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PC SOFTWARE FOR CRYSTALLOGRAPHIC SPACE GROUPS AND ITS APPLICATION IN SYMMETRY ANALYSIS OF DOMAIN STRUCTURES

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Abstract: An integrated package of programs has been developed to investigate the structures and representations of crystallographic space groups. The programs, written in PASCAL and C, are made user friendly by additional programs using the Oakland C-scape Interface Management System. A Microsoft Windows version of the software is currently being developed using Borland Delphi. For a given phase transition the software identifies all domain states and finds inter alia (i) symmetry groups of all domain states in algebraic form as a conjugate subgroup stratum, (ii) all operations that transform a given domain state into another domain state, (iii) classes of crystallographically equivalent domain pairs, (iv) symmetry groups of ordered and unordered domain pairs. As an illustrative example software results for the triply commensurate charge-density-wave domain states in the $2H$ polytype $TaSe_2$ are presented.

1 Group-theoretical analysis

Here we consider structural phase transitions which are accompanied by a symmetry reduction. Thus, the space group $\mathfrak{H}$ of the *distorted* phase is a proper subgroup of the space group $\mathfrak{G}$ of the *parent* phase which implies $\mathfrak{H} \subset \mathfrak{G}$. Due to the symmetry reduction at the phase transition the distorted phase can appear in several homogeneous simultaneously coexisting states which have the same structure but different orientations and/or locations in space when referring to a particular coordinate system. Due to lack of space we demonstrate only some applications of the software in the symmetry analysis of domain structures, others will be described elsewhere. The theoretical background of the symmetry analysis can be found in many papers from which we mention only some, namely Refs. [1], [2], [3], [4], [5], [6].

Group-theoretical properties of single domain states: These homogeneous structures are usually called *structural variants* or *single domain states* (SDS's) and are denoted by the symbols $\mathbb{S}_1, \mathbb{S}_2, \cdots, \mathbb{S}_n$ respectively. By definition, SDS's are called *crystallographically equivalent* if the set of all SDS's forms a single $\mathfrak{G}$-orbit which implies that for each pair $\mathbb{S}_j$ and $\mathbb{S}_k$ there exists a suitable space group element $g \in \mathfrak{G}$ such that $\mathbb{S}_k = g \circ \mathbb{S}_j$ is valid. Thus, it is immaterial from which SDS one starts to generate the complete set of SDS's. