ISOSUBGROUP: an internet tool for generating isotropy subgroups of crystallographic space groups

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ISOSUBGROUP, the newest member of the ISOTROPY Software Suite (http://iso.byu.edu), generates isotropy subgroups of crystallographic space groups based on superpositions of multiple irreducible representations, along with a wealth of information about each one. Like the original ISOTROPY program, its scope is general rather than being restricted to common types of order parameters of a user-specified parent structure. But like the newer ISODISTORT program, its user-friendly interface has menu-driven selections. This combination of features has been oft requested but unavailable until now. Program output includes information about the subgroup symmetry, ferroic species, phase-transition continuity, active **k** vectors, domains and secondary order parameters.

The methods of group representation theory have been applied with much success to many different areas of crystallography (Landau & Lifshitz, 1969; Bradley & Cracknell, 1972; Perez-Mato *et al.*, 2010; Kerman *et al.*, 2012). Over the years, we have been developing tools in the *ISOTROPY Software Suite* (http://iso.byu.edu) that apply such methods to explore a variety of distortions in crystals, including those that appear in real structural phase transitions. By 'distortions', we mean to include any physical change that lowers the symmetry of the crystal in a well defined way, such as lattice strains, atomic displacements, magnetic ordering, occupational ordering *etc*.
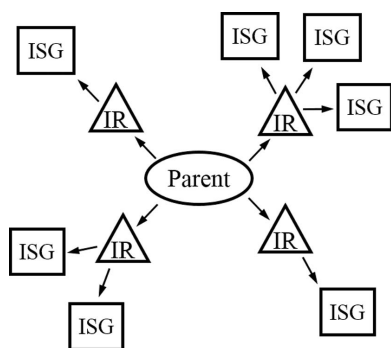
The centerpiece of these group theoretical methods is the irreducible representation (IR), which maps the space-group operators g onto a set of n-dimensional square matrices $D(g)$. It is a well known but still remarkable fact that any crystal distortion can be decomposed or expanded as a linear combination of IR basis functions. We call these basis functions 'symmetry modes'. They are modes that extend throughout the entire crystal. In the case of displacive symmetry breaking, for example, each IR symmetry mode is a pattern of atomic displacements. Symmetry modes come in groups of n: $\{\varphi_1, \varphi_2, \ldots, \varphi_n\}$, one for each dimension of the IR they belong to. These n symmetry modes are related by symmetry operators g in the parent:

$$g\varphi_i = \sum_{j=1}^{n} \varphi_j D_{ji}(g), \qquad (1)$$

which means that they transform like the columns of the IR matrices under the parent symmetry operations.

Let

$$\varphi = \sum_{i=1}^{n} \eta_i \varphi_i \qquad (2)$$

be the contribution to the overall distortion from a specific set of symmetry modes belonging to an n-dimensional IR. The n-dimensional vector $\boldsymbol{\eta}$ consisting of the coefficients of the decomposition is called the order parameter of the IR. When its components are treated as abstract variables, we refer to it as the order parameter direction (OPD) within the space of possible IR-generated distortions. The OPD indicates any symmetry relationships that might exist between its components, and thereby indicates special constraints on how the corresponding symmetry modes of the IR are to be combined. The special $(a, -a, 0, 0)$ OPD, for example, indicates a significantly smaller degree of symmetry breaking than the general (a, b, c, d) OPD.

Combining equations (1) and (2), we obtain the result of the operation of g on a distortion,

$$g\varphi = \sum_{i=1}^{n} \sum_{j=1}^{n} D_{ji}(g)\eta_i \varphi_j = \sum_{j=1}^{n} (g\eta)_j \varphi_j, \quad (3)$$

where

$$g\eta = D(g)\eta \quad (4)$$

so that the operation of g on the distortion can be viewed as an operation on the OPD rather than the symmetry modes themselves.

For a given IR and OPD ($\boldsymbol{\eta}$), the space group G of the distorted structure consists of all symmetry operators g of the parent space group G_0 which satisfy $D(g)\boldsymbol{\eta} = \boldsymbol{\eta}$. We refer to G as an isotropy subgroup (ISG) of G_0. Two OPDs, $\boldsymbol{\eta}_1$ and $\boldsymbol{\eta}_2$, are said to be equivalent if there exists a parent symmetry operator g such than $\boldsymbol{\eta}_2 = g\boldsymbol{\eta}_1$. Their corresponding ISGs are also equivalent. For a given space-group IR, the list of inequivalent OPDs, and hence ISGs, is always finite.

