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Crystallographic data of double antisymmetry space groups

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This paper presents crystallographic data of double antisymmetry space groups, including symmetry-element diagrams, general-position diagrams and positions, with multiplicities, site symmetries, coordinates, spin vectors, roto vectors and displacement vectors.

1. Introduction

Double antisymmetry space groups are symmetry groups that describe rotation-reversal and time-reversal symmetry in crystals. These groups were introduced to generalize the symmetry classification of rigid static rotations in crystals (Gopalan & Litvin, 2011). There are two independent anti-identities representing time reversal and rotation reversal, which are labeled $1'$ and 1^*, respectively. In addition, there is an anti-identity that is the product of the two independent ones, labeled $1'^*$. Colors are used to distinguish the identity and three anti-identities. If one would denote a spin vector as $\mathbf{S}(\mathbf{r})$, a roto-vector as $\mathbf{V}(\mathbf{r})$ and a displacement vector as $\mathbf{U}(\mathbf{r})$, the colors of the identity and the anti-identities and their actions on spin, roto and displacement vectors are listed in Table 1. Here we use 'spin vector' to refer to an arbitrary axial vector that is reversed under the action of $1'$ and is invariant under the action of 1^*; thus we are not necessarily limited to physical spins. Similarly, we use 'roto vector' to refer to an arbitrary axial vector that is reversed under the action of 1^* and invariant under $1'$. We also use 'displacement vector' to refer to an arbitrary polar vector that is reversed under the action of 1^* and invariant under $1'$.

A full list of the 17 803 proper affine classes of double antisymmetry space groups was presented by VanLeeuwen *et al.* (2014). These classes are referred to as the 17 803 double antisymmetry space-group types or the 17 803 double anti-symmetry space groups. For each set of groups belonging to the same double antisymmetry space-group type, one representative is chosen and listed (VanLeeuwen *et al.*, 2014). The document referred to in the present work gives the crystallographic data of these representatives.[1]

The structure of the document is similar to the tables found in *International Tables for Crystallography* Volumes A (Hahn, 2006) and E (Kopsky & Litvin, 2010), and in tables of magnetic space groups (Litvin, 2013). The document was generated by computer code based on the machine-readable file from VanLeeuwen *et al.* (2014) and *International Tables for Crystallography* Volume A (abbreviated as ITC-A). Given the extreme length of the document (over 30 000 pages), each page could not be manually checked; however, through several iterations of the document, hundreds of pages have been checked manually for systematic errors. The details of the format and content of the document are discussed in §2.

2. Crystallographic data of double antisymmetry space groups

The document contains crystallographic properties for all 17 803 double antisymmetry space-group types. A description is given for each double antisymmetry space group. A description starts a new page in the document.

Each description contains: (i) headline; (ii) lattice diagram; (iii) diagram of symmetry elements and general-position diagram; (iv) asymmetric unit; (v) symmetry operations; (vi) generators selected; (vii) general and special positions.

For example, the description for the double antisymmetry space group $P(1,1^*,1)\ mm'a^*$ is shown in Fig. 1.

2.1. Headline

A headline is placed at the top left of the first page for each description. Each headline consists of two lines, which read from left to right. A headline consists of the following information.

First line:

(i) The serial number of the double antisymmetry space group. The serial numbers of the double antisymmetry space groups follow the numbering system of VanLeeuwen *et al.* (2014).

(ii) International (Hermann–Mauguin) symbol of the double antisymmetry space group. The symbols are those

[1] An electronic document *Crystallographic Data of Double Antisymmetry Space Groups* is available from the IUCr electronic archives (Reference: PC5035). This document may also be downloaded from http://sites.psu.edu/gopalan/research/symmetry/. The document is a pdf file and is ~280 MB in size.

