(\mathbf{H}_2)\{\mathbf{K}_2\}$ are of the same double antisymmetry space-group type.

(iv) From each set of groups belonging to the same type, we list one representative double antisymmetry space group.

Further details for each of these steps are given in §5.

3. Tables of double antisymmetry space groups

3.1. Double antisymmetry space-group types

The serial number, symbol and symmetry operations of a representative group of each of the 17 803 double antisymmetry space-group types are given in the supplementary material 'Double Antisymmetry Space Groups.pdf'.[1] The double antisymmetry space-group symbols are based on the Hermann–Mauguin symbol of the colorblind parent space group, *e.g.* $C2'/m^*$ is based on $C2/m$.

The first part of the symbol gives the lattice centering (or more precisely the translational subgroup). If there are no colored translations in the group, then this part of the symbol is given as *P* (primitive), *C* (*C*-face centered), *A* (*A*-face centered), *I* (body centered), *F* (all-face centered) or *R* (rhombohedrally centered). If there are colored translations, then *P*, *C*, *A*, *I*, *F* or *R* is followed by three color operations in parentheses, *e.g.* $C(1,1'^*,1')2/m'^*$. These three color operations denote the coloring of a minimal set of generating lattice translations indicated in Table 2. For example, consider

[1] Supplementary material for this paper is available from the IUCr electronic archives (Reference: PC5029). Some of this material is available at: http://sites.psu.edu/gopalan/research/symmetry/.

Table 2
Positions of generating translations.

Lattice symbol P(1,1,1)	First position P(**1**,1,1)	Second position P(1,**1**,1)	Third position P(1,1,**1**)
P	$t_{[100]}$	$t_{[010]}$	$t_{[001]}$
C	$t_{[100]}$	$t_{[001]}$	$t_{[\frac{1}{2}\frac{1}{2}0]}$
A	$t_{[100]}$	$t_{[010]}$	$t_{[0\frac{1}{2}\frac{1}{2}]}$
I	$t_{[100]}$	$t_{[001]}$	$t_{[\frac{1}{2}\frac{1}{2}\frac{1}{2}]}$
F	$t_{[0\frac{1}{2}\frac{1}{2}]}$	$t_{[\frac{1}{2}0\frac{1}{2}]}$	$t_{[\frac{1}{2}\frac{1}{2}0]}$
R	$t_{[001]}$	$t_{[\frac{2}{3}\frac{1}{3}\frac{1}{3}]}$	$t_{[\frac{1}{3}\frac{2}{3}\frac{2}{3}]}$

$C(1,1'^*,1')2/m'^*$: 1 is in the first position, $1'^*$ is in the second position and $1'$ is in the third position. Looking up the lattice symbol '*C*' in the first column of Table 2, we find that the first, second and third positions correspond to $t_{[100]}$, $t_{[001]}$ and $t_{[\frac{1}{2}\frac{1}{2}0]}$, respectively. The translations of $C(1,1'^*,1')2/m'^*$ are therefore generated by $t_{[100]}$, $t_{[001]}{}'^*$ and $t_{[\frac{1}{2}\frac{1}{2}0]}{}'$.

The second part of the symbol gives the remaining generators for the double antisymmetry space group. This is also based on the corresponding part of the Hermann–Mauguin symbol of the colorblind parent space group. The Seitz notation of each character is given in 'secondPartOfSymbolGenerators.pdf' in the supplementary material.

Finally, if the group is a member of category (2), (4), (5), (6), (8), (9) or (10), then $1'$, 1^*, $1'1^*$, 1^*, $1'^*$, $1'$, $1'^*$ or $1'^*$, respectively, is appended to the end of the symbol.

3.2. Using the Computable Document Format (CDF) file

The Computable Document Format (CDF) file 'Double antisymmetry space groups.cdf' (supplementary material) provides an interactive way to find the symbols and operations of double antisymmetry space groups. The file is opened with the Wolfram CDF Player which can be downloaded from http://www.wolfram.com/cdf-player/. After opening the file, click 'Enable Dynamics' if prompted. Provide the necessary input with the drop-down menus.

A tutorial with screenshots is given in 'Double antisymmetry space groups CDF tutorial.pdf (supplementary material).

3.3. Using the PDF file

In the PDF file 'Double Antisymmetry Space Groups.pdf' (supplementary material), the 17 803 double antisymmetry space groups are listed sequentially. The first portion of the file contains links to each group entry. These links are sorted by the colorblind parent group, *e.g.* $C2'/m^*$ is listed under the space-group number of $C2/m$ (*i.e.* 'SG. 12').

The first line of each entry gives the sequential serial number (1 through 17 803), the double antisymmetry space-group symbol and the X-ray diffraction symmetry group (*i.e.* the symmetry group obtained by removing all of the starred and prime–starred operations and changing all of the primed operations to colorless operations). The second line gives the number of the colorblind parent group, the double antisymmetry point group and the crystal system. The remaining lines give the symmetry operations of the group: a set of coset representatives of the group with respect to the translational subgroup generated by translations of the conventional unit cell. These symmetry operations are given in *International Tables* Volume A notation and Seitz notation. Three examples from the listings of double antisymmetry space groups are given in Table 3.

3.4. Machine-readable file

The 'machine-readable' file 'DASGMachineReadable.txt' (supplementary material) is intended to provide a simple way to use the double antisymmetry space groups in code or software such as *MatLab* or *Mathematica*. The structure of the file is given in the supplementary material file called 'Using the Machine Readable File.pdf'. The file 'Import DASGMachineReadable.nb' (supplementary material) has been provided to facilitate loading into *Mathematica*.

4. Symmetry diagrams

Symmetry diagrams have been made for the example double antisymmetry space groups listed in Table 3. These diagrams are intended to extend the conventional space-group diagrams such as those in *International Tables for Crystallography* Volume A.

In Fig. 4(*a*), double antisymmetry space group No. 8543, $C2'/m^*$, is projected along the *b* axis. In Fig. 4(*b*), double antisymmetry space group No. 16490, $I4^*/mm'm'^*$, is projected along the *c* axis. In Fig. 4(*c*), double antisymmetry space group No. 13461, $Ib'^*c'a'$, is projected along the *c* axis. As with Fig. 4(*a*), the symbols in these diagrams are naturally extended from those used for conventional space groups in *International Tables for Crystallography* Volume A.

5. Computation details

The majority of the computation was performed in *Mathematica* using 4 × 4 augmented matrices to represent space-group operations and unit-cell transformations (more generally, affine transformations). The use of augmented matrices to represent space-group operations and unit-cell transformations is described in *International Tables for Crystallography* Volume A, Chapters 5.1 and 8.1. These matrices were downloaded for each space-group type from the *GENPOS* tool on the Bilbao Crystallographic Server, http://www.cryst.ehu.es/cryst/get_gen.html (Aroyo, Kirov *et al.*, 2006; Aroyo, Perez-Mato *et al.*, 2006; Aroyo *et al.*, 2011). The standard setting was used for each of the 230 space-group types as given in *International Tables for Crystallography* Volume A.

5.1. Augmented matrices

Every space-group operation can be broken up into a linear transformation **R** and a translation **t** which transform the coordinates (r_1, r_2, r_3) into (r_1', r_2', r_3'):

Table 3
Examples of double antisymmetry space-group listings.

No. 8543	$C2'/m^*$	$C2$
SG. 12	$2'/m^*$	**Monoclinic**

Symmetry Operations

For $(0,0,0)+$ **set**

(1) 1 $(1\|000)$	(2) $2'\ 0,y,0$ $(2_y\|000)'$	(3) $\bar{1}'^*\ 0,0,0$ $(\bar{1}\|000)'^*$	(4) $m^*\ x,0,z$ $(m_y\|000)^*$

For $(\frac{1}{2},\frac{1}{2},0)+$ **set**

(1) $t(\frac{1}{2},\frac{1}{2},0)$ $(1\|\frac{1}{2}\frac{1}{2}0)$	(2) $2(0,\frac{1}{2},0)'\ \frac{1}{4},y,0$ $(2_y\|\frac{1}{2}\frac{1}{2}0)'$	(3) $\bar{1}'^*\ \frac{1}{4},\frac{1}{4},0$ $(\bar{1}\|\frac{1}{2}\frac{1}{2}0)'^*$	(4) $a^*\ x,\frac{1}{4},z$ $(m_y\|\frac{1}{2}\frac{1}{2}0)^*$

No. 16490	$I4^*/mm'm'^*$	$Immm$
SG. 139	$4^*/mm'm'^*$	**Tetragonal**

Symmetry Operations

For $(0,0,0)+$ **set**

(1) 1 $(1\|000)$	(2) $2\ 0,0,z$ $(2_z\|000)$	(3) $4^{+*}\ 0,0,z$ $(4_z\|000)^*$	(4) $4^{-*}\ 0,0,z$ $(4_z{}^{-1}\|000)^*$
(5) $2'\ 0,y,0$ $(2_y\|000)'$	(6) $2'\ x,0,0$ $(2_x\|000)'$	(7) $2'^*\ x,x,0$ $(2_{xy}\|000)'^*$	(8) $2'^*\ x,\bar{x},0$ $(2_{x\bar{y}}\|000)'^*$
(9) $\bar{1}\ 0,0,0$ $(\bar{1}\|000)$	(10) $m\ x,y,0$ $(m_z\|000)$	(11) $\bar{4}^{+*}\ 0,0,z;0,0,0$ $(\bar{4}_z\|000)^*$	(12) $\bar{4}^{-*}\ 0,0,z;0,0,0$ $(\bar{4}_z{}^{-1}\|000)^*$
(13) $m'\ x,0,z$ $(m_y\|000)'$	(14) $m'\ 0,y,z$ $(m_x\|000)'$	(15) $m'^*\ x,\bar{x},z$ $(m_{xy}\|000)'^*$	(16) $m'^*\ x,x,z$ $(m_{x\bar{y}}\|000)'^*$

For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$ **set**

(1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ $(1\|\frac{1}{2}\frac{1}{2}\frac{1}{2})$	(2) $2(0,0,\frac{1}{2})\ \frac{1}{4},\frac{1}{4},z$ $(2_z\|\frac{1}{2}\frac{1}{2}\frac{1}{2})$	(3) $4^+(0,0,\frac{1}{2})^*\ 0,\frac{1}{2},z$ $(4_z\|\frac{1}{2}\frac{1}{2}\frac{1}{2})^*$	(4) $4^-(0,0,\frac{1}{2})^*\ \frac{1}{2},0,z$ $(4_z{}^{-1}\|\frac{1}{2}\frac{1}{2}\frac{1}{2})^*$
(5) $2(0,\frac{1}{2},0)'\ \frac{1}{4},y,\frac{1}{4}$ $(2_y\|\frac{1}{2}\frac{1}{2}\frac{1}{2})'$	(6) $2(\frac{1}{2},0,0)'\ x,\frac{1}{4},\frac{1}{4}$ $(2_x\|\frac{1}{2}\frac{1}{2}\frac{1}{2})'$	(7) $2(\frac{1}{2},\frac{1}{2},0)'^*\ x,x,\frac{1}{4}$ $(2_{xy}\|\frac{1}{2}\frac{1}{2}\frac{1}{2})'^*$	(8) $2'^*\ x,\bar{x}+\frac{1}{2},\frac{1}{4}$ $(2_{x\bar{y}}\|\frac{1}{2}\frac{1}{2}\frac{1}{2})'^*$
(9) $\bar{1}\ \frac{1}{4},\frac{1}{4},\frac{1}{4}$ $(\bar{1}\|\frac{1}{2}\frac{1}{2}\frac{1}{2})$	(10) $n(\frac{1}{2},\frac{1}{2},0)\ x,y,\frac{1}{4}$ $(m_z\|\frac{1}{2}\frac{1}{2}\frac{1}{2})$	(11) $\bar{4}^{+*}\ \frac{1}{2},0,z;\frac{1}{2},0,\frac{1}{4}$ $(\bar{4}_z\|\frac{1}{2}\frac{1}{2}\frac{1}{2})^*$	(12) $\bar{4}^{-*}\ 0,\frac{1}{2},z;0,\frac{1}{2},\frac{1}{4}$ $(\bar{4}_z{}^{-1}\|\frac{1}{2}\frac{1}{2}\frac{1}{2})^*$
(13) $n(\frac{1}{2},0,\frac{1}{2})'\ x,\frac{1}{4},z$ $(m_y\|\frac{1}{2}\frac{1}{2}\frac{1}{2})'$	(14) $n(0,\frac{1}{2},\frac{1}{2})'\ \frac{1}{4},y,z$ $(m_x\|\frac{1}{2}\frac{1}{2}\frac{1}{2})'$	(15) $c'^*\ x+\frac{1}{2},\bar{x},z$ $(m_{xy}\|\frac{1}{2}\frac{1}{2}\frac{1}{2})'^*$	(16) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})'^*\ x,x,z$ $(m_{x\bar{y}}\|\frac{1}{2}\frac{1}{2}\frac{1}{2})'^*$

No. 13461	$Ib'^*c'a'$	$Iba2$ $c,a,b+\frac{1}{4}$
SG. 73	$m'^*m'm'$	**Orthorhombic**

Symmetry Operations

For $(0,0,0)+$ **set**

(1) 1 $(1\|000)$	(2) $2(0,0,\frac{1}{2})^*\ \frac{1}{4},0,z$ $(2_z\|\frac{1}{2}0\frac{1}{2})^*$	(3) $2(0,\frac{1}{2},0)^*\ 0,y,\frac{1}{4}$ $(2_y\|0\frac{1}{2}\frac{1}{2})^*$	(4) $2(\frac{1}{2},0,0)\ x,\frac{1}{4},0$ $(2_x\|\frac{1}{2}\frac{1}{2}0)$
(5) $\bar{1}'^*\ 0,0,0$ $(\bar{1}\|000)'^*$	(6) $a'\ x,y,\frac{1}{4}$ $(m_z\|\frac{1}{2}0\frac{1}{2})'$	(7) $c'\ x,\frac{1}{4},z$ $(m_y\|0\frac{1}{2}\frac{1}{2})'$	(8) $b'^*\ \frac{1}{4},y,z$ $(m_x\|\frac{1}{2}\frac{1}{2}0)'^*$

For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$ **set**

(1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ $(1\|\frac{1}{2}\frac{1}{2}\frac{1}{2})$	(2) $2^*\ 0,\frac{1}{4},z$ $(2_z\|0\frac{1}{2}0)^*$	(3) $2^*\ \frac{1}{4},y,0$ $(2_y\|\frac{1}{2}00)^*$	(4) $2\ x,0,\frac{1}{4}$ $(2_x\|00\frac{1}{2})$
(5) $\bar{1}'^*\ \frac{1}{4},\frac{1}{4},\frac{1}{4}$ $(\bar{1}\|\frac{1}{2}\frac{1}{2}\frac{1}{2})'^*$	(6) $b'\ x,y,0$ $(m_z\|0\frac{1}{2}0)'$	(7) $a'\ x,0,z$ $(m_y\|\frac{1}{2}00)'$	(8) $c'^*\ 0,y,z$ $(m_x\|00\frac{1}{2})'^*$

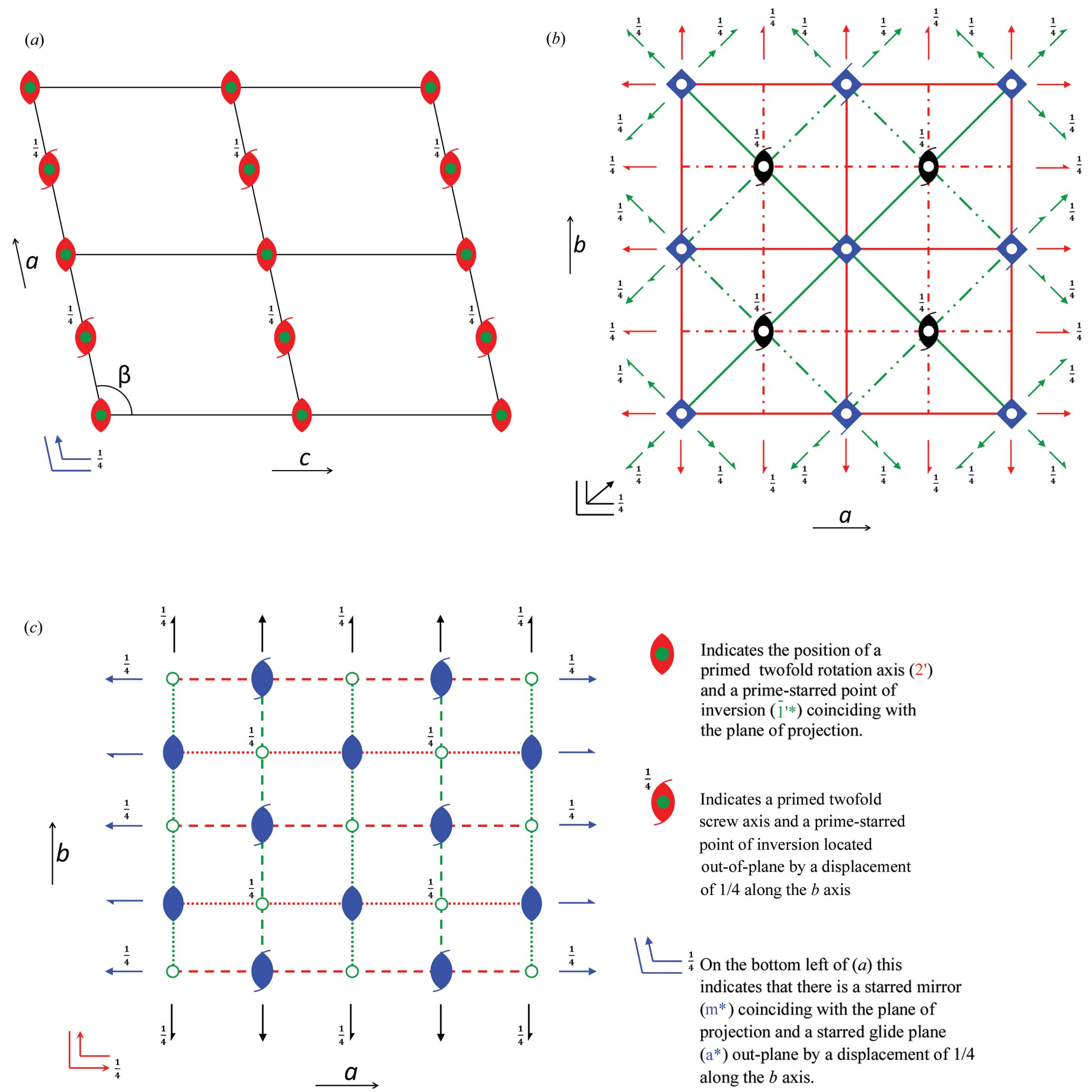


Figure 4
Example double antisymmetry space-group diagrams. (*a*) No. 8543 *C*2′/*m**, (*b*) No. 16490 *I*4*/*mm*′*m*′*, (*c*) No. 13461, *Ib*′**c*′*a*′. The legend relates to part (*a*).

$$\mathbf{r}' = \mathbf{R}\mathbf{r} + \mathbf{t},$$

$$\begin{pmatrix} r'_1 \\ r'_2 \\ r'_3 \end{pmatrix} = \begin{pmatrix} R_{11} & R_{12} & R_{13} \\ R_{21} & R_{22} & R_{23} \\ R_{31} & R_{32} & R_{33} \end{pmatrix} \begin{pmatrix} r_1 \\ r_2 \\ r_3 \end{pmatrix} + \begin{pmatrix} t_1 \\ t_2 \\ t_3 \end{pmatrix}. \quad (1)$$

It is convenient to condense this linear transformation and translation into a single square matrix called an *augmented matrix*:

$$\begin{pmatrix} r'_1 \\ r'_2 \\ r'_3 \\ 1 \end{pmatrix} = \begin{pmatrix} R_{11} & R_{12} & R_{13} & t_1 \\ R_{21} & R_{22} & R_{23} & t_2 \\ R_{31} & R_{32} & R_{33} & t_3 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} r_1 \\ r_2 \\ r_3 \\ 1 \end{pmatrix}. \quad (2)$$

Note that the final row is necessary to make a square 4×4 matrix but contains no information specific to the transformation. When using these augmented matrices to represent space-group operations, the product of two space-group operations is evaluated by matrix multiplication, *i.e.* g_1g_2 is performed by multiplying the matrices which represent g_1 and g_2 to get a product matrix which is also an augmented matrix that represents a space-group operation. The inverse of a space-group operation is represented by the matrix inverse of the operation's augmented matrix. The sign of the determinant of an augmented matrix representing a space-group operation determines if it is proper (orientation-preserving). A positive determinant means that it is proper.