Each space-group IR is associated with a $\mathbf{k}$ vector in the first Brillouin zone. IRs defined at distinct $\mathbf{k}$ vectors (not related by a reciprocal-lattice translation or a point operator of G_0) are distinct. A $\mathbf{k}$ vector on the surface of the symmetry-unique portion of the Brillouin zone lies on either a vertex (a special point of symmetry), an edge (a line of symmetry) or a face (a plane of symmetry). Otherwise, it is a general $\mathbf{k}$ vector in the zone interior.

In 1988, Stokes and Hatch published a exhaustive list of the ISGs arising from the complete space-group IRs at each of the special $\mathbf{k}$ points of each of the 230 crystallographic space groups, along with detailed information about each one. Shortly afterwards, Stokes and Hatch wrote an interactive software program called *ISOTROPY*, which later became the first component of what we now call the *ISOTROPY Software Suite* of online crystallographic software tools (http://iso.byu.edu). The *ISOTROPY* program performs real-time calculation of the IRs and ISGs at special or non-special $\mathbf{k}$ vectors,

including superpositions of multiple IRs. The ISG that results from the superposition of multiple IRs is simply the intersection of the ISGs of the individual IRs. *ISOTROPY*'s most important feature is its ability to explore the symmetry modes of a crystal structure that has been distorted *via* the IRs of its parent space group.

Because *ISOTROPY* is a command-line program with its own internal language and syntax and a very flexible feature set, considerable technical knowledge is required to use it effectively. The steep learning curve may have discouraged some potential users. More recently, Campbell *et al.* (2006) developed a new tool called *ISODISTORT*, which targets the needs of the materials research community, requires a minimum of technical knowledge beyond that common to those familiar with mainstream crystallographic tools, and

IR	OPD	k-active	Subgroup	Basis	Origin	Size	Index	cont	spec
GM1+	P1 (a)	(0,0,0)	221 Pm-3m	(1,0,0),(0,1,0),(0,0,1)	(0,0,0)	1	1	no	
GM2+	P1 (a)	(0,0,0)	200 Pm-3	(1,0,0),(0,1,0),(0,0,1)	(0,0,0)	1	2	yes	
GM3+	P1 (a,0)	(0,0,0)	123 P4/mmm	(1,0,0),(0,1,0),(0,0,1)	(0,0,0)	1	3	no	pfs
GM3+	C1 (a,b)	(0,0,0)	47 Pmmm	(1,0,0),(0,1,0),(0,0,1)	(0,0,0)	1	6	no	pfs
GM4+	P1 (a,0,0)	(0,0,0)	83 P4/m	(0,1,0),(0,0,1),(1,0,0)	(0,0,0)	1	6	yes	ifs
GM4+	P2 (a,a,0)	(0,0,0)	12 C2/m	(1,-1,0),(1,1,0),(0,0,1)	(0,0,0)	1	12	no	ifs
GM4+	P3 (a,a,a)	(0,0,0)	148 R-3	(1,-1,0),(0,1,-1),(1,1,1)	(0,0,0)	1	8	yes	ifs
GM4+	S1 (a,b,c)	(0,0,0)	2 P-1	(1,0,0),(0,1,0),(0,0,1)	(0,0,0)	1	24	no	ifs
GM5+	P1 (a,0,0)	(0,0,0)	65 Cmmm	(1,1,0),(-1,1,0),(0,0,1)	(0,0,0)	1	6	no	pfs
GM5+	P3 (a,a,a)	(0,0,0)	166 R-3m	(1,-1,0),(0,1,-1),(1,1,1)	(0,0,0)	1	4	no	pfs
GM5+	C2 (a,a,b)	(0,0,0)	12 C2/m	(1,0,1),(1,0,-1),(0,1,0)	(0,0,0)	1	12	no	pfs
GM5+	S1 (a,b,c)	(0,0,0)	2 P-1	(1,0,0),(0,1,0),(0,0,1)	(0,0,0)	1	24	no	pfs
GM1-	P1 (a)	(0,0,0)	207 P432	(1,0,0),(0,1,0),(0,0,1)	(0,0,0)	1	2	yes	
GM2-	P1 (a)	(0,0,0)	215 P-43m	(1,0,0),(0,1,0),(0,0,1)	(0,0,0)	1	2	yes	
GM3-	P1 (a,0)	(0,0,0)	111 P-42m	(1,0,0),(0,1,0),(0,0,1)	(0,0,0)	1	6	yes	ifs
GM3-	P2 (0,a)	(0,0,0)	89 P422	(1,0,0),(0,1,0),(0,0,1)	(0,0,0)	1	6	yes	ifs
GM3-	C1 (a,b)	(0,0,0)	16 P222	(1,0,0),(0,1,0),(0,0,1)	(0,0,0)	1	12	no	ifs
GM4-	P1 (a,0,0)	(0,0,0)	99 P4mm	(0,1,0),(0,0,1),(1,0,0)	(0,0,0)	1	6	yes	ifs,pfc
GM4-	P2 (a,a,0)	(0,0,0)	38 Amm2	(0,0,1),(1,-1,0),(1,1,0)	(0,0,0)	1	12	no	ifs,pfc
GM4-	P3 (a,a,a)	(0,0,0)	160 R3m	(1,-1,0),(0,1,-1),(1,1,1)	(0,0,0)	1	8	yes	ifs,pfc
GM4-	C1 (a,b,0)	(0,0,0)	6 Pm	(0,1,0),(0,0,1),(1,0,0)	(0,0,0)	1	24	no	ifs,pfc
GM4-	C2 (a,a,b)	(0,0,0)	8 Cm	(1,1,0),(-1,1,0),(0,0,1)	(0,0,0)	1	24	no	ifs,pfc
GM4-	S1 (a,b,c)	(0,0,0)	1 P1	(1,0,0),(0,1,0),(0,0,1)	(0,0,0)	1	48	no	ifs,pfc
GM5-	P1 (a,0,0)	(0,0,0)	115 P-4m2	(1,0,0),(0,1,0),(0,0,1)	(0,0,0)	1	6	yes	ifs
GM5-	P2 (a,a,0)	(0,0,0)	38 Amm2	(0,1,0),(1,0,1),(1,0,-1)	(0,0,0)	1	12	no	ifs,ifc
GM5-	P3 (a,a,a)	(0,0,0)	155 R32	(1,-1,0),(0,1,-1),(1,1,1)	(0,0,0)	1	8	yes	ifs
GM5-	C1 (a,b,0)	(0,0,0)	6 Pm	(1,0,0),(0,1,0),(0,0,1)	(0,0,0)	1	24	no	ifs,ifc
GM5-	C2 (a,a,b)	(0,0,0)	5 C2	(1,0,1),(1,0,-1),(0,1,0)	(0,0,0)	1	24	no	ifs,ifc
GM5-	S1 (a,b,c)	(0,0,0)	1 P1	(1,0,0),(0,1,0),(0,0,1)	(0,0,0)	1	48	no	ifs,ifc

Figure 1
Detailed descriptions of each of the ISGs of each of the IRs of space group $Pm\bar{3}m$ (No. 221) at $\mathbf{k} = (0, 0, 0)$, also called the Γ (GM) point. The dimension of the matrices of a given IR is equal to the number of components of the OPD vector. Observe differences in the space group, subgroup index, continuity and ferroic species from one IR and ISG to the next.

Domain	OPD	k-active	Subgroup	Basis	Origin	Size	Index	cont	spec
(1) 1,1,1 (x,y,z)	C1 (a,0,b)	(0,1/2,0),(0,0,1/2)	50 Pban	(0,2,0),(0,0,2),(1,0,0)	(0,0,0)	4	24	no	ifs
(7) 1,1,2 (x,y,z+1)	C1 (a,0,-b)	(0,1/2,0),(0,0,1/2)	50 Pban	(0,2,0),(0,0,2),(1,0,0)	(0,0,1)	4	24	no	ifs
(13) 1,1,3 (x,y+1,z)	C1 (-a,0,b)	(0,1/2,0),(0,0,1/2)	50 Pban	(0,2,0),(0,0,2),(1,0,0)	(0,1,0)	4	24	no	ifs
(19) 1,1,4 (x,y+1,z+1)	C1 (-a,0,-b)	(0,1/2,0),(0,0,1/2)	50 Pban	(0,2,0),(0,0,2),(1,0,0)	(0,1,1)	4	24	no	ifs
(2) 2,1,1 (y,z,x)	C1 (b,a,0)	(0,1/2,0),(1/2,0,0)	50 Pban	(2,0,0),(0,2,0),(0,0,1)	(0,0,0)	4	24	no	ifs
(8) 2,1,2 (y,z+1,x)	C1 (-b,a,0)	(0,1/2,0),(1/2,0,0)	50 Pban	(2,0,0),(0,2,0),(0,0,1)	(0,1,0)	4	24	no	ifs
(14) 2,1,3 (y+1,z,x)	C1 (b,-a,0)	(0,1/2,0),(1/2,0,0)	50 Pban	(2,0,0),(0,2,0),(0,0,1)	(1,0,0)	4	24	no	ifs
(20) 2,1,4 (y+1,z+1,x)	C1 (-b,-a,0)	(0,1/2,0),(1/2,0,0)	50 Pban	(2,0,0),(0,2,0),(0,0,1)	(1,1,0)	4	24	no	ifs
(3) 3,1,1 (z,x,y)	C1 (0,b,a)	(1/2,0,0),(0,0,1/2)	50 Pban	(0,0,2),(2,0,0),(0,1,0)	(0,0,0)	4	24	no	ifs
(9) 3,1,2 (z+1,x,y)	C1 (0,-b,a)	(1/2,0,0),(0,0,1/2)	50 Pban	(0,0,2),(2,0,0),(0,1,0)	(1,0,0)	4	24	no	ifs
(15) 3,1,3 (z,x,y+1)	C1 (0,b,-a)	(1/2,0,0),(0,0,1/2)	50 Pban	(0,0,2),(2,0,0),(0,1,0)	(0,0,1)	4	24	no	ifs
(21) 3,1,4 (z+1,x,y+1)	C1 (0,-b,-a)	(1/2,0,0),(0,0,1/2)	50 Pban	(0,0,2),(2,0,0),(0,1,0)	(1,0,1)	4	24	no	ifs
(4) 4,1,1 (-y,-x,-z)	C1 (0,-a,-b)	(1/2,0,0),(0,0,1/2)	50 Pban	(-2,0,0),(0,0,-2),(0,-1,0)	(0,0,0)	4	24	no	ifs
(10) 4,1,2 (-y,-x,-z-1)	C1 (0,-a,b)	(1/2,0,0),(0,0,1/2)	50 Pban	(-2,0,0),(0,0,-2),(0,-1,0)	(0,0,-1)	4	24	no	ifs
(16) 4,1,3 (-y-1,-x,-z)	C1 (0,a,-b)	(1/2,0,0),(0,0,1/2)	50 Pban	(-2,0,0),(0,0,-2),(0,-1,0)	(-1,0,0)	4	24	no	ifs
(22) 4,1,4 (-y-1,-x,-z-1)	C1 (0,a,b)	(1/2,0,0),(0,0,1/2)	50 Pban	(-2,0,0),(0,0,-2),(0,-1,0)	(-1,0,-1)	4	24	no	ifs
(5) 5,1,1 (-x,-z,-y)	C1 (-b,0,-a)	(0,1/2,0),(0,0,1/2)	50 Pban	(0,0,-2),(0,-2,0),(-1,0,0)	(0,0,0)	4	24	no	ifs
(11) 5,1,2 (-x,-z-1,-y)	C1 (b,0,-a)	(0,1/2,0),(0,0,1/2)	50 Pban	(0,0,-2),(0,-2,0),(-1,0,0)	(0,-1,0)	4	24	no	ifs
(17) 5,1,3 (-x,-z,-y-1)	C1 (-b,0,a)	(0,1/2,0),(0,0,1/2)	50 Pban	(0,0,-2),(0,-2,0),(-1,0,0)	(0,0,-1)	4	24	no	ifs
(23) 5,1,4 (-x,-z-1,-y-1)	C1 (b,0,a)	(0,1/2,0),(0,0,1/2)	50 Pban	(0,0,-2),(0,-2,0),(-1,0,0)	(0,-1,-1)	4	24	no	ifs
(6) 6,1,1 (-z,-y,-x)	C1 (-a,-b,0)	(0,1/2,0),(1/2,0,0)	50 Pban	(0,-2,0),(-2,0,0),(0,0,-1)	(0,0,0)	4	24	no	ifs
(12) 6,1,2 (-z-1,-y,-x)	C1 (-a,b,0)	(0,1/2,0),(1/2,0,0)	50 Pban	(0,-2,0),(-2,0,0),(0,0,-1)	(-1,0,0)	4	24	no	ifs
(18) 6,1,3 (-z,-y-1,-x)	C1 (a,-b,0)	(0,1/2,0),(1/2,0,0)	50 Pban	(0,-2,0),(-2,0,0),(0,0,-1)	(0,-1,0)	4	24	no	ifs
(24) 6,1,4 (-z-1,-y-1,-x)	C1 (a,b,0)	(0,1/2,0),(1/2,0,0)	50 Pban	(0,-2,0),(-2,0,0),(0,0,-1)	(-1,-1,0)	4	24	no	ifs

Figure 2
Detailed descriptions of each of the equivalent domains of each of the ISG of the X3+(a,b,0) IR/OPD of space group $Pm\bar{3}m$ (No. 221) at $\mathbf{k} = (1/2, 0, 0)$. Observe differences in the OPD, active $\mathbf{k}$ vectors, basis and origin from one domain to the next.

OPD	k-active	Subgroup	Basis	Origin	Size	Index	cont	spec
P1 (a,0)	(1/2,1/2,1/2)	139 I4/mmm	(1,1,0),(-1,1,0),(0,0,2)	(0,0,0)	2	6	yes	ifs
SOP:[0,0,0]GM1+(a)	(0,0,0)	221 Pm-3m	(0,-1,0),(-1,0,0),(0,0,-1)	(0,0,0)	1	1		
SOP:[0,0,0]GM3+(a,0)	(0,0,0)	123 P4/mmm	(1,0,0),(0,1,0),(0,0,1)	(0,0,0)	1	3		pfs
SOP:[1/2,1/2,1/2]R1+(a)	(1/2,1/2,1/2)	225 Fm-3m	(0,-2,0),(-2,0,0),(0,0,-2)	(0,0,0)	2	2		
P2 (0,a)	(1/2,1/2,1/2)	140 I4/mcm	(1,1,0),(-1,1,0),(0,0,2)	(1/2,1/2,0)	2	6	yes	ifs
SOP:[0,0,0]GM1+(a)	(0,0,0)	221 Pm-3m	(0,-1,0),(-1,0,0),(0,0,-1)	(0,0,0)	1	1		
SOP:[0,0,0]GM3+(a,0)	(0,0,0)	123 P4/mmm	(1,0,0),(0,1,0),(0,0,1)	(0,0,0)	1	3		pfs
SOP:[1/2,1/2,1/2]R2+(a)	(1/2,1/2,1/2)	226 Fm-3c	(0,-2,0),(-2,0,0),(0,0,-2)	(0,0,0)	2	2		
C1 (a,b)	(1/2,1/2,1/2)	69 Fmmm	(2,0,0),(0,2,0),(0,0,2)	(0,0,0)	2	12	no	ifs
SOP:[0,0,0]GM1+(a)	(0,0,0)	221 Pm-3m	(0,-1,0),(-1,0,0),(0,0,-1)	(0,0,0)	1	1		
SOP:[0,0,0]GM2+(a)	(0,0,0)	200 Pm-3	(0,0,-1),(0,-1,0),(-1,0,0)	(0,0,0)	1	2		
SOP:[0,0,0]GM3+(a,b)	(0,0,0)	47 Pmmm	(-1,0,0),(0,0,1),(0,1,0)	(0,0,0)	1	6		pfs
SOP:[1/2,1/2,1/2]R1+(a)	(1/2,1/2,1/2)	225 Fm-3m	(0,-2,0),(-2,0,0),(0,0,-2)	(0,0,0)	2	2		
SOP:[1/2,1/2,1/2]R2+(a)	(1/2,1/2,1/2)	226 Fm-3c	(0,-2,0),(-2,0,0),(0,0,-2)	(0,0,0)	2	2		

Figure 3
Detailed descriptions of each of the secondary order parameters of each of the ISGs of the R3+ IR of space group $Pm\bar{3}m$ (No. 221) at $\mathbf{k} = (1/2, 1/2, 1/2)$. Each entry whose OPD label begins with 'SOP' indicates a secondary order parameter of the current ISG. The data set for a given ISG begins with an entry for its primary order parameter the OPD label of which does not begin with 'SOP'. Observe that the ISGs of the special $(a, 0)$ and $(0, a)$ OPDs both have three secondary order parameters, while the general (a, b) OPD has five secondary order parameters.

allows one to quickly generate and explore the distorted structures generated by the space-group IRs of a specific user-uploaded parent structure. Its applications are similar to those of the *AMPLIMODES* tool from the Bilbao Crystallographic Server (Orobengoa *et al.*, 2009).

We report here on the *ISOSUBGROUP* software, the newest online component of the *ISOTROPY Software Suite*, which fills an important gap in the capabilities of the other components of the suite. It combines much of the generality of the original *ISOTROPY* tool with the user-friendly interface of *ISODISTORT*. Whereas *ISODISTORT* uses only the IRs that produce common distortion types (*e.g.* lattice strains, atomic displacements, magnetic moments and occupational orderings) of a user-specified parent space-group symmetry and crystal structure, *ISOSUBGROUP* will generate the ISGs of any IR of any space group. Unlike *ISOTROPY* or *ISODISTORT*, *ISOSUBGROUP* cannot be used to project or decompose the symmetry modes of a distorted structure. Its key feature is that it provides a great deal of general information about each ISG that is not tied to a specific parent structure.

ISOSUBGROUP provides dropdown menus for selecting a parent space group, a $\mathbf{k}$ vector, and an IR of that space group and $\mathbf{k}$ vector. For each inequivalent OPD of the IR, a wealth of information about the resulting ISG is provided. Check boxes allow the user to determine which information will actually be displayed. The user has the option of simultaneously generating ISG output for all of the IRs defined at a single $\mathbf{k}$ vector. They can also specify multiple IRs (at one or more $\mathbf{k}$ vectors) to be superposed, and generate the resulting ISG output.

(1) The IR is indicated in the notation of Cracknell *et al.* (1979). The order parameter direction is

expressed as an *n*-dimensional vector $\boldsymbol{\eta}$ with one or more free parameters, following the notation used by the *ISOTROPY Software Suite* (Stokes & Hatch, 1988; Campbell *et al.*, 2006). The components of the OPD are actually partitioned into blocks of equal length, one for each of the arms of the star of the **k** vector, as described by Stokes *et al.* (2013). Only the **k** vectors of the star of **k**, *i.e.* those corresponding to the nonzero components of the OPD, are displayed. The OPDs of superposed IRs are strung together into a single joint OPD, but visually separated by semicolons.

(2) The basic properties of each ISG are presented, including (*a*) the basis vectors of the subgroup lattice in terms of the basis vectors of the parent lattice, (*b*) the origin of the subgroup with respect to the origin of the parent, given in parent coordinates, (*c*) the size of the subgroup's primitive unit cell relative to the parent's primitive unit cell, and (*d*) the index of the subgroup, which is the ratio of the number of parent operators to the number of subgroup operators.

(3) The properties of the IR matrices and OPD of the ISG determine whether or not a phase transition from the parent symmetry to the subgroup symmetry is allowed to be continuous *via* either Landau theory or renormalization-group theory. Those for which continuity is allowed by Landau theory have been further tested under the more stringent conditions of renormalization-group theory. *ISOSUBGROUP* reports 'no' for an ISG rejected by either theory, and 'yes' otherwise (Kim, Hatch & Stokes, 1986; Kim, Stokes & Hatch, 1986; Stokes *et al.*, 1987).

(4) The ferroic order-parameter types reported by *ISOSUBGROUP* include ferroelectric (fc), ferroelastic (fs) and ferromagnetic (fm). If the ISG allows the ferroic species as a primary order parameter, its label is prefaced by the letter 'p' for 'proper' (*e.g.* pfc for proper ferroelectric). If the ISG only allows the ferroic species as a secondary order parameter, its label is prefaced by the letter 'i' for 'improper"' (*e.g.* 'ifs' for improper ferroelelastic).

(5) The number of domains of an ISG is equal to its index, one for each coset of the subgroup with respect to the parent. Each coset is represented by a symmetry operator of the parent that is not retained in the subgroup. If requested by the user, *ISOSUBGROUP* displays a complete ISG entry for each domain of the ISG. The domains of an ISG are indexed with three integers, which indicate (1) the external orientation domain of the subgroup lattice relative to the parent lattice, (2) the internal orientation domain of the point group of the subgroup relative to the point group of the lattice of the subgroup, and (3) the translation domain of the subgroup origin relative to the parent origin.

(6) In addition to the primary IR and OPD used to generate the ISG, *ISOSUBGROUP* can calculate each of the secondary IRs and secondary order parameters (SOPs) that are compatible with the ISG (*i.e.* they can contribute order parameters to the ISG without further lowering the symmetry but may not generate the ISG alone). A full ISG entry is displayed for each secondary IR/OPD if requested by the user, and can be distinguished from the primary ISG entry by the letters 'SOP' at the front of the ISG label. The subgroup details presented in an SOP entry are for the ISG that would result if the SOP were considered by itself. Note that *ISOSUBGROUP* will not allow the user to display both domain and SOP information at the same time owing to the lengthy pages that would result.

As a result of new developments within the *ISOTROPY Software Suite* (Stokes *et al.*, 2007, 2011, 2013; Stokes & Campbell, 2016; van Smaalen *et al.*, 2013), *ISOSUBGROUP* is able to treat ISGs with superspace-group symmetry, which result from incommensurate order parameters. In such a case, the user must specify the number of incommensurate **k** vectors for each IR. When employing incommensurate **k** vectors, the parent is implicitly assumed to be a superspace extension of the specified space group, with extra dimensions for continuously infinite phase shifts of zero-amplitude modulations.

OPD	k-active	Subgroup	Basis	Origin	Size	Index	cont	spec
P1(1)P1(1) (a,0,0;b,0,0)	(0,0,0);(1/2,1/2,0)	65.486 Cmm'm'	(2,0,0),(0,2,0),(0,0,1)	(1/2,-1/2,0)	2	24	no	fs,fm
P1(1)P1(3) (a,0,0;0,0,b)	(0,0,0);(0,1/2,1/2)	127.393 P4/mb'm'	(0,1,1),(0,-1,1),(1,0,0)	(0,0,0)	2	12	no	fs,fm
P2(1)P1(1) (a,a,0;b,0,0)	(0,0,0);(1/2,1/2,0)	55.358 Pb'am'	(1,-1,0),(1,1,0),(0,0,1)	(0,0,0)	2	24	no	fs,fm
C1(1)P1(1) (a,b,0;c,0,0)	(0,0,0);(1/2,1/2,0)	10.46 P2'/m'	(-1,1,0),(0,0,1),(1,1,0)	(0,0,0)	2	48	no	fs,fm
C1(1)P1(2) (a,b,0;0,c,0)	(0,0,0);(1/2,0,1/2)	12.62 C2'/m'	(2,0,0),(0,0,2),(0,-1,0)	(1/2,0,1/2)	2	48	no	fs,fm
C2(1)P1(1) (a,a,b;c,0,0)	(0,0,0);(1/2,1/2,0)	14.79 P2_1'/c'	(0,0,1),(1,-1,0),(1,1,0)	(0,0,0)	2	48	no	fs,fm
S1(1)P1(1) (a,b,c;d,0,0)	(0,0,0);(1/2,1/2,0)	2.4 P-1	(0,0,1),(1,1,0),(-1,1,0)	(0,0,0)	2	96	no	fs,fm
P3(1)P3(1) (a,a,a;b,b,b)	(0,0,0);(1/2,1/2,0),(1/2,0,1/2),(0,1/2,1/2)	148.17 R-3	(-2,2,0),(2,0,-2),(-1,-1,-1)	(0,0,0)	4	64	no	fs,fm
P1(1)P2(2) (a,0,0;b,b,0)	(0,0,0);(1/2,1/2,0),(1/2,0,1/2)	139.537 I4/mm'm'	(0,2,0),(0,0,2),(2,0,0)	(1/2,-1/2,1/2)	4	24	no	fs,fm
P2(1)P2(3) (a,a,0;0,b,b)	(0,0,0);(1/2,0,1/2),(0,1/2,1/2)	69.524 Fm'm'm	(0,0,2),(-2,2,0),(-2,-2,0)	(-3/2,-1/2,1/2)	4	48	no	fs,fm
C2(1)P2(3) (a,a,b;0,c,c)	(0,0,0);(1/2,0,1/2),(0,1/2,1/2)	12.62 C2'/m'	(0,0,2),(2,-2,0),(1,1,-1)	(1/2,-1/2,1/2)	4	96	no	fs,fm
P1(1)S1(1) (a,0,0;b,c,d)	(0,0,0);(1/2,1/2,0),(1/2,0,1/2),(0,1/2,1/2)	71.536 Im'm'm	(0,2,0),(0,0,2),(2,0,0)	(1/2,-1/2,1/2)	4	48	no	fs,fm
C1(1)S1(1) (a,b,0;c,d,e)	(0,0,0);(1/2,1/2,0),(1/2,0,1/2),(0,1/2,1/2)	12.62 C2'/m'	(2,-2,0),(0,0,2),(0,-2,0)	(1/2,-1/2,1/2)	4	96	no	fs,fm
S1(1)S1(1) (a,b,c;d,e,f)	(0,0,0);(1/2,1/2,0),(1/2,0,1/2),(0,1/2,1/2)	2.4 P-1	(1,1,1),(1,1,-1),(-1,1,1)	(0,0,0)	4	192	no	fs,fm

Figure 4
Detailed descriptions of each of the ISGs resulting from the intersection of the magnetic mGM4+ IR at **k** = (0, 0, 0) with the nonmagnetic M3+ IR at **k** = (1/2, 1/2, 0), for space group $Pm\bar{3}m$ (No. 221). Note that the magnetic space group of each ISG is indicated.