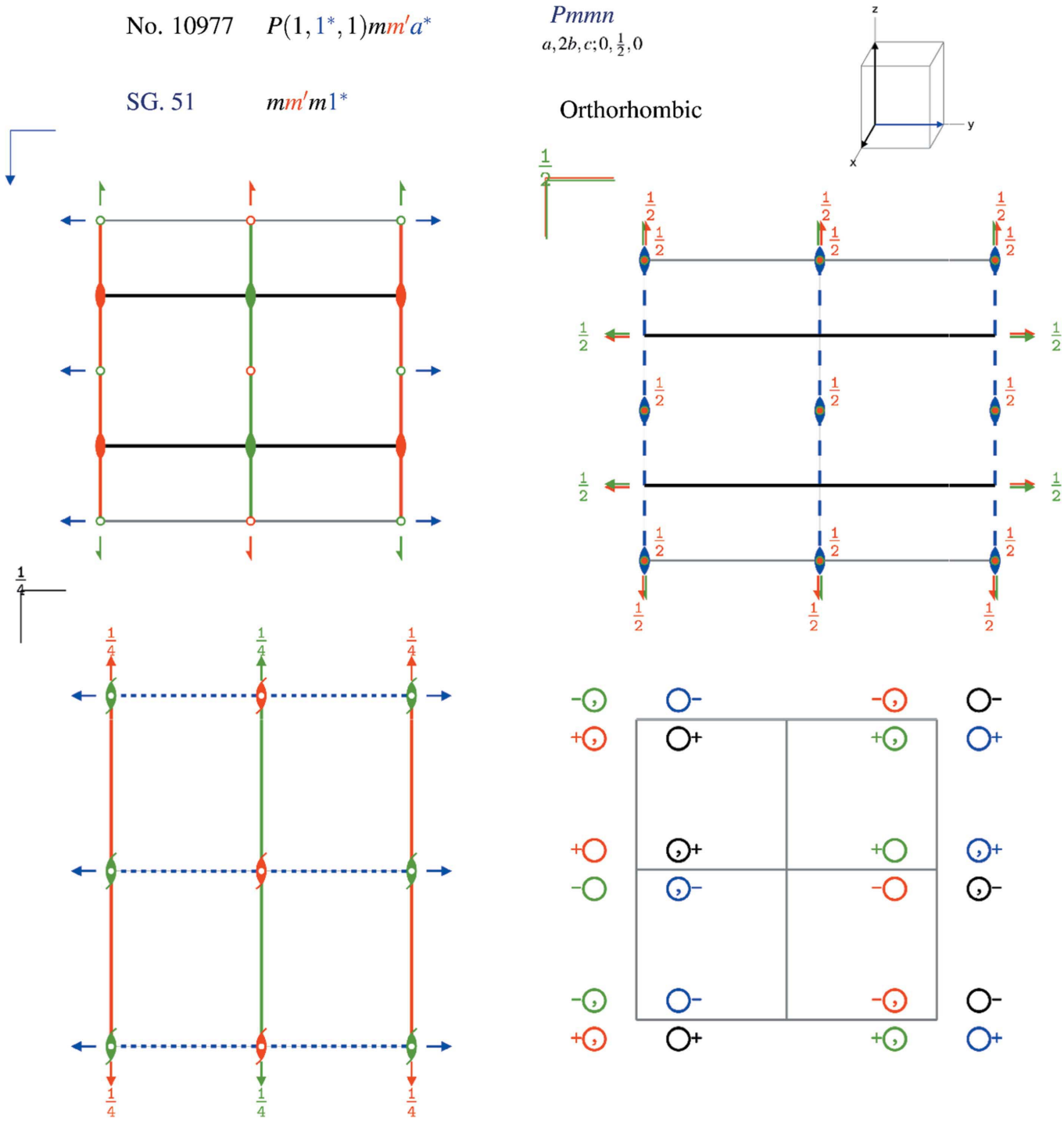


Figure 1
Crystallographic data of the double antisymmetry space group $P(1,1^*,1)\ mm'a^*$, No. 10977.

Table 1
Identity and the three anti-identities of double antisymmetry space groups.

Identity or anti-identity	Color	Action on spin vectors **S**(**r**), roto vectors **V**(**r**) and displacement vectors **U**(**r**)
1	Black	$1\mathbf{S}(\mathbf{r}) = \mathbf{S}(\mathbf{r})$; $1\mathbf{V}(\mathbf{r}) = \mathbf{V}(\mathbf{r})$; $1\mathbf{U}(\mathbf{r}) = \mathbf{U}(\mathbf{r})$
1′	Red	$1'\mathbf{S}(\mathbf{r}) = -\mathbf{S}(\mathbf{r})$; $1'\mathbf{V}(\mathbf{r}) = \mathbf{V}(\mathbf{r})$; $1'\mathbf{U}(\mathbf{r}) = \mathbf{U}(\mathbf{r})$
1*	Blue	$1^*\mathbf{S}(\mathbf{r}) = \mathbf{S}(\mathbf{r})$; $1^*\mathbf{V}(\mathbf{r}) = -\mathbf{V}(\mathbf{r})$; $1^*\mathbf{U}(\mathbf{r}) = -\mathbf{U}(\mathbf{r})$
1′*	Green	$1'^*\mathbf{S}(\mathbf{r}) = -\mathbf{S}(\mathbf{r})$; $1'^*\mathbf{V}(\mathbf{r}) = -\mathbf{V}(\mathbf{r})$; $1'^*\mathbf{U}(\mathbf{r}) = -\mathbf{U}(\mathbf{r})$

introduced by VanLeeuwen *et al.* (2014) based on the Hermann–Mauguin symbol of the *colorblind parent space group*. By removing all anti-identities coupled with symmetry operations from the group, one has one of the 230 crystallographic space groups which we shall refer to as the colorblind parent space group associated with the double antisymmetry group. The colorblind parent space group of a double antisymmetry space group is the space group based on which the double antisymmetry space group is generated, and is denoted by **Q** by VanLeeuwen *et al.* (2014). For example, if all anti-identities are removed from $P(1,1^*,1)$ $mm'a^*$, one has *Pmma*, so *Pmma* is the colorblind parent space group of $P(1,1^*,1)$ $mm'a^*$.

The International symbol is composed of two parts. The first part of the symbol gives the translational subgroup. If the group has no translations coupled with anti-identities, the symbol is given as *P* (primitive), *C* (*c*-centering), *A* (*a*-centering), *I* (body centering), *F* (face centering) and *R* (rhombohedral centering). If there are translations coupled with anti-identities, three color operations in parentheses are given after the *P*, *C*, *A*, *I*, *F* and *R* symbol. The three color operations denote the generating lattice translations and are listed in Table 2 (VanLeeuwen *et al.*, 2014).

Table 2
Three color operations denoting the generating lattice translations in the International symbol of a double antisymmetry space group.

Lattice symbol	First position	Second position	Third position
P	$t[100]$	$t[010]$	$t[001]$
C	$t[100]$	$t[001]$	$t[\frac{11}{22}0]$
A	$t[100]$	$t[010]$	$t[0\frac{11}{22}]$
I	$t[100]$	$t[001]$	$t[\frac{111}{222}]$
F	$t[0\frac{11}{22}]$	$t[\frac{1}{2}0\frac{1}{2}]$	$t[\frac{11}{22}0]$
R	$t[001]$	$t[\frac{211}{333}]$	$t[\frac{122}{333}]$

For example, consider $P(1,1^*,1)$ $mm'a^*$: 1 is in the first position, 1^* is in the second position and 1 is in the third position. In Table 2, the lattice symbol '*P*' is in the first row, which shows that the first, second and third positions correspond to $t_{[100]}$, $t_{[010]}$ and $t_{[001]}$, respectively. Therefore the translations of $P(1,1^*,1)$ $mm'a^*$ are generated by $t_{[100]}$, $t_{[010]}{}^*$ and $t_{[001]}$.

The second part of the symbol gives the remaining generators for the group. It is based on the corresponding part of the Hermann–Mauguin symbol of the colorblind parent space group.

The symmetry operations of the representative group are given later in §2.5 on symmetry operations.

(iii) X-ray diffraction symmetry group. This is the symmetry which would be expected to be indicated by the typical methods of analysis of X-ray diffraction patterns (one of the 230 conventional space groups). This group comes from converting all primed operations to colorless operations (because X-ray scattering is invariant under the action of time reversal) and removing all starred and prime–starred operations (because X-ray scattering is non-invariant under the action of rotation reversal). If the standard setting of the X-ray diffraction symmetry group differs from that of the double antisymmetry space group, the affine transformation relating the two is given. The notation for this transformation is meant to be shorthand for the 4×4 augmented matrix of the transformation, *i.e.*

$$\begin{pmatrix} R_{11} & R_{12} & R_{13} & t_1 \\ R_{21} & R_{22} & R_{23} & t_2 \\ R_{31} & R_{32} & R_{33} & t_3 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

would be given as $R_{11}a + R_{21}b + R_{31}c$, $R_{12}a + R_{22}b + R_{32}c$, $R_{13}a + R_{23}b + R_{33}c$; t_1, t_2, t_3. For example, the transformation matrix relating the X-ray diffraction symmetry group *Pmmn* and the double antisymmetry space group $P(1,1^*,1)$ $mm'a^*$

Positions			Coordinates	
8	l	1	$\{x,y,z\}[a,b,c][d,e,f][u,v,w]$	$\{\bar{x}+\frac{1}{2},\bar{y},z\}[a,b,\bar{c}][\bar{d},\bar{e},f][\bar{u},\bar{v},w]$
			$\{\bar{x},y,\bar{z}\}[\bar{a},b,\bar{c}][d,\bar{e},f][u,\bar{v},w]$	$\{x+\frac{1}{2},\bar{y},\bar{z}\}[\bar{a},b,c][\bar{d},e,f][\bar{u},v,w]$
			$\{\bar{x},\bar{y},\bar{z}\}[\bar{a},\bar{b},\bar{c}][\bar{d},\bar{e},\bar{f}][u,v,w]$	$\{x+\frac{1}{2},y,\bar{z}\}[\bar{a},\bar{b},c][d,e,\bar{f}][\bar{u},\bar{v},w]$
			$\{x,\bar{y},z\}[a,\bar{b},c][\bar{d},e,\bar{f}][u,\bar{v},w]$	$\{\bar{x}+\frac{1}{2},y,z\}[a,\bar{b},\bar{c}][d,\bar{e},\bar{f}][\bar{u},v,w]$
4	k	$m..$	$\{\frac{1}{4},y,z\}[a,0,0][d,0,0][0,v,w]$	$\{\frac{1}{4},\bar{y},z\}[a,0,0][\bar{d},0,0][0,\bar{v},w]$
			$\{\frac{3}{4},y,\bar{z}\}[\bar{a},0,0][d,0,0][0,\bar{v},w]$	$\{\frac{3}{4},\bar{y},\bar{z}\}[\bar{a},0,0][\bar{d},0,0][0,v,w]$
4	j	$.m'^*.$	$\{x,\frac{1}{2},z\}[a,0,c][d,0,f][0,v,0]$	$\{\bar{x}+\frac{1}{2},\frac{1}{2},z\}[a,0,\bar{c}][d,0,\bar{f}][0,v,0]$
			$\{\bar{x},\frac{1}{2},\bar{z}\}[\bar{a},0,\bar{c}][d,0,f][0,\bar{v},0]$	$\{x+\frac{1}{2},\frac{1}{2},\bar{z}\}[\bar{a},0,c][d,0,\bar{f}][0,\bar{v},0]$
4	i	$.m'.$	$\{x,0,z\}[a,0,c][0,e,0][u,0,w]$	$\{\bar{x}+\frac{1}{2},0,z\}[a,0,\bar{c}][0,\bar{e},0][\bar{u},0,w]$
			$\{\bar{x},0,\bar{z}\}[\bar{a},0,\bar{c}][0,\bar{e},0][u,0,w]$	$\{x+\frac{1}{2},0,\bar{z}\}[\bar{a},0,c][0,e,0][\bar{u},0,w]$
4	h	$.2^*.$	$\{0,y,\frac{1}{2}\}[0,b,0][d,0,f][u,0,w]$	$\{\frac{1}{2},\bar{y},\frac{1}{2}\}[0,b,0][\bar{d},0,f][\bar{u},0,w]$
			$\{0,\bar{y},\frac{1}{2}\}[0,\bar{b},0][\bar{d},0,\bar{f}][u,0,w]$	$\{\frac{1}{2},y,\frac{1}{2}\}[0,\bar{b},0][d,0,\bar{f}][\bar{u},0,w]$
4	g	$.2^*.$	$\{0,y,0\}[0,b,0][d,0,f][u,0,w]$	$\{\frac{1}{2},\bar{y},0\}[0,b,0][\bar{d},0,f][\bar{u},0,w]$
			$\{0,\bar{y},0\}[0,\bar{b},0][\bar{d},0,\bar{f}][u,0,w]$	$\{\frac{1}{2},y,0\}[0,\bar{b},0][d,0,\bar{f}][\bar{u},0,w]$
2	f	$mm'^*2'^*$	$\{\frac{1}{4},\frac{1}{2},z\}[a,0,0][d,0,0][0,v,0]$	$\{\frac{3}{4},\frac{1}{2},\bar{z}\}[\bar{a},0,0][d,0,0][0,\bar{v},0]$
2	e	$mm'2'$	$\{\frac{1}{4},0,z\}[a,0,0][0,0,0][0,0,w]$	$\{\frac{3}{4},0,\bar{z}\}[\bar{a},0,0][0,0,0][0,0,w]$
2	d	$.2^*/m'^*.$	$\{0,\frac{1}{2},\frac{1}{2}\}[0,0,0][d,0,f][0,0,0]$	$\{\frac{1}{2},\frac{1}{2},\frac{1}{2}\}[0,0,0][d,0,\bar{f}][0,0,0]$
2	c	$.2^*/m'.$	$\{0,0,\frac{1}{2}\}[0,0,0][0,0,0][u,0,w]$	$\{\frac{1}{2},0,\frac{1}{2}\}[0,0,0][0,0,0][\bar{u},0,w]$
2	b	$.2^*/m'^*.$	$\{0,\frac{1}{2},0\}[0,0,0][d,0,f][0,0,0]$	$\{\frac{1}{2},\frac{1}{2},0\}[0,0,0][d,0,\bar{f}][0,0,0]$
2	a	$.2^*/m'.$	$\{0,0,0\}[0,0,0][0,0,0][u,0,w]$	$\{\frac{1}{2},0,0\}[0,0,0][0,0,0][\bar{u},0,w]$