For a set of 4×4 matrices $\mathbf{S}$ and a 4×4 matrix A, we will denote the set formed by the similarity transformation of each element of $\mathbf{S}$ by A as $A\mathbf{S}A^{-1}$, *i.e.* $A\mathbf{S}A^{-1} = \{AsA^{-1} : s \in \mathbf{S}\}$.

5.2. Index-2 subgroups

To evaluate the formulae in Table 1 for any given colorblind parent space group $\mathbf{Q}$, the index-2 subgroups of $\mathbf{Q}$ are needed. The index-2 subgroups of a space group are also space groups themselves. As such, every index-2 subgroup of space group $\mathbf{Q}$ must be one of the 230 types of space groups. Using this, we can specify an index-2 subgroup of $\mathbf{Q}$ by specifying the type of the subgroup (1 to 230) and a transformation from a standard representative group of that type. This is to say that $\mathbf{H}$, a subgroup of $\mathbf{Q}$, can be specified by a standard representative group $\mathbf{H}_0$ and the transformation T such that $\mathbf{H} = T\mathbf{H}_0T^{-1}$. Note, this is just the usual linear algebra change-of-basis formula; we are simply using T to transform from the standard conventional basis to the basis which makes $\mathbf{H}$ a subgroup of $\mathbf{Q}$.

$\mathbf{Q}$, $\mathbf{H}$ and $\mathbf{H}_0$ are each represented by a set of 4×4 real matrices. T is represented by a single 4×4 real matrix. For every element h in $\mathbf{H}$ there is an element h_0 in $\mathbf{H}_0$ such that $h = Th_0T^{-1}$. Thus, we make the set of matrices representing $\mathbf{H}$ by computing Th_0T^{-1} for each matrix in the set representing $\mathbf{H}_0$.

The index-2 subgroup data were downloaded from the Bilbao Crystallographic Server. Altogether there are 1848 index-2 subgroups among the 230 representative space groups. Each entry (out of 1848) consisted of: a number between 1 and 230 for the space-group type of $\mathbf{Q}$, a number between 1 and 230 for the space-group type of $\mathbf{H}_0$ and a 4×4 matrix for T.

5.3. Normalizer method for evaluating the proper affine equivalence of Q(H){K} groups

The proper affine equivalence relation can be defined as: two groups, $\mathbf{G}_1$ and $\mathbf{G}_2$, are equivalent if and only if $\mathbf{G}_1$ can be bijectively mapped to $\mathbf{G}_2$ by a proper affine transformation, a. Expressed in mathematical shorthand, this is

$$\mathbf{G}_2 \sim \mathbf{G}_1 \equiv \exists a \in \mathscr{A}^+ : \left(\mathbf{G}_2 = a\mathbf{G}_1a^{-1}\right), \qquad (3)$$

where $\sim$ is the proper affine equivalence relational operator, $\equiv$ is logical equivalence ('is logically equivalent to'), $\exists a$ is the existential quantification of a ('there exists a'), $\in$ means 'an element of', : means 'such that' and $\mathscr{A}^+$ is the group of proper affine transformations. An *affine transformation* is the combination of a linear transformation and a translation. A *proper affine transformation* is an affine transformation that preserves chirality.

For evaluating the proper affine equivalence of a pair of $\mathbf{Q}(\mathbf{H})\{\mathbf{K}\}$ groups, if the space-group types of $\mathbf{Q}$, $\mathbf{H}$ and $\mathbf{K}$ of one of the $\mathbf{Q}(\mathbf{H})\{\mathbf{K}\}$ groups are not the same as those of the other, then the proper affine equivalence relation fails and no further work is necessary. For a pair of $\mathbf{Q}(\mathbf{H})\{\mathbf{K}\}$ groups where they are the same, we have derived a method to evaluate proper affine equivalence based on affine normalizer groups. To begin this derivation, we can expand the proper affine equivalence for $\mathbf{Q}(\mathbf{H})\{\mathbf{K}\}$ groups to

$$\mathbf{Q}(\mathbf{H}_2)\{\mathbf{K}_2\} \sim \mathbf{Q}(\mathbf{H}_1)\{\mathbf{K}_1\} \equiv \exists a \in \mathscr{A}^+ : \left(\mathbf{Q} = a\mathbf{Q}a^{-1}\right) \wedge \left(\mathbf{H}_2 = a\mathbf{H}_1a^{-1}\right) \wedge \left(\mathbf{K}_2 = a\mathbf{K}_1a^{-1}\right), \qquad (4)$$

where $\wedge$ denotes logical conjunction ('and'). The subscripts have been omitted for $\mathbf{Q}_1$ and $\mathbf{Q}_2$ because we are testing the equivalence of $\mathbf{Q}(\mathbf{H})\{\mathbf{K}\}$ groups where $\mathbf{Q}_1 = \mathbf{Q}_2$. We can use the definition of the proper affine normalizer group of $\mathbf{Q}$, *i.e.* $\mathbf{N}_{\mathscr{A}^+}(\mathbf{Q}) = \{a \in \mathscr{A}^+ : \mathbf{Q} = a\mathbf{Q}a^{-1}\}$[2] (Opechowski, 1986), to get

$$\mathbf{Q}(\mathbf{H}_2)\{\mathbf{K}_2\} \sim \mathbf{Q}(\mathbf{H}_1)\{\mathbf{K}_1\} \equiv \exists a \in \mathbf{N}_{\mathscr{A}^+}(\mathbf{Q}) : \left(\mathbf{H}_2 = a\mathbf{H}_1a^{-1}\right) \wedge \left(\mathbf{K}_2 = a\mathbf{K}_1a^{-1}\right). \qquad (5)$$

$\mathbf{H}_1$ and $\mathbf{H}_2$ are mapped by proper affine transformations, T_{H_1} and T_{H_2}, respectively, from a standard representative group, $\mathbf{H}_0$, as follows: $\mathbf{H}_1 = T_{H_1}\mathbf{H}_0{T_{H_1}}^{-1}$ and $\mathbf{H}_2 = T_{H_2}\mathbf{H}_0{T_{H_2}}^{-1}$. Likewise, $\mathbf{K}_1$ and $\mathbf{K}_2$ are mapped by proper affine transformations, T_{K_1} and T_{K_2}, respectively, from a standard representative group, $\mathbf{K}_0$, as follows: $\mathbf{K}_1 = T_{K_1}\mathbf{K}_0{T_{K_1}}^{-1}$ and $\mathbf{K}_2 = T_{K_2}\mathbf{K}_0{T_{K_2}}^{-1}$. Thus, by substitution, $(\mathbf{H}_2 = a\mathbf{H}_1a^{-1}) \wedge (\mathbf{K}_2 = a\mathbf{K}_1a^{-1})$ is equivalent to $(T_{H_2}\mathbf{H}_0T_{H_2}^{-1} = aT_{H_1}\mathbf{H}_0T_{H_1}^{-1}a^{-1}) \wedge (T_{K_2}\mathbf{K}_0T_{K_2}^{-1} = aT_{K_1}\mathbf{K}_0T_{K_1}^{-1}a^{-1})$, which can be rearranged to $(\mathbf{H}_0 = (T_{H_2}^{-1}aT_{H_1})\mathbf{H}_0(T_{H_2}^{-1}aT_{H_1})^{-1}) \wedge (\mathbf{K}_0 = (T_{K_2}^{-1}aT_{K_1})\mathbf{K}_0(T_{K_2}^{-1}aT_{K_1})^{-1})$. By applying the definition of a normalizer group again, we find that $T_{H_2}^{-1}aT_{H_1} \in \mathbf{N}_{\mathscr{A}^+}(\mathbf{H}_0)$ and $T_{K_2}^{-1}aT_{K_1} \in \mathbf{N}_{\mathscr{A}^+}(\mathbf{K}_0)$, which rearrange to $a \in T_{H_2}\mathbf{N}_{\mathscr{A}^+}(\mathbf{H}_0)T_{H_1}^{-1}$ and $a \in T_{K_2}\mathbf{N}_{\mathscr{A}^+}(\mathbf{K}_0)T_{K_1}^{-1}$, respectively. Therefore, the proper affine equivalence of $\mathbf{Q}(\mathbf{H}_1)\{\mathbf{K}_1\}$ and $\mathbf{Q}(\mathbf{H}_2)\{\mathbf{K}_2\}$ is logically equivalent to the existence of a non-empty intersection of $\mathbf{N}_{\mathscr{A}^+}(\mathbf{Q})$, $T_{H_2}\mathbf{N}_{\mathscr{A}^+}(\mathbf{H}_0)T_{H_1}^{-1}$ and $T_{K_2}\mathbf{N}_{\mathscr{A}^+}(\mathbf{K}_0)T_{K_1}^{-1}$:

$$\mathbf{Q}(\mathbf{H}_1)\{\mathbf{K}_1\} \sim \mathbf{Q}(\mathbf{H}_2)\{\mathbf{K}_2\} \equiv \mathbf{N}_{\mathscr{A}^+}(\mathbf{Q}) \cap T_{H_2}\mathbf{N}_{\mathscr{A}^+}(\mathbf{H}_0)T_{H_1}^{-1} \cap T_{K_2}\mathbf{N}_{\mathscr{A}^+}(\mathbf{K}_0)T_{K_1}^{-1} \neq \emptyset. \qquad (6)$$

This simplifies the problem of evaluating the equivalence relation to either proving that the intersection has at least one member or proving that it does not. To do this, we applied *Mathematica*'s built-in 'FindInstance' function. As with the subgroup data, the normalizer group data were downloaded from the Bilbao Crystallographic Server. As previously discussed, the formulae in Table 1 generate 38 290 double antisymmetry space groups when applied to all 230 representative space groups. With the aid of *Mathematica*, these 38 290 double antisymmetry space groups were partitioned by

[2] If $\mathbf{Q}$ contains improper motions, then $\mathbf{N}_{\mathscr{A}^+}(\mathbf{Q})$ is not actually a normalizer group because $\mathbf{Q} \not\subset \mathscr{A}^+$. In these cases, $\mathbf{N}_{\mathscr{A}^+}(\mathbf{Q})$ can be interpreted as $\mathbf{N}_{\mathscr{A}}(\mathbf{Q}) \cap \mathscr{A}^+$. This does not affect the results.

Table 4
Double antisymmetry space-group generating sets listed by Zamorzaev & Palistrant (1980).

The numbers in the second and third columns refer to the number of unique types obtained by the permutation of anti-identities.

Generating line from Zamorzaev & Palistrant (1980)	Symbol in present work	No. of types (Zamorzaev & Palistrant)	Actual number (present work)	Difference
$\{a, b, \frac{a+b+c}{2}\}\left(\frac{c}{2}2' \cdot \frac{b}{2}m : \frac{a}{2}2^{*}_{\frac{b}{4}}\right)$	$Ibc'a'^{*}$	6	3	−3
$\{a, b, \frac{a+b+c}{2}\}\left(\frac{c}{2}2' \cdot \frac{b}{2}m^{*} : \frac{a}{2}2^{*}_{\frac{b}{4}}\right)$	$Ib^{*}c'^{*}a'$	2	1	−1

the equivalence relation given in equation (3) into 17 803 proper affine equivalence classes, *i.e.* 17 803 *double antisymmetry space-group types*.

This method can be easily generalized to other types of antisymmetry and color symmetry. For example, for antisymmetry groups formed from one index-2 subgroup, such as $\mathbf{Q}(\mathbf{H})$ groups, the condition simply reduces to the following:

$$\mathbf{Q}(\mathbf{H}_1) \sim \mathbf{Q}(\mathbf{H}_2) \equiv N_{\mathscr{A}^+}(\mathbf{Q}) \cap T_{H_2} N_{\mathscr{A}^+}(\mathbf{H}_0) T_{H_1}^{-1} \neq \emptyset. \quad (7)$$

For finding the double antisymmetry space-group types, only conditions for $\mathbf{Q}(\mathbf{H})$ and $\mathbf{Q}(\mathbf{H})\{\mathbf{K}\}$ groups are necessary. This is because it is trivial to map these results to all the other categories of double antisymmetry space groups. This normalizer method is demonstrated in Appendix *B* to derive all double antisymmetry space-group types where $\mathbf{Q} = Cc$.

6. Number of types of double antisymmetry space groups

The total number of types of double antisymmetry space groups listed by the present work is 17 803. The total number of $\mathbf{Q}(\mathbf{H})\{\mathbf{K}\}$ types listed by the present work is 9507. These values differ from those given by Zamorzaev & Palistrant (1980). We have found four fewer $\mathbf{Q}(\mathbf{H})\{\mathbf{K}\}$ types where $\mathbf{Q}$ = *Ibca* (No. 73 in *International Tables for Crystallography* Volume A). Since there are only a small number of discrepancies between our listing and the numbers calculated by Zamorzaev & Palistrant, each will be addressed explicitly.

Zamorzaev & Palistrant (1980) gave a list of double antisymmetry space-group generators in noncoordinate notation (Koptsik & Shubnikov, 1974). For *Ibca* [21*a* in Zamorzaev & Palistrant (1980)] the following generators are used:

$$\left\{a, b, \frac{a+b+c}{2}\right\}\left(\frac{c}{2}2 \cdot \frac{b}{2}m : \frac{a}{2}2_{\frac{b}{4}}\right).$$

$a, b, \frac{a+b+c}{2}, \frac{c}{2}2, \frac{b}{2}m$ and $\frac{a}{2}2_{\frac{b}{4}}$ can be interpreted, in Seitz notation, as $(1|100)$, $(1|010)$, $(1|\frac{1}{2}\frac{1}{2}\frac{1}{2})$, $(2_z|\frac{1}{2}0\frac{1}{2})$, $(m_x|\frac{1}{2}\frac{1}{2}0)$ and $(2_x|\frac{1}{2}\frac{1}{2}0)$, respectively.

Zamorzaev & Palistrant (1980) couple these generators with anti-identities to give generating sets for double antisymmetry space groups. However, unlike the more explicit listing given in the present work, Zamorzaev & Palistrant give only generating sets and only those that are unique under the permutations of the elements of $\mathbf{1'1^*}$ that preserve the group structure, *i.e.* the automorphisms of $\mathbf{1'1^*}$. Because of this concise method of listing generating sets (only 1846 $\mathbf{Q}(\mathbf{H})\{\mathbf{K}\}$ generating sets are necessary), a single generating set given by Zamorzaev & Palistrant (1980) can represent up to six types under the proper affine equivalence relation. The six possible types correspond to the six automorphisms of $\mathbf{1'1^*}$.

The automorphisms of $\mathbf{1'1^*}$ correspond to the possible permutations of the three anti-identities of double antisymmetry: $(1', 1^*, 1'^*)$, $(1', 1'^*, 1^*)$, $(1^*, 1', 1'^*)$, $(1^*, 1'^*, 1')$, $(1'^*, 1', 1^*)$ and $(1'^*, 1^*, 1')$, *i.e.* $\mathrm{Aut}(\mathbf{1'1^*}) \cong \mathbf{S}_3$. Zamorzaev & Palistrant give the number of types represented by each line, but not which automorphisms must be applied to get them. This is discussed in the supplementary material file called 'Color Automorphisms of Double Antisymmetry.pdf'. There are only two lines of generators from Zamorzaev & Palistrant for which their resulting number of $\mathbf{Q}(\mathbf{H})\{\mathbf{K}\}$ types differs from this work. These lines are given in Table 4.

Applying the six automorphisms of $\mathbf{1'1^*}$ to $Ibc'a'^*$ from the first line of Table 4, we get $Ibc'a'^*$, $Ibc'a^*$, $Ibc^*a'^*$, Ibc^*a', Ibc'^*a^* and Ibc'^*a'. According to Zamorzaev & Palistrant, these are six distinct types whereas there are actually only three distinct types. $Ibc'a'^*$ and Ibc'^*a' are of type No. 13460. $Ibc'a^*$ and Ibc^*a' are of type No. 13462. $Ibc^*a'^*$ and Ibc'^*a^* are of type No. 13450. Applying the six automorphisms of $\mathbf{1'1^*}$ to $Ib^*c'^*a'$ from the second line of Table 4, we get $Ib^*c'^*a'$, Ib'^*c^*a', $Ib'c'^*a^*$, $Ib'^*c'a^*$, $Ib'c^*a'^*$ and $Ib^*c'a'^*$. According to Zamorzaev & Palistrant, these correspond to two distinct types whereas they are actually all the same type, No. 13447.

Consequently, the generators in the first line of Table 4 map to three types and the generators in the second line map to one type, not six and two, respectively. Thus, there are four fewer $\mathbf{Q}(\mathbf{H})\{\mathbf{K}\}$ types than the number given by Zamorzaev & Palistrant (1980), *i.e.* 9507 rather than 9511. This error likely affects the number of higher-order multiple antisymmetry groups calculated by Zamorzaev & Palistrant as well. We conjecture that there are 24 fewer non-trivial triple antisymmetry space groups than calculated by Zamorzaev & Palistrant but that the numbers for other multiple antisymmetries are correct. If we are correct, this would mean that the numbers in the final column of Table 1 of 'Generalized Antisymmetry' by Zamorzaev (1988) should read 230, 1191, 9507, 109115, 1640955, 28331520 and 419973120, rather than 230, 1191, 9511, 109139, 1640955, 28331520 and 419973120 (the numbers which differ are underlined). Similarly, if we are correct, the final column of Table 3 of the same work should read 230, 1651, 17803, 287574, 6879260, 240768842 and 12209789596, rather than 230, 1651, 17807, 287658, 6880800, 240800462 (mistyped as 240900462) and 12210589024.

Our results also confirm that there are 5005 types of $\mathbf{Q}(\mathbf{H})\{\mathbf{K}\}$ Mackay groups (Jablan, 1993*a*, 2002; Radovic & Jablan, 2005).

7. Concluding remarks

It was found that there are 17 803 types of double antisymmetry space groups. This is four fewer than previously stated by Zamorzaev (1988). When rotation-reversal symmetry and time-reversal symmetry are considered together with the periodic spatial symmetry of a three-dimensional crystal, our results show that there are 17 803 distinct types of symmetry that a crystal may exhibit.

APPENDIX *A*
Visual representation of category structures using Venn diagrams

The set structure of each category is visually represented in Fig. 5. These category symbols, *e.g.* **Q(H){K}**, were introduced by Litvin *et al.* (1994, 1995). They are intended as a generalization of the widely used **Q(H)** notation for magnetic groups. The '()' brackets enclose a subset which is not primed. The '{ }' brackets enclose a subset which is not starred. The **1′**, **1***, **1′*** or **1′1*** at the end of a symbol indicates that 1′, 1*, 1′*, or 1′ and 1*, respectively, are elements of the group.

APPENDIX *B*
Additional examples of generating double antisymmetry groups

2/*m* has four elements: $\{1,2,m,-1\}$. **2/*m*** has three index-2 subgroups: $\{1,2\}$, $\{1,m\}$ and $\{1,-1\}$, which will be referred to as **2**, ***m*** and **−1**, respectively.

Category (1): $\mathbf{Q}$
1. $\mathbf{Q} = \mathbf{2/m} \rightarrow \mathbf{Q} = \{1,2,m,-1\}$

Category (2): $\mathbf{Q} + \mathbf{Q}1'$
2. $\mathbf{Q} = \mathbf{2/m} \rightarrow \mathbf{Q1'} = \{1,2,m,-1,1',2',m',-1'\}$

Category (3): $\mathbf{H} + (\mathbf{Q} - \mathbf{H})1'$
3. $\mathbf{Q} = \mathbf{2/m}$, $\mathbf{H} = \mathbf{2} \rightarrow \mathbf{Q(H)} = \{1,2,m',-1'\}$
4. $\mathbf{Q} = \mathbf{2/m}$, $\mathbf{H} = \boldsymbol{m} \rightarrow \mathbf{Q(H)} = \{1,2',m,-1'\}$
5. $\mathbf{Q} = \mathbf{2/m}$, $\mathbf{H} = \mathbf{-1} \rightarrow \mathbf{Q(H)} = \{1,2',m',-1\}$

Category (4): $\mathbf{Q} + \mathbf{Q}1^*$
6. $\mathbf{Q} = \mathbf{2/m} \rightarrow \mathbf{Q1^*} = \{1,2,m,-1,1^*,2^*,m^*,-1^*\}$

Category (5): $\mathbf{Q} + \mathbf{Q}1' + \mathbf{Q}1^* + \mathbf{Q}1'^*$
7. $\mathbf{Q} = \mathbf{2/m} \rightarrow \mathbf{Q1'1^*} = \{1,2,m,-1,1',2',m',-1',1^*,2^*,m^*,-1^*,1'^*,2'^*,m'^*,-1'^*\}$

Category (6): $\mathbf{H} + (\mathbf{Q} - \mathbf{H})1' + \mathbf{H}1^* + (\mathbf{Q} - \mathbf{H})1'^*$
8. $\mathbf{Q} = \mathbf{2/m}$, $\mathbf{H} = \mathbf{2} \rightarrow \mathbf{Q(H)1^*} = \{1,2,m',-1',1^*,2^*,m'^*,-1'^*\}$
9. $\mathbf{Q} = \mathbf{2/m}$, $\mathbf{H} = \boldsymbol{m} \rightarrow \mathbf{Q(H)1^*} = \{1,2',m,-1',1^*,2'^*,m^*,-1'^*\}$
10. $\mathbf{Q} = \mathbf{2/m}$, $\mathbf{H} = \mathbf{-1} \rightarrow \mathbf{Q(H)1^*} = \{1,2',m',-1,1^*,2'^*,m'^*,-1^*\}$

Category (7): $\mathbf{H} + (\mathbf{Q} - \mathbf{H})1^*$
11. $\mathbf{Q} = \mathbf{2/m}$, $\mathbf{H} = \mathbf{2} \rightarrow \mathbf{Q\{H\}} = \{1,2,m^*,-1^*\}$
12. $\mathbf{Q} = \mathbf{2/m}$, $\mathbf{H} = \boldsymbol{m} \rightarrow \mathbf{Q\{H\}} = \{1,2^*,m,-1^*\}$
13. $\mathbf{Q} = \mathbf{2/m}$, $\mathbf{H} = \mathbf{-1} \rightarrow \mathbf{Q\{H\}} = \{1,2^*,m^*,-1\}$

Category (8): $\mathbf{Q} + \mathbf{Q}1'^*$
14. $\mathbf{Q} = \mathbf{2/m} \rightarrow \mathbf{Q1'^*} = \{1,2,m,-1,1'^*,2'^*,m'^*,-1'^*\}$

Category (9): $\mathbf{H} + (\mathbf{Q} - \mathbf{H})1^* + \mathbf{H}1' + (\mathbf{Q} - \mathbf{H})1'^*$
15. $\mathbf{Q} = \mathbf{2/m}$, $\mathbf{H} = \mathbf{2} \rightarrow \mathbf{Q\{H\}1'} = \{1,2,m^*,-1^*,1',2',m'^*,-1'^*\}$
16. $\mathbf{Q} = \mathbf{2/m}$, $\mathbf{H} = \boldsymbol{m} \rightarrow \mathbf{Q\{H\}1'} = \{1,2^*,m,-1^*,1',2'^*,m',-1'^*\}$
17. $\mathbf{Q} = \mathbf{2/m}$, $\mathbf{H} = \mathbf{-1} \rightarrow \mathbf{Q\{H\}1'} = \{1,2^*,m^*,-1,1',2'^*,m'^*,-1'\}$

Category (10): $\mathbf{H} + (\mathbf{Q} - \mathbf{H})1' + \mathbf{H}1'^* + (\mathbf{Q} - \mathbf{H})1^*$
18. $\mathbf{Q} = \mathbf{2/m}$, $\mathbf{H} = \mathbf{2} \rightarrow \mathbf{Q(H)1'^*} = \{1,2,m',-1',1'^*,2'^*,m^*,-1^*\}$
19. $\mathbf{Q} = \mathbf{2/m}$, $\mathbf{H} = \boldsymbol{m} \rightarrow \mathbf{Q(H)1'^*} = \{1,2',m,-1',1'^*,2^*,m'^*,-1^*\}$
20. $\mathbf{Q} = \mathbf{2/m}$, $\mathbf{H} = \mathbf{-1} \rightarrow \mathbf{Q(H)1'^*} = \{1,2',m',-1,1'^*,2^*,m^*,-1'^*\}$

Category (11): $\mathbf{H} + (\mathbf{Q} - \mathbf{H})1'^*$
21. $\mathbf{Q} = \mathbf{2/m}$, $\mathbf{H} = \mathbf{2} \rightarrow \mathbf{Q(H)\{H\}} = \{1,2,m'^*,-1'^*\}$
22. $\mathbf{Q} = \mathbf{2/m}$, $\mathbf{H} = \boldsymbol{m} \rightarrow \mathbf{Q(H)\{H\}} = \{1,2'^*,m,-1'^*\}$
23. $\mathbf{Q} = \mathbf{2/m}$, $\mathbf{H} = \mathbf{-1} \rightarrow \mathbf{Q(H)\{H\}} = \{1,2'^*,m'^*,-1\}$

Category (12): $\mathbf{H} \cap \mathbf{K} + (\mathbf{H} - \mathbf{K})1^* + (\mathbf{K} - \mathbf{H})1' + (\mathbf{Q} - (\mathbf{H} + \mathbf{K}))1'^*$
24. $\mathbf{Q} = \mathbf{2/m}$, $\mathbf{H} = \boldsymbol{m}$, $\mathbf{K} = \mathbf{-1} \rightarrow \mathbf{Q(H)\{K\}} = \{1,2'^*,m^*,-1'\}$
25. $\mathbf{Q} = \mathbf{2/m}$, $\mathbf{H} = \mathbf{2}$, $\mathbf{K} = \mathbf{-1} \rightarrow \mathbf{Q(H)\{K\}} = \{1,2^*,m'^*,-1'\}$
26. $\mathbf{Q} = \mathbf{2/m}$, $\mathbf{H} = \mathbf{2}$, $\mathbf{K} = \boldsymbol{m} \rightarrow \mathbf{Q(H)\{K\}} = \{1,2^*,m',-1'^*\}$
27. $\mathbf{Q} = \mathbf{2/m}$, $\mathbf{H} = \mathbf{-1}$, $\mathbf{K} = \boldsymbol{m} \rightarrow \mathbf{Q(H)\{K\}} = \{1,2'^*,m',-1^*\}$
28. $\mathbf{Q} = \mathbf{2/m}$, $\mathbf{H} = \mathbf{-1}$, $\mathbf{K} = \mathbf{2} \rightarrow \mathbf{Q(H)\{K\}} = \{1,2',m'^*,-1^*\}$
29. $\mathbf{Q} = \mathbf{2/m}$, $\mathbf{H} = \boldsymbol{m}$, $\mathbf{K} = \mathbf{2} \rightarrow \mathbf{Q(H)\{K\}} = \{1,2',m^*,-1'^*\}$.

Both **2/*m*** and **222** (given as an example in §2) have three index-2 subgroups. Consequently, they generate the same number of double antisymmetry groups: 29. However, unlike with **222**, none of the 29 groups formed from **2/*m*** are in the same equivalence class. This may seem surprising given that **2/*m*** is isomorphic to **222**. This can be thought of as being a consequence of the fact that none of the elements of **2/*m*** can be rotated into one another, whereas the three twofold axes of **222** can. Another way to look at it is to consider that **2/*m***'s proper affine normalizer group (∞**2**) does not contain non-trivial automorphisms whereas **222**'s proper affine normalizer group (**432**) does.

As with all crystallographic space groups, *Cc* has an infinite number of elements due to the infinite translational subgroup. *Cc*'s elements will be represented as $(t_{[100]},t_{[001]},t_{[\frac{1}{2}\frac{1}{2}0]})\{1,c\}$ where $(t_{[100]},t_{[001]},t_{[\frac{1}{2}\frac{1}{2}0]})$ represent the generators of the translation subgroup and $\{1,c\}$ are coset representatives of the corresponding decomposition. *Cc* has three index-2 subgroups: $(t_{[100]},t_{[001]},t_{[\frac{1}{2}\frac{1}{2}0]})\{1\}$, $(t_{[100]},t_{[010]},t_{[001]})\{1,c\}$ and $(t_{[100]},t_{[010]},t_{[001]})\{1, t_{[\frac{1}{2}\frac{1}{2}0]}\cdot c\}$.

Category (1): $\mathbf{Q}$
1. $\mathbf{Q} = Cc \rightarrow \mathbf{Q} = (t_{[100]},t_{[001]},t_{[\frac{1}{2}\frac{1}{2}0]})\{1,c\}$

Category (2): $\mathbf{Q} + \mathbf{Q}1'$
2. $\mathbf{Q} = Cc \rightarrow \mathbf{Q1'} = (t_{[100]},t_{[001]},t_{[\frac{1}{2}\frac{1}{2}0]})\{1,c,1',c'\}$

Category (3): $\mathbf{H} + (\mathbf{Q} - \mathbf{H})1'$
3. $\mathbf{Q} = Cc$, $\mathbf{H} = (t_{[100]},t_{[001]},t_{[\frac{1}{2}\frac{1}{2}0]})\{1\} \rightarrow \mathbf{Q(H)} = (t_{[100]},t_{[001]},t_{[\frac{1}{2}\frac{1}{2}0]})\{1,c'\}$
4. $\mathbf{Q} = Cc$, $\mathbf{H} = (t_{[100]},t_{[010]},t_{[001]})\{1,c\} \rightarrow \mathbf{Q(H)} = (t_{[100]},t_{[001]},t_{[\frac{1}{2}\frac{1}{2}0]}{}')\{1,c\}$
5. $\mathbf{Q} = Cc$, $\mathbf{H} = (t_{[100]},t_{[010]},t_{[001]})\{1,t_{[\frac{1}{2}\frac{1}{2}0]}\cdot c\} \rightarrow \mathbf{Q(H)} = (t_{[100]},t_{[001]},t_{[\frac{1}{2}\frac{1}{2}0]}{}')\{1,c'\}$

Category (4): $\mathbf{Q} + \mathbf{Q}1^*$
6. $\mathbf{Q} = Cc \rightarrow \mathbf{Q1^*} = (t_{[100]},t_{[001]},t_{[\frac{1}{2}\frac{1}{2}0]})\{1,c,1^*,c^*\}$

Category (5): $\mathbf{Q} + \mathbf{Q}1' + \mathbf{Q}1^* + \mathbf{Q}1'^*$

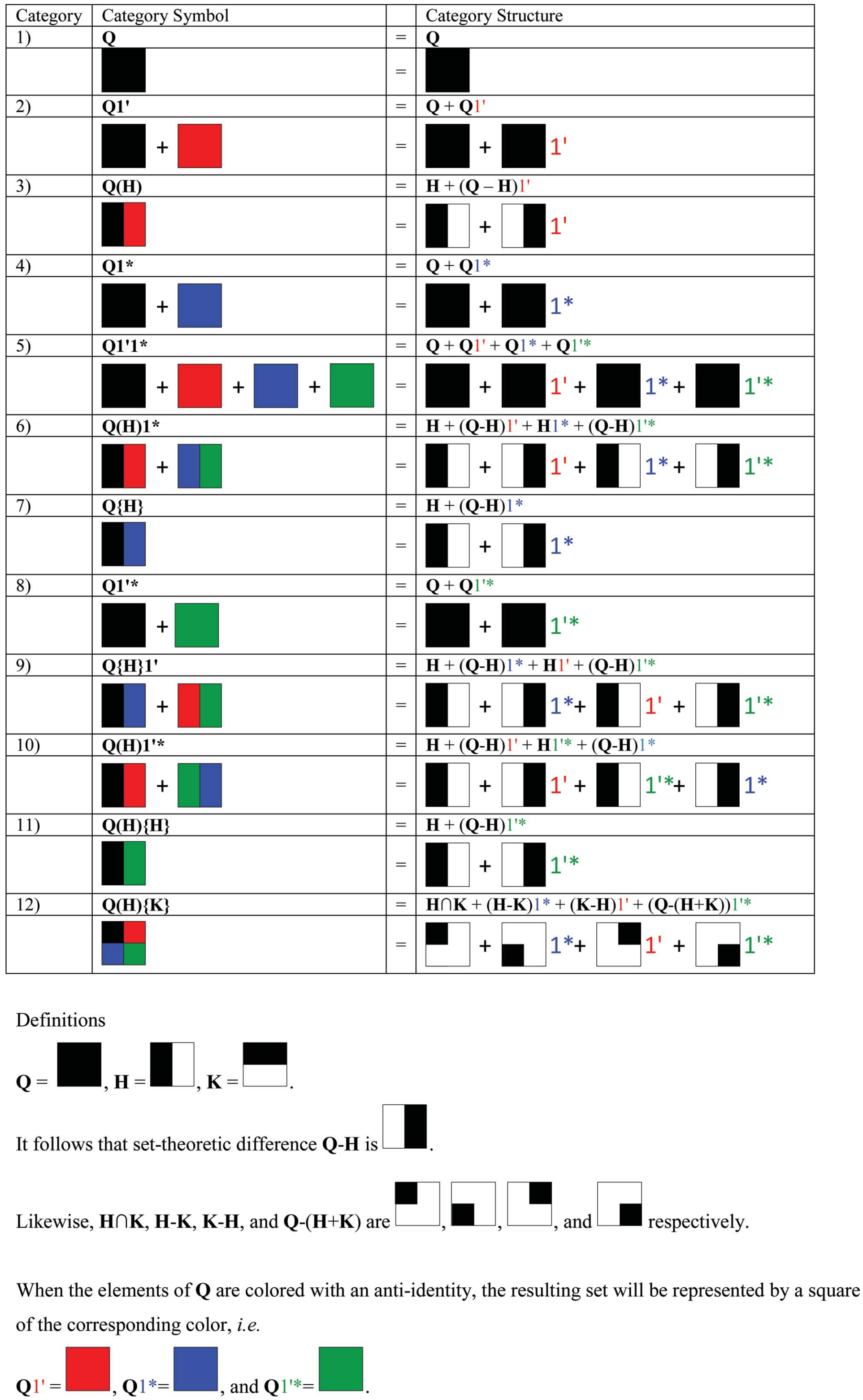


Figure 5
Representation of the 12 categories of double antisymmetry groups.

7. $\mathbf{Q} = Cc \rightarrow \mathbf{Q1'1^*} = (t_{[100]},t_{[001]},t_{[\frac{1}{2}\frac{1}{2}0]})\{1,c,1',c',1^*,c^*,1'^*,c'^*\}$
Category (6): $\mathbf{H} + (\mathbf{Q} - \mathbf{H})1' + \mathbf{H}1^* + (\mathbf{Q} - \mathbf{H})1'^*$

8. $\mathbf{Q} = Cc$, $\mathbf{H} = (t_{[100]},t_{[001]},t_{[\frac{1}{2}\frac{1}{2}0]})\{1\} \rightarrow \mathbf{Q(H)1^*} = (t_{[100]},t_{[001]},t_{[\frac{1}{2}\frac{1}{2}0]})\{1,c',1^*,c'^*\}$

9. $\mathbf{Q} = Cc$, $\mathbf{H} = (t_{[100]},t_{[010]},t_{[001]})\{1,c\} \rightarrow \mathbf{Q(H)1^*} = (t_{[100]},t_{[001]},t_{[\frac{1}{2}\frac{1}{2}0]}{}')\{1,c,1^*,c^*\}$

10. $\mathbf{Q} = Cc$, $\mathbf{H} = (t_{[100]},t_{[010]},t_{[001]})\{1,t_{[\frac{1}{2}\frac{1}{2}0]}\cdot c\} \rightarrow \mathbf{Q(H)1^*} = (t_{[100]},t_{[001]},t_{[\frac{1}{2}\frac{1}{2}0]}{}')\{1,c',1^*,c'^*\}$

Category (7): $\mathbf{H} + (\mathbf{Q} - \mathbf{H})1^*$

11. $\mathbf{Q} = Cc$, $\mathbf{H} = (t_{[100]},t_{[001]},t_{[\frac{1}{2}\frac{1}{2}0]})\{1\} \rightarrow \mathbf{Q\{H\}} = (t_{[100]},t_{[001]},t_{[\frac{1}{2}\frac{1}{2}0]})\{1,c^*\}$

12. $\mathbf{Q} = Cc$, $\mathbf{H} = (t_{[100]},t_{[010]},t_{[001]})\{1,c\} \rightarrow \mathbf{Q\{H\}} = (t_{[100]},t_{[001]},t_{[\frac{1}{2}\frac{1}{2}0]}{}^*)\{1,c\}$

13. $\mathbf{Q} = Cc$, $\mathbf{H} = (t_{[100]},t_{[010]},t_{[001]})\{1,t_{[\frac{1}{2}\frac{1}{2}0]}\cdot c\} \rightarrow \mathbf{Q\{H\}} = (t_{[100]},t_{[001]},t_{[\frac{1}{2}\frac{1}{2}0]}{}^*)\{1,c^*\}$

Category (8): $\mathbf{Q} + \mathbf{Q}1'^*$

14. $\mathbf{Q} = Cc \rightarrow \mathbf{Q1'^*} = (t_{[100]},t_{[001]},t_{[\frac{1}{2}\frac{1}{2}0]})\{1,c,1'^*,c'^*\}$

Category (9): $\mathbf{H} + (\mathbf{Q} - \mathbf{H})1^* + \mathbf{H}1' + (\mathbf{Q} - \mathbf{H})1'^*$

15. $\mathbf{Q} = Cc$, $\mathbf{H} = (t_{[100]},t_{[001]},t_{[\frac{1}{2}\frac{1}{2}0]})\{1\} \rightarrow \mathbf{Q\{H\}1'} = (t_{[100]},t_{[001]},t_{[\frac{1}{2}\frac{1}{2}0]})\{1,c^*,1',c'^*\}$

16. $\mathbf{Q} = Cc$, $\mathbf{H} = (t_{[100]},t_{[010]},t_{[001]})\{1,c\} \rightarrow \mathbf{Q\{H\}1'} = (t_{[100]},t_{[001]},t_{[\frac{1}{2}\frac{1}{2}0]}{}^*)\{1,c,1',c'\}$

17. $\mathbf{Q} = Cc$, $\mathbf{H} = (t_{[100]},t_{[010]},t_{[001]})\{1,t_{[\frac{1}{2}\frac{1}{2}0]}\cdot c\} \rightarrow \mathbf{Q\{H\}1'} = (t_{[100]},t_{[001]},t_{[\frac{1}{2}\frac{1}{2}0]}{}^*)\{1,c^*,1',c'^*\}$

Category (10): $\mathbf{H} + (\mathbf{Q} - \mathbf{H})1' + \mathbf{H}1'^* + (\mathbf{Q} - \mathbf{H})1^*$

18. $\mathbf{Q} = Cc$, $\mathbf{H} = (t_{[100]},t_{[001]},t_{[\frac{1}{2}\frac{1}{2}0]})\{1\} \rightarrow \mathbf{Q(H)1'^*} = (t_{[100]},t_{[001]},t_{[\frac{1}{2}\frac{1}{2}0]})\{1,c',1'^*,c^*\}$

19. $\mathbf{Q} = Cc$, $\mathbf{H} = (t_{[100]},t_{[010]},t_{[001]})\{1,c\} \rightarrow \mathbf{Q(H)1'^*} = (t_{[100]},t_{[001]},t_{[\frac{1}{2}\frac{1}{2}0]}{}')\{1,c,1'^*,c'^*\}$

20. $\mathbf{Q} = Cc$, $\mathbf{H} = (t_{[100]},t_{[010]},t_{[001]})\{1,t_{[\frac{1}{2}\frac{1}{2}0]}\cdot c\} \rightarrow \mathbf{Q(H)1'^*} = (t_{[100]},t_{[001]},t_{[\frac{1}{2}\frac{1}{2}0]}{}')\{1,c',1'^*,c^*\}$

Category (11): $\mathbf{H} + (\mathbf{Q} - \mathbf{H})1'^*$

21. $\mathbf{Q} = Cc$, $\mathbf{H} = (t_{[100]},t_{[001]},t_{[\frac{1}{2}\frac{1}{2}0]})\{1\} \rightarrow \mathbf{Q(H)\{H\}} = (t_{[100]},t_{[001]},t_{[\frac{1}{2}\frac{1}{2}0]})\{1,c'^*\}$

22. $\mathbf{Q} = Cc$, $\mathbf{H} = (t_{[100]},t_{[010]},t_{[001]})\{1,c\} \rightarrow \mathbf{Q(H)\{H\}} = (t_{[100]},t_{[001]},t_{[\frac{1}{2}\frac{1}{2}0]}{}'^*)\{1,c\}$

23. $\mathbf{Q} = Cc$, $\mathbf{H} = (t_{[100]},t_{[010]},t_{[001]})\{1,t_{[\frac{1}{2}\frac{1}{2}0]}\cdot c\} \rightarrow \mathbf{Q(H)\{H\}} = (t_{[100]},t_{[001]},t_{[\frac{1}{2}\frac{1}{2}0]}{}'^*)\{1,c'^*\}$

Category (12): $\mathbf{H} \cap \mathbf{K} + (\mathbf{H} - \mathbf{K})1^* + (\mathbf{K} - \mathbf{H})1' + (\mathbf{Q} - (\mathbf{H} + \mathbf{K}))1'^*$

24. $\mathbf{Q} = Cc$, $\mathbf{H} = (t_{[100]},t_{[010]},t_{[001]})\{1,c\}$, $\mathbf{K} = (t_{[100]},t_{[010]},t_{[001]})\{1,t_{[\frac{1}{2}\frac{1}{2}0]}\cdot c\} \rightarrow \mathbf{Q(H)\{K\}} = (t_{[100]},t_{[001]},t_{[\frac{1}{2}\frac{1}{2}0]}{}'^*)\{1,c^*\}$

25. $\mathbf{Q} = Cc$, $\mathbf{H} = (t_{[100]},t_{[001]},t_{[\frac{1}{2}\frac{1}{2}0]})\{1\}$, $\mathbf{K} = (t_{[100]},t_{[010]},t_{[001]})\{1,t_{[\frac{1}{2}\frac{1}{2}0]}\cdot c\} \rightarrow \mathbf{Q(H)\{K\}} = (t_{[100]},t_{[001]},t_{[\frac{1}{2}\frac{1}{2}0]}{}^*)\{1,c'^*\}$

26. $\mathbf{Q} = Cc$, $\mathbf{H} = (t_{[100]},t_{[001]},t_{[\frac{1}{2}\frac{1}{2}0]})\{1\}$, $\mathbf{K} = (t_{[100]},t_{[010]},t_{[001]})\{1,c\} \rightarrow \mathbf{Q(H)\{K\}} = (t_{[100]},t_{[001]},t_{[\frac{1}{2}\frac{1}{2}0]}{}^*)\{1,c'\}$

27. $\mathbf{Q} = Cc$, $\mathbf{H} = (t_{[100]},t_{[010]},t_{[001]})\{1,t_{[\frac{1}{2}\frac{1}{2}0]}\cdot c\}$, $\mathbf{K} = (t_{[100]},t_{[010]},t_{[001]})\{1,c\} \rightarrow \mathbf{Q(H)\{K\}} = (t_{[100]},t_{[001]},t_{[\frac{1}{2}\frac{1}{2}0]}{}'^*)\{1,c'\}$

28. $\mathbf{Q} = Cc$, $\mathbf{H} = (t_{[100]},t_{[010]},t_{[001]})\{1,t_{[\frac{1}{2}\frac{1}{2}0]}\cdot c\}$, $\mathbf{K} = (t_{[100]},t_{[001]},t_{[\frac{1}{2}\frac{1}{2}0]})\{1\} \rightarrow \mathbf{Q(H)\{K\}} = (t_{[100]},t_{[001]},t_{[\frac{1}{2}\frac{1}{2}0]}{}')\{1,c'^*\}$

29. $\mathbf{Q} = Cc$, $\mathbf{H} = (t_{[100]},t_{[010]},t_{[001]})\{1,c\}$, $\mathbf{K} = (\mathrm{t}_{[100]},t_{[001]},t_{[\frac{1}{2}\frac{1}{2}0]})\{1\} \rightarrow \mathbf{Q(H)\{K\}} = (t_{[100]},t_{[001]},t_{[\frac{1}{2}\frac{1}{2}0]}{}')\{1,c^*\}$.

Note that although 29 double antisymmetry space groups are generated from using *Cc* as a colorblind parent group, they are not all of unique types. This is because there exist proper affine transformations which map some of these into each other. We show this by applying the results of §5.3.

To do this, we need to know the transformation matrices mapping the standard representative groups to the actual subgroups, and the proper affine normalizer groups of *Cc* and its index-2 subgroups. For *Cc*'s three index-2 subgroups:

$(t_{[100]},t_{[001]},t_{[\frac{1}{2}\frac{1}{2}0]})\{1\}$ is type $P1$ and can be mapped from the standard $P1$ by

$$\begin{pmatrix} 1/2 & 1/2 & 0 & 0 \\ -1/2 & 1/2 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

$(t_{[100]},t_{[010]},t_{[001]})\{1,c\}$ is type Pc and can be mapped from the standard Pc by

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

$(t_{[100]},t_{[010]},t_{[001]})\{1,t_{[\frac{1}{2}\frac{1}{2}0]}\cdot c\}$ is type Pc and can be mapped from the standard Pc by

$$\begin{pmatrix} 1 & 0 & -1 & 0 \\ 0 & 1 & 0 & 1/4 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

The proper affine normalizers of *Cc* are

$$\mathbf{N}_{\mathscr{A}^+}(Cc) = \left\{ \begin{pmatrix} 2n_1+1 & 0 & 2n_2+p & r \\ 0 & \pm 1 & 0 & (2n_3+p)/4 \\ 2n_4 & 0 & 2n_5+1 & t \\ 0 & 0 & 0 & 1 \end{pmatrix} \in \mathscr{A}^+ : r,t \in \mathbb{R} \wedge n_i \in \mathbb{Z} \wedge (p=0 \vee p=1) \right\}.$$

The proper affine normalizers of the standard representative groups of the two types of subgroups ($P1$ and Pc) are:

$P1$ normalizers $\mathbf{N}^+_{\mathscr{A}}(P1) =$

$$\left\{ \begin{pmatrix} n_{11} & n_{12} & n_{13} & r \\ n_{21} & n_{22} & n_{23} & s \\ n_{31} & n_{32} & n_{33} & t \\ 0 & 0 & 0 & 1 \end{pmatrix} \in \mathscr{A}^+ : r,s,t \in \mathbb{R} \wedge n_{ij} \in \mathbb{Z} \right\};$$

Pc normalizers $\mathbf{N}_{\mathscr{A}^+}(Pc) =$

$$\left\{ \begin{pmatrix} 2n_6+1 & 0 & 2n_7 & r \\ 0 & \pm 1 & 0 & n_8/2 \\ n_9 & 0 & 2n_{10}+1 & t \\ 0 & 0 & 0 & 1 \end{pmatrix} \in \mathscr{A}^+ : r,t \in \mathbb{R} \wedge n_i \in \mathbb{Z} \right\}.$$

Having collected all this information, we can now evaluate the proper affine equivalence of the 29 double antisymmetry groups generated from $\mathbf{Q} = Cc$.

We know that groups from different categories can never be equivalent; therefore categories (1), (2), (4), (5) and (8) must contain only one type as only one group has been generated.

For category (3), we have three generated groups. Thus there are three pairs for which we can test for equivalence, $3 \sim 4, 3 \sim 5$ and $4 \sim 5$. For group 3, $\mathbf{H}$ is $P1$ type whereas for 4 and 5 **H** is *Pc* type. Therefore, 3 $\sim$ 4 and 3 $\sim$ 5 are false. For 4 $\sim$ 5, we can evaluate:

$$\mathbf{Q}(\mathbf{H}_2) \sim \mathbf{Q}(\mathbf{H}_1) \equiv \mathbf{N}_{\mathscr{A}^+}(\mathbf{Q}) \cap T_{H_2}\mathbf{N}_{\mathscr{A}^+}(\mathbf{H}_0)T_{H_1}^{-1} \neq \emptyset. \quad (8)$$

In this case,

$$T_{H_2}\mathbf{N}_{\mathscr{A}^+}(\mathbf{H}_0)T_{H_1}^{-1} = \left\{\begin{pmatrix}1&0&-1&0\\0&1&0&\frac{1}{4}\\0&0&1&0\\0&0&0&1\end{pmatrix}\begin{pmatrix}2n_6+1&0&2n_7&r\\0&\pm1&0&n_8/2\\n_9&0&2n_{10}+1&t\\0&0&0&1\end{pmatrix}\times\begin{pmatrix}1&0&0&0\\0&1&0&0\\0&0&1&0\\0&0&0&1\end{pmatrix}^{-1} \in \mathscr{A}^+ : r,t\in\mathbb{R}\wedge n_i\in\mathbb{Z}\right\}$$

and

$$\mathbf{N}_{\mathscr{A}^+}(\mathbf{Q}) = \left\{\begin{pmatrix}2n_1+1&0&2n_2+p&r\\0&\pm1&0&(2n_3+p)/4\\2n_4&0&2n_5+1&t\\0&0&0&1\end{pmatrix} \in \mathscr{A}^+ : r,t\in\mathbb{R}\wedge n_i\in\mathbb{Z}\wedge(p=0\vee p=1)\right\}.$$

From substituting these in and simplifying, we can show that 4 $\sim$ 5 is logically equivalent to the existence of a solution with a positive determinant to the following:

$$\begin{pmatrix}2n_1+1&0&2n_2+p&r\\0&\pm1&0&(2n_3+p)/4\\2n_4&0&2n_5+1&t\\0&0&0&1\end{pmatrix} = \begin{pmatrix}2n_6+1-n_9&0&-1-2n_{10}+2n_7&r-t\\0&\pm1&0&(2n_8+1)/4\\n_9&0&2n_{10}+1&t\\0&0&0&1\end{pmatrix}. \quad (9)$$

There are clearly many solutions, *e.g.* one solution is where $n_2 = -1$, $n_{i\neq2} = r = t = 0$ and $p = 1$. Thus, 4 and 5 are equivalent and therefore for category (3) there are only two types of groups where **Q** = *Cc*. It is trivial to extend these results to show that categories (6), (7), (9), (10) and (11) similarly have two types.