IR	OPD	Subgroup	Basis	Origin	Size	Index	spec
DT1	P (a,0,0,0,0,0)	123.1.19.1 P4/mmm(0,0,g)0000	(1,0,0,0),(0,0,1,0),(0,-1,0,0),(0,0,0,1)	(0,0,0,0)	1	3	ifs
DT2	P (a,0,0,0,0,0)	123.1.19.4 P4/mmm(0,0,g)s00s	(1,0,0,0),(0,0,1,0),(0,-1,0,0),(0,0,0,1)	(0,0,0,0)	1	3	ifs
DT3	P (a,0,0,0,0,0)	123.1.19.2 P4/mmm(0,0,g)s0s0	(1,0,0,0),(0,0,1,0),(0,-1,0,0),(0,0,0,1)	(0,0,0,3/4)	1	3	ifs
DT4	P (a,0,0,0,0,0)	123.1.19.3 P4/mmm(0,0,g)00ss	(1,0,0,0),(0,0,1,0),(0,-1,0,0),(0,0,0,1)	(0,0,0,3/4)	1	3	ifs
DT5	P (a,a,a,a,0,0,0,0,0,0)	89.1.19.2 P422(0,0,g)q00	(1,0,0,0),(0,0,1,0),(0,-1,0,0),(0,0,0,1)	(0,0,0,1/4)	1	6	ifs
DT5	P (a,0,a,0,0,0,0,0,0,0)	47.1.9.2 Pmmm(0,0,g)s00	(0,0,-1,0),(-1,0,0,0),(0,1,0,0),(0,0,0,1)	(0,0,0,3/4)	1	6	ifs
DT5	P (a,a,-a,a,0,0,0,0,0,0)	65.1.13.2 Cmmm(0,0,g)s00	(-1,0,1,0),(-1,0,-1,0),(0,-1,0,0),(0,0,0,1)	(0,0,0,0)	1	6	ifs
DT5	C (a,b,a,b,0,0,0,0,0,0)	16.1.9.2 P222(0,0,g)00s	(-1,0,0,0),(0,0,1,0),(0,1,0,0),(0,0,0,1)	(0,0,0,1/4)	1	12	ifs
DT5	C (a,a,b,-b,0,0,0,0,0,0)	21.1.13.2 C222(0,0,g)00s	(-1,0,1,0),(-1,0,-1,0),(0,-1,0,0),(0,0,0,1)	(0,0,0,1/4)	1	12	ifs
DT5	C (a,b,-a,b,0,0,0,0,0,0)	10.1.5.5 P2/m(0,0,g)s0	(0,0,1,0),(1,0,0,0),(0,1,0,0),(0,0,0,1)	(0,0,0,0)	1	12	ifs
DT5	4D (a,b,c,d,0,0,0,0,0,0)	3.1.5.4 P2(0,0,g)s	(0,0,1,0),(1,0,0,0),(0,1,0,0),(0,0,0,1)	(0,0,0,0)	1	24	ifs,ifc

Figure 5
Detailed descriptions of each of the ISGs of each of the IRs of space group $Pm\bar{3}m$ (No. 221) at incommensurate modulation vector $\mathbf{k} = (0, \beta, 0)$. The symmetry group of each ISG in this case is a $(3 + 1)$-dimensional superspace group.

Some ISG information is not presented for incommensurate cases: active $\mathbf{k}$ vectors, which are inferable from the super-space-group symbol, secondary order parameters associated with higher harmonics of the fundamental modulation vectors, the domains of the basic space group of the ISG (may be added later) and phase-transition continuity indicators (may be added later).

ISOSUBGROUP further allows the user to include magnetic IRs, which result in ISGs with magnetic space-group symmetry (or even magnetic superspace-group symmetry in incommensurate cases). When magnetic IRs are selected, the parent symmetry is implicitly assumed to be the paramagnetic (gray) symmetry group obtained by adding a pure time reversal to the specified space group.

The screen shots in Figs. 1–5 demonstrate *ISOSUBGROUP* output for several specific examples involving parent space group $Pm\bar{3}m$. These examples were selected to illustrate a variety of different scenarios, including output from all IRs and OPDs at a single $\mathbf{k}$ vector, multi-domain output for a specific IR/OPD, secondary order parameter output for a specific IR/OPD, a magnetic ISG, an incommensurate ISG, and ISGs resulting from the superposition of IRs at multiple $\mathbf{k}$ vectors. The details of each example are provided in the corresponding figure caption.

ISOSUBGROUP provides online menu-driven access to isotropy subgroups of the irreducible representations of any crystallographic space group at arbitrary superpositions of commensurate and incommensurate $\mathbf{k}$ vectors, including magnetic cases, without reference to any parent structure or order-parameter type. The output for each isotropy subgroup includes information about the symmetry group, basis and origin relative to the parent, active $\mathbf{k}$ vectors, ferroic species, phase-transition continuity, subgroup domains, and secondary order parameters. It builds on and complements other programs of the *ISOTROPY Software Suite* by combining the generality of the *ISOTROPY* tool with the user-friendly interface of *ISODISTORT*, while focusing on isotropy subgroups rather than projected order parameters.

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