Figure 1 (continued)

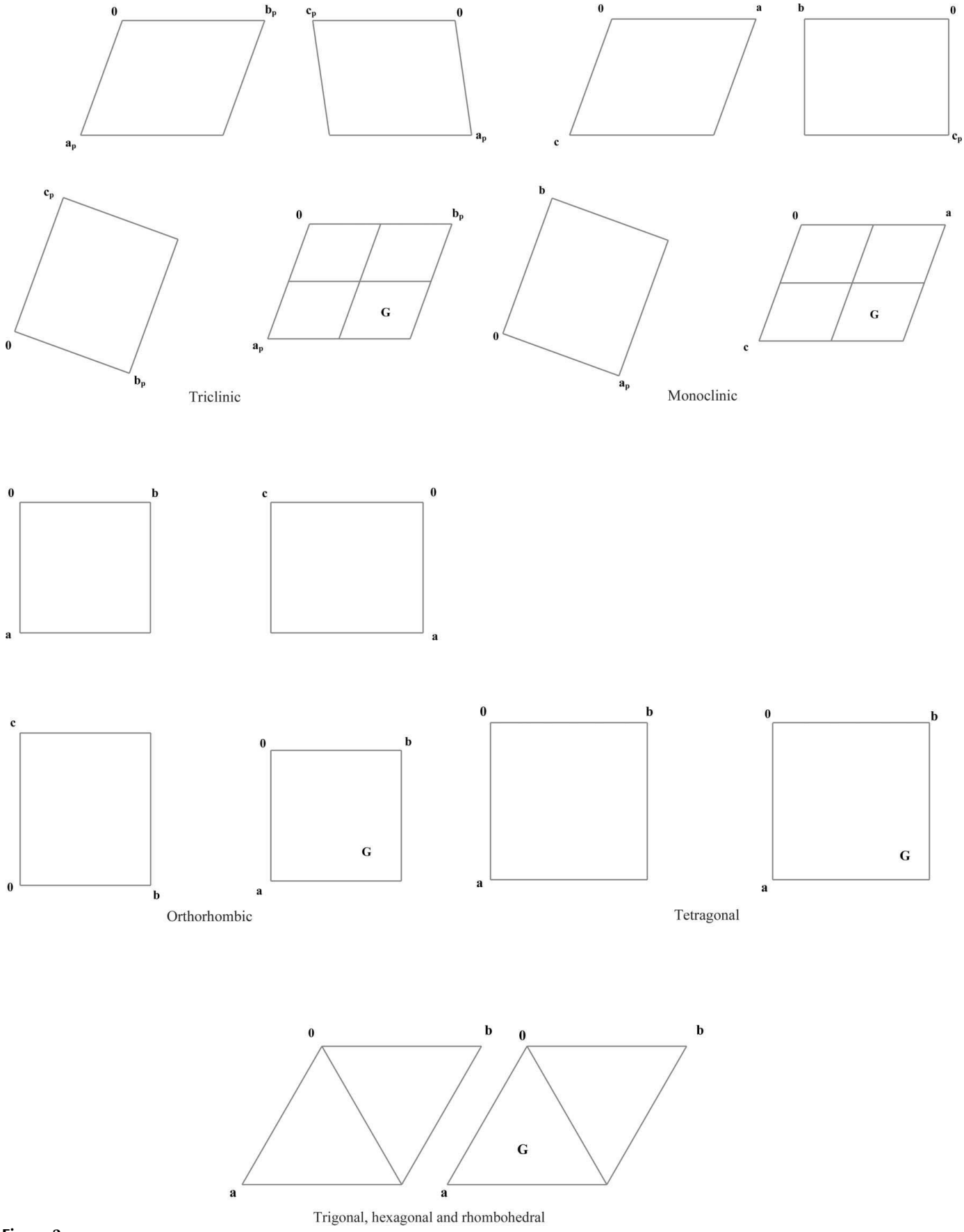


Figure 2
Schematic representations of the general-position and symmetry-element diagrams for different crystal systems (**G** = general-position diagram).

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 2 & 0 & \frac{1}{2} \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

is given as a, $2b$, c; 0, $\frac{1}{2}$, 0.

Second line:

(i) The serial number of the colorblind parent space-group type in ITC-A. For example, the colorblind parent space group of $P(1,1^*,1)$ $mm'a^*$ is *Pmma*. Therefore, 51 is shown as the serial number of *Pmma* in ITC-A.

(ii) Double antisymmetry point-group symbol. The double antisymmetry point group is the point group obtained from the double antisymmetry space group by setting all translations equal to zero.

For example, setting all translations of the $P(1,1^*,1)$ $mm'a^*$ to zero gives double antisymmetry point group $mm'm1^*$.

(iii) The name of the crystal system of the group. Note: information for only one origin choice is given for each group. The choice of origin follows the origin choice of the colorblind parent group in ITC-A if there is only one origin choice for it. The 'Origin 2' setting is selected when the colorblind parent space group has two origin choices in ITC-A.

2.2. Lattice diagram

A three-dimensional lattice diagram is given for each double antisymmetry space group in the upper right corner of the first page, which describes the conventional lattice cell of the colorblind parent group of the group with the generators of the translation subgroup of the group. The color of each arrow indicates whether it is a pure colorless translation (black), a primed translation (red), a starred translation (blue) or a prime–starred translation (green). The translations can be derived from the International symbol according to §2.1 and are explicitly listed in the section of generators selected. For example, the lattice diagram of group $P(1,1^*,1)$ $mm'a^*$ is shown in the upper right corner of Fig. 1. It shows an orthorhombic $P(1,1^*,1)$ lattice. The black arrows along the x and z axes represent unit-cell translations that are not coupled with anti-identity. The blue arrow along y represents a translation along y coupled with 1^*. Thus the generators of the translation subgroup are $t_{[100]}$, $t_{[010]}{}^*$ and $t_{[001]}$.

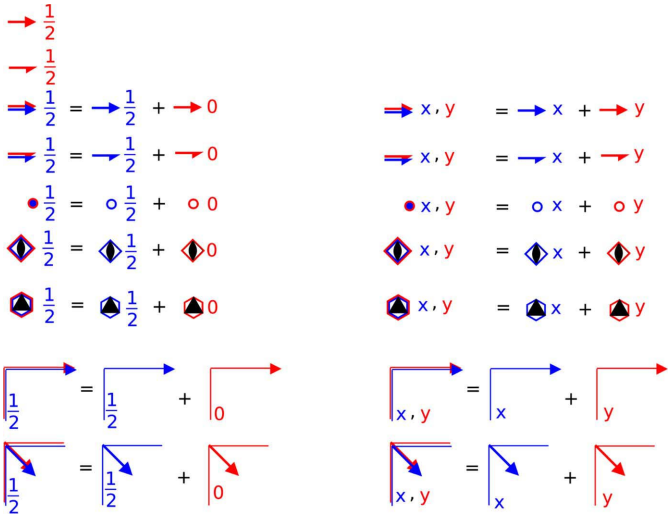


Figure 3
Heights of symmetry operations above the plane of projection. The text besides the symbols indicates the height of the symbols, x and y represent arbitrary heights.

Table 3
Symmetry axes parallel to the plane of projection.

Symmetry axis	Graphical symbol	Screw vector of a right-handed screw axis in units of colorblind unit-cell translation parallel to the axis	Printed symbol
Twofold primed rotation axis		None	$2'$
Twofold primed screw axis		1/2	$2_1'$
Fourfold primed rotation axis		None	$4'$
Fourfold primed screw axis		1/4	$4_1'$
Fourfold primed screw axis		2/4	$4_2'$
Fourfold primed screw axis		3/4	$4_3'$
Four-bar primed inversion		None	$\bar{4}'$

2.3. Asymmetric unit

An asymmetric unit of a double antisymmetry space group is defined as a simply connected smallest part of space, which can exactly fill the whole space by application of all symmetry operations of the double antisymmetry space group. The asymmetric unit of a double antisymmetry space group is defined by setting the limits of the coordinates of points contained in the symmetric unit. For example, the asymmetric unit of $P(1,1^*,1)$ $mm'a^*$ is defined as

$$0 \le x \le 1/2;\ 0 \le y \le 1/2;\ 0 \le z \le 1/4.$$

Because the asymmetric unit is invariant with the introduction of anti-identities, all double antisymmetry space groups derived from the same colorblind parent space group have identical asymmetric units.

2.4. Diagrams of symmetry elements and general positions

Following the headline and the lattice diagram, diagrams of symmetry elements and general positions are given. The symmetry-element diagrams show the relative locations and orientations of the symmetry elements and the general-position diagrams show the locations of a set of general positions.

Two types of unit cell are defined for a double antisymmetry space group. Here we define the conventional unit cell of the colorblind parent group of a double antisymmetry space group

Table 4
Symmetry axes normal to the plane of projection.

If a center of symmetry is on a rotation axis, the symbol of the center of symmetry is placed onto the symbol of the rotation axis.

Symmetry axis or symmetry point	Graphical symbol	Screw vector of a right-handed screw axis in units of colorblind unit-cell translation parallel to the axis	Printed symbol
Identity	None	None	1
Primed center of symmetry		None	$\bar{1}'$
Primed center of symmetry and starred center of symmetry		None	$\bar{1}'$, $\bar{1}$*
Twofold primed rotation axis		None	$2'$
Twofold primed screw axis		1/2	$2_1'$
Threefold primed rotation axis		None	$3'$
Threefold primed screw axis		1/3	$3_1'$
Threefold primed screw axis		2/3	$3_2'$
Fourfold primed rotation axis		None	$4'$
Fourfold primed screw axis		1/4	$4_1'$
Fourfold primed screw axis		2/4	$4_2'$
Fourfold primed screw axis		3/4	$4_3'$
Fourfold primed inversion		None	$\bar{4}'$
Sixfold primed rotation axis		None	$6'$
Sixfold primed screw axis		1/6	$6_1'$
Sixfold primed screw axis		2/6	$6_2'$
Sixfold primed screw axis		3/6	$6_3'$
Sixfold primed screw axis		4/6	$6_4'$
Six-fold primed screw axis		5/6	$6_5'$
Six-bar primed inversion		None	$\bar{6}'$

as the *colorblind unit cell*, and the unit cell that can fill the space with colorless translations as the *colorless unit cell*. A colorless translation is a translation that is not coupled with any anti-identity. A colored translation is a translation coupled with one of the three anti-identities, and is printed in the same color as the anti-identity to denote the coupling. The colorblind unit cell and the colorless unit cell are different for double antisymmetry space groups in which the colorblind unit-cell translations are coupled with anti-identities. For example, in a $P(1,1^*,1)$ lattice, the colorblind unit cell is the same as that of the colorblind parent space group, which has a size of $1\times1\times1$, while the colorless unit cell has a size of $1\times2\times1$.

The arrangement of the diagrams for different crystal systems is shown in Fig. 2. The projection direction for all diagrams is perpendicular to the plane of the figure. The *b* axis is selected as the unique axis for monoclinic groups. Symmetry-element diagrams projected along *a*, *b* and *c* directions are given for triclinic, monoclinic and orthorhombic groups. Symmetry-element diagrams projected along the *c* axis are given for tetragonal, hexagonal and trigonal groups. For face-centered cubic groups, the symmetry-element diagrams show only the upper-left quadrant of the colorblind unit cell. General-position diagrams projected along the *b* axis are given for monoclinic groups. General-position diagrams projected along the *c* axis are given for all other non-cubic groups. For cubic groups, general-position diagrams are not shown.

The color of a graphical symbol of a symmetry element indicates that the symmetry element is coupled with an anti-identity associated with that color or not coupled with any anti-identity if the color is black. Similarly, the color of a graphical symbol of a general position indicates that the position is generated from an arbitrary black position by a symmetry operation coupled with the anti-identity associated with that color or not coupled with any anti-identity if the color is black. The colors associated with antisymmetry identities follow the coloring schemes of VanLeeuwen *et al.* (2014) which are listed in Table 1.

The diagrams only consider the unit cell of the colorblind parent group of a double antisymmetry space group, *i.e.* the colorblind unit cell. The diagrams only show the symmetry elements within the colorblind unit cell because the diagrams can be easily extended as the symmetry-element diagrams are periodic in the directions of translation, and general-position diagrams are periodic in the direction of a colorless translation and the color alternates according to the color operation rule in the direction of a colored translation.

2.4.1. Diagrams of symmetry elements. The symbols used in diagrams of symmetry elements are extensions of those used in ITC-A. The meaning of each symbol is given in Appendix *A*.

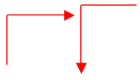
The heights of centers of symmetry, rotoinversions, and axes and planes parallel to the plane of projection are printed next to the graphical symbol if the heights are non-zero. Some symmetry elements sit on top of each other in the projected diagram; these are addressed by the formats given in Fig. 3.

If a group has a colored unit-cell translation, *e.g.* $(1|010)^*$, and there is a mirror plane, *e.g.* $(m_x|\frac{1}{2}00)$ so that the translation direction is parallel to the mirror plane, combination of the translation and the mirror operation will result in a coplanar glide plane $(m_x|\frac{1}{2}10)^*$. Such glide planes are not explicitly shown in the diagrams as they can be derived from the original two operations. For example, in the symmetry-element diagram of $P(1,1^*,1)$ $mm'a^*$, $(m_x|\frac{1}{2}10)^*$ is not shown. Because the original mirror plane and the coplanar glide plane share the same plane, showing both would unnecessarily complicate these diagrams. This also applies to any coaxial screw axes that come from a rotation axis coupled with a colored unit-cell translation along the same axis. For example, in the symmetry-element diagram of $P(1,1^*,1)$ $mm'a^*$, the combination of $(1|010)^*$ and $(2_y|000)^*$, $(2_y|010)$, is not shown.

Table 5
Symmetry planes normal to the plane of projection.

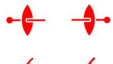
Symmetry plane	Graphical symbol	Glide vector in units of colorblind unit-cell translation parallel to the projection plane	Printed symbol
Primed mirror plane		None	m'
Primed glide plane		1/2 lattice vector along line in projection plane	a', b' or c'
Primed glide plane		1/2 lattice vector normal to projection plane	a', b' or c'
Primed glide plane		One glide vector with two components: 1/2 along line parallel to projection plane, 1/2 normal to projection plane	n'
Primed glide plane and starred glide plane		Two glide vectors: 1/2 along line parallel to projection plane primed and 1/2 normal to projection plane starred	$e1'$ and $e2^*$
Primed glide plane		1/4 along line parallel to projection plane, combined with 1/4 normal to projection plane (arrow indicates direction parallel to the projection plane for which the normal component is positive)	d'

Table 6
Symmetry planes parallel to the plane of projection.

Symmetry plane	Graphical symbol	Glide vector in units of colorblind unit-cell translation parallel to the projection plane	Printed symbol
Primed mirror plane		None	m'
Primed glide plane		1/2	a', b' or c'
Primed glide plane		One glide vector with two components, 1/2 in the direction of the arrow	n'
Primed glide plane and starred glide plane		Two glide vectors, 1/2 in either of the directions of the two arrows	$e1'$ and $e2^*$

The main benefit of this way of presenting the symmetry-element diagrams is that the diagram of a double antisymmetry space group will show exactly the same elements as the symmetry-element diagram of its colorblind parent group, with only additional colors to indicate the coupled anti-identities.

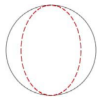
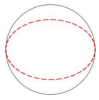
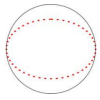
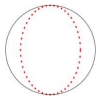
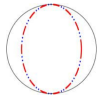
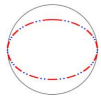
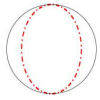
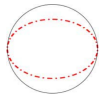
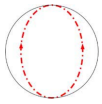
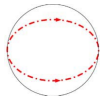
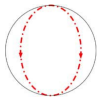
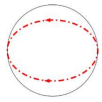
Table 7
Symmetry axes inclined to the plane of projection (cubic groups only).

Symmetry axis	Graphical symbol	Screw vector of a right-handed screw axis in units of colorblind unit-cell translation parallel to the axis	Printed symbol
Twofold primed rotation axis		None	$2'$
Twofold primed screw axis		1/2	$2_1'$
Threefold primed rotation axis		None	$3'$
Threefold primed screw axis		1/3	$3_1'$
Threefold primed screw axis		2/3	$3_2'$

2.4.2. Diagrams of general positions. A diagram of general positions is given for each non-cubic double antisymmetry space group. The symbols used in diagrams of general positions are extensions of those used in ITC-A. Each position is represented by a circle colored with the color of the position and a height notation beside the circle indicating the z component of the position. For positions with a z component of '$+z$' or '$-z$', the height notation is '+' or '−', respectively. For positions with a z component of '$h + z$' or '$h - z$', the height notation is 'h+' or 'h−', respectively. If two general positions have the same x and y component and z components of $+z$ and $-z$, respectively, the two positions are represented as

Each half of the symbol corresponds to a unique position. The height notations are placed on either side of the symbol. For positions with a reversed chirality with respect to the starting position, a comma is added into the circle or the half of the circle that represents that position.

Table 8
Symmetry planes inclined to the plane of projection (cubic groups only).

Symmetry plane	Graphical symbol for planes normal to [011] and [01$\bar{1}$]	Graphical symbol for planes normal to [101] and [10$\bar{1}$]	Glide vector in units of colorblind unit-cell translation for planes normal to [011] and [01$\bar{1}$]	Glide vector in units of colorblind unit-cell translation for planes normal to [101] and [10$\bar{1}$]	Printed symbol
Primed mirror plane			None	None	m'
Primed glide plane			1/2 lattice vector along [100]	1/2 lattice vector along [010]	a' or b'
Primed glide plane			1/2 lattice vector along [01$\bar{1}$] or along [011]	1/2 lattice vector along [10$\bar{1}$] or along [101]	a' or b'
Primed glide plane and starred glide plane			Two glide vectors: 1/2 along [100] primed and 1/2 along [01$\bar{1}$] or along [011] starred	Two glide vectors: 1/2 along [010] primed and 1/2 along [10$\bar{1}$] or along [101] starred	$e1'$ and $e2^*$
Primed glide plane			One glide vector: 1/2 along [11$\bar{1}$] or along [111]	One glide vector: 1/2 along [11$\bar{1}$] or along [111]	n'
Primed glide plane			1/2 along [1$\bar{1}$1] or along [111]	1/2 along [$\bar{1}$11] or along [111]	d'
Primed glide plane			1/2 along [$\bar{1}\bar{1}$1] or along [$\bar{1}$11]	1/2 along [$\bar{1}\bar{1}$1] or along [1$\bar{1}$1]	d'

2.5. Symmetry operations

The modified ITC-A notation and Seitz notation for the symmetry operations are listed under the heading *Symmetry operations*. The symbolism follows Section 11.1.2 of ITC-A with the addition of the use of prime, star and prime–star to denote coupled anti-identities. For glide planes and screw axes, the glide and screw vectors are given in units of the length of the colorblind unit cell. In addition, Seitz notation is also given for each symmetry operation.

For double antisymmetry space groups with centered cells, the symmetry operations are given in several blocks. Groups without centering translations only have one block. For groups with centering translations, the number of blocks in addition to the origin (0, 0, 0)+ block equals the number of the centering translations. For example, in a group with a body-centering translation coupled with $1'$, two blocks (0, 0, 0)+ and $(1/2, 1/2, 1/2)'$+ are shown.

2.6. Generators selected

The first generator selected is the identity operation given by (1). This is followed by the generating translations. The other generating symmetry operations are listed as numbers (p) that refer to the corresponding symmetry operations in the first block of *Symmetry operations*. If the group includes anti-identities, then anti-identities are appended to the end of other generating symmetry operations.

2.7. General and special positions with spin vectors, roto vectors and displacement vectors

The position table of a double antisymmetry space group under *Positions* consists of general positions and special positions. These positions are called Wyckoff positions. The first block of the table is the general positions, which shows the points that are left invariant only by identity operations or anti-identity operations. The remaining blocks of the table are the special positions, which are the points that are left invariant by at least one non-identity operation. For each entry, the columns contain the following information from left to right: (i) multiplicity of the Wyckoff position; (ii) Wyckoff letter; (iii) oriented site-symmetry symbol; (iv) coordinates and vectors on sites.

2.7.1. Multiplicity. The multiplicity is the number of equivalent positions in the conventional unit cell of the colorblind parent space group of the double antisymmetry space group.

2.7.2. Wyckoff letter. The letter is a coding scheme for the blocks of positions, starting with a at the bottom block and continuing upwards in alphabetical order.

2.7.3. Oriented site-symmetry symbol. The site-symmetry group of the first position of each block of positions is given by an oriented symbol. The group is isomorphic to a subgroup of the point group of the double antisymmetry space group. The symbol shows how the symmetry elements of the site-symmetry group are oriented at the site. The symmetry-element symbol was placed according to the sequence of symmetry directions in the space-group symbol. The symmetry directions that do not contribute any element to the site symmetry are represented by dots. For example, the site-symmetry symbol . m'*. at special positions with Wyckoff letter *j* listed for *P*(1,1*,1) $mm'a$* means that there is a mirror plane coupled with 1′* perpendicular to the secondary direction, which is [010] for orthorhombic groups.

2.7.4. Coordinates and vectors on sites. For each block of positions, the coordinates of the positions are given. Immediately to the right of each set of coordinates are components of the symmetry-allowed spin vectors, roto vectors and displacement vectors. The symmetry-allowed components of spin vectors, roto vectors and displacement vectors on the first position are determined from the site-symmetry group. For example, at the special positions with Wyckoff letter *b*, we have

2 b . 2*/m'* . {0,$\frac{1}{2}$,0}[0,0,0][d,0,f][0,0,0] {$\frac{1}{2}$, $\frac{1}{2}$,0}[0,0,0][d,0,$\bar{f}$][0,0,0].

The site symmetry at 0, $\frac{1}{2}$, 0 is . 2*/m'* and, consequently, the spin vector is [0, 0, 0], the roto vector is [*d*, 0, *f*] and the displacement vector is [0, 0, 0]. The components at the remaining positions are determined by applying symmetry operations to the components at the first position. Applying the operation (m_x|$\frac{1}{2}$ 00) to the spin vector [0, 0, 0], roto vector [*d*, 0, *f*] and displacement vector [0, 0, 0] at 0, $\frac{1}{2}$, 0, we obtain the spin vector [0, 0, 0], roto vector [*d*, 0, $\bar{f}$] and displacement vector [0, 0, 0] at the second position $\frac{1}{2}$, $\frac{1}{2}$, 0.

For double antisymmetry space groups with centering translations or translations coupled with anti-identity, the translations such as (0, 0, 0)+ (1/2, 1/2, 1/2)′+ are listed above the ordinate triplets. The symbol '+' means that the components
of the translation coordinates should be added to the listed coordinate triplets to obtain the positions coupled with the translation and the anti-identity coupled with the translation should be acted on the listed spin vectors, roto vectors and displacement vectors to obtain the components of the three types of vectors on the positions coupled with the translation.

APPENDIX *A*
Double antisymmetry space-group diagram symbols

Most symbols used in the double antisymmetry space-group diagrams have the same shapes as those used in ITC-A. The symbols are colored according to the anti-identity coupled with the operation. Extra symbols come from colored unit-cell translations on the projection direction of the diagrams. When the unit-cell translation is coupled with an anti-identity, there will be symmetry elements with different colors that are located at the same position on the projection plane but at different positions along the projection direction. Both the original and the extra symbols used are listed in Tables 3 to 8. The symbols are based on the symmetry-element font *cryst* created by Ulrich Müller from http://www.iucr.org/resources/symmetry-font.

For simplicity, any symmetry element that has only one color associated with it is represented by a symmetry element coupled with 1′ (red) in Tables 3 to 8. 1′ can be substituted by identity or any anti-identity (1′, 1* or 1′*) and the coloring should be substituted (to black, red, blue or green) respectively. Similarly, symmetry elements with two colors are represented by symmetry elements with 1′ and 1* (red and blue) in Tables 3 to 8 where 1′ and 1* can be substituted by any two anti-identities and the colorings should be substituted respectively.

If a center of symmetry is on a rotation axis, the symbol of the center of symmetry is placed onto the symbol of the rotation axis.

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