For category (12), we have six generated groups. Thus there are 15 pairs for which we can test for equivalence. Only three of the 15 have the same **H** and **K** types (26 $\sim$ 25, 24 $\sim$ 27 and 28 $\sim$ 29) and therefore only these need to be evaluated using

$$\mathbf{Q}(\mathbf{H}_1)\{\mathbf{K}_1\} \sim \mathbf{Q}(\mathbf{H}_2)\{\mathbf{K}_2\} \equiv \mathbf{N}_{\mathscr{A}^+}(\mathbf{Q}) \cap T_{H_2}\mathbf{N}_{\mathscr{A}^+}(\mathbf{H}_0)T_{H_1}^{-1} \cap T_{K_2}\mathbf{N}_{\mathscr{A}^+}(\mathbf{K}_0)T_{K_1}^{-1} \neq \emptyset. \quad (10)$$

For 26 $\sim$ 25,

$$T_{H_2}\mathbf{N}_{\mathscr{A}^+}(\mathbf{H}_0)T_{H_1}^{-1} = \left\{\begin{pmatrix}1&0&-1&0\\0&1&0&\frac{1}{4}\\0&0&1&0\\0&0&0&1\end{pmatrix}\begin{pmatrix}2n_6+1&0&2n_7&r\\0&\pm1&0&n_8/2\\n_9&0&2n_{10}+1&t\\0&0&0&1\end{pmatrix}\times\begin{pmatrix}1&0&0&0\\0&1&0&0\\0&0&1&0\\0&0&0&1\end{pmatrix}^{-1} \in \mathscr{A}^+ : r,t\in\mathbb{R}\wedge n_i\in\mathbb{Z}\right\},$$

$$T_{K_2}\mathbf{N}_{\mathscr{A}^+}(\mathbf{K}_0)T_{K_1}^{-1} = \left\{\begin{pmatrix}\frac{1}{2}&\frac{1}{2}&0&0\\-\frac{1}{2}&\frac{1}{2}&0&0\\0&0&1&0\\0&0&0&1\end{pmatrix}\begin{pmatrix}n_{11}&n_{12}&n_{13}&r\\n_{21}&n_{22}&n_{23}&s\\n_{31}&n_{32}&n_{33}&t\\0&0&0&1\end{pmatrix}\times\begin{pmatrix}\frac{1}{2}&\frac{1}{2}&0&0\\-\frac{1}{2}&\frac{1}{2}&0&0\\0&0&1&0\\0&0&0&1\end{pmatrix}^{-1} \in \mathscr{A}^+ : r,s,t\in\mathbb{R}\wedge n_{ij}\in\mathbb{Z}\right\}$$

and

$$\mathbf{N}_{\mathscr{A}^+}(\mathbf{Q}) = \left\{\begin{pmatrix}2n_1+1&0&2n_2+p&r\\0&\pm1&0&(2n_3+p)/4\\2n_4&0&2n_5+1&t\\0&0&0&1\end{pmatrix} \in \mathscr{A}^+ : r,t\in\mathbb{R}\wedge n_i\in\mathbb{Z}\wedge(p=0\vee p=1)\right\}.$$

From substituting these in and simplifying, we can show that 26 $\sim$ 25 is logically equivalent to the existence of a solution with a positive determinant to the following:

$$\begin{pmatrix}2n_1+1&0&2n_2+p&r\\0&\pm1&0&(2n_3+p)/4\\2n_4&0&2n_5+1&t\\0&0&0&1\end{pmatrix} = \begin{pmatrix}2n_6+1-n_9&0&-1-2n_{10}+2n_7&r-t\\0&\pm1&0&(2n_8+1)/4\\n_9&0&2n_{10}+1&t\\0&0&0&1\end{pmatrix} = \begin{pmatrix}n_{11}-n_{31}&n_{12}-n_{32}&n_{13}-n_{33}&r-t\\n_{21}&n_{22}&n_{23}&s+1/4\\n_{31}&n_{32}&n_{33}&t\\0&0&0&1\end{pmatrix}. \quad (11)$$

There are clearly many solutions, *e.g.* one solution is where $n_2 = -1$, $n_{i\neq2} = r = t = s = 0$, $p = 1$, $n_{i=j} = 1$ and $n_{i\neq j} = 0$. Thus 25 and 26 are equivalent. Since 24, 27, 28 and 29 can be related to 25 and 26 by automorphisms of **1′1***, 26 $\sim$ 25 implies 24 $\sim$ 27 and 28 $\sim$ 29. Therefore there are only three types of category (12) groups and a total of 20 double antisymmetry space-group types for $\mathbf{Q} = Cc$.

APPENDIX C
Equivalence classes, proper affine classes (types), Mackay groups and color-permuting classes

An *equivalence relation* can be used to partition a set of groups into *equivalence classes*. For example, an equivalence relation can be applied to partition the set of crystallographic space groups (which is uncountably infinite) into a finite number of classes. The proper affine equivalence relation is used to classify space groups into 230 *proper affine classes* or 'types'. The proper affine equivalence relation can be defined as: two groups, $\mathbf{G}_1$ and $\mathbf{G}_2$, are equivalent if and only if $\mathbf{G}_1$ can be bijectively mapped to $\mathbf{G}_2$ by a proper affine transformation, a.

$$\mathbf{G}_2 \sim \mathbf{G}_1 \equiv \exists a \in \mathscr{A}^+ : \left(\mathbf{G}_2 = a\mathbf{G}_1 a^{-1}\right). \tag{12}$$

If it is known that $\mathbf{G}_1$ and $\mathbf{G}_2$ have the same colorblind parent group $\mathbf{Q}$, then, instead of using the entire proper affine group $\mathscr{A}^+$, it is sufficient to use the proper affine normalizer group of $\mathbf{Q}$, denoted $\mathbf{N}_{\mathscr{A}^+}(\mathbf{Q})$ (see footnote 2).

The proper affine equivalence relation does not allow for any permutations of anti-identities. Other works give another set of equivalence classes of antisymmetry groups called Mackay groups (Jablan, 1993*a*, 2002; Radovic & Jablan, 2005). The equivalence relation of Mackay groups allows some color permutations in addition to proper affine transformation. For double antisymmetry, the Mackay equivalence relation allows for $1'$ and 1^* to be permuted, *i.e.* all the primed operations become starred and *vice versa*:

$$\mathbf{G}_2 \sim \mathbf{G}_1 \equiv \exists a \in \mathscr{A}^+ \wedge \exists p \in \{1, 1' \leftrightarrow 1^*\} : \left(\mathbf{G}_2 = ap(\mathbf{G}_1)a^{-1}\right). \tag{13}$$

The Mackay equivalence relation does not allow for $1'^*$ to be permuted (Radovic & Jablan, 2005). Note that Radovic & Jablan do give the Mackay equivalence relation as permuting 'anti-identities' but $1'^*$ is not considered an anti-identity in their work (it is simply the product of $1'$ and 1^*). They also conclude that Mackay groups are the minimal representation of 'Zamorzaev groups'. This seems potentially inconsistent with the aforementioned restriction on color permutation. If we instead allow for all possible color permutations that preserve the group structure of $\mathbf{1'1^*}$, *i.e.* the automorphisms of $\mathbf{1'1^*}$, then we can clearly further reduce the representation beyond that of the Mackay groups, contrary to what has been claimed. This is demonstrated by Zamorzaev & Palistrant's listing of double antisymmetry space-group-generating sets. In their listing, they gave only those sets which were unique up to the automorphisms of $\mathbf{1'1^*}$ (Zamorzaev & Palistrant, 1980). Such a listing only needs to contain 1846 $\mathbf{Q(H)\{K\}}$ generating sets, far fewer than the 5005 Mackay equivalence classes of $\mathbf{Q(H)\{K\}}$ groups.

If all possible color permutations that preserve the group structure of $\mathbf{1'1^*}$, *i.e.* the automorphisms of $\mathbf{1'1^*}$, are allowed, then the equivalence relation can be expressed as

$$\mathbf{G}_2 \sim \mathbf{G}_1 \equiv \exists a \in \mathscr{A}^+ \wedge \exists p \in \mathrm{Aut}(\mathbf{1'1^*}) : \left(\mathbf{G}_2 = ap(\mathbf{G}_1)a^{-1}\right). \tag{14}$$

This proper affine *color equivalence relation* results in 1846 classes for category (12) $\mathbf{Q(H)\{K\}}$ groups. The equivalence classes of this kind of relation are similar to what Koptsik & Shubnikov (1974) refer to as 'Belov groups'.

Generalized to an arbitrary coloring scheme, $\mathbf{P}$, the *color equivalence relation*, can be defined as

$$\mathbf{G}_2 \sim \mathbf{G}_1 \equiv \exists a \in \mathscr{A}^+ \wedge \exists p \in \mathrm{Aut}(\mathbf{P}) : \left(\mathbf{G}_2 = ap(\mathbf{G}_1)a^{-1}\right). \tag{15}$$

The advantage of using the color equivalence relation to reduce the number of equivalence classes becomes greater as the number of colors (the order of $\mathbf{P}$) increases. For example, for non-trivial double antisymmetry space groups (where $\mathbf{P} \cong \mathbb{Z}_2{}^2$ and thus $|\mathbf{P}| = 4$), there are 9507 proper affine equivalence classes [equation (12)], 5005 Mackay equivalence classes [equation (13)] and 1846 color equivalence classes [equation (14)]. Whereas for non-trivial sextuple antisymmetry space groups (where $\mathbf{P} \cong \mathbb{Z}_2{}^6$ and thus $|\mathbf{P}| = 64$), there are 419 973 120 proper affine equivalence classes, 598 752 Mackay equivalence classes and just one color equivalence class. Although the number of colors only increased from four to 64 by going from non-trivial double antisymmetry space groups to non-trivial sextuple antisymmetry space groups, the number of proper affine classes [equation (12)] increased from 9507 to 419 973 120 whereas the number of color equivalence classes [equation (15)] actually decreased from 1846 to one.

Although these color-permuting equivalence relations reduce the number of equivalence classes significantly, they are not suitable when the differences between the colors are important. With time-reversal as $1'$ and rotation-reversal as 1^*, the differences are clearly very important. However, there may be applications where the color equivalence relation is suitable, for example, in making patterns for aesthetic purposes.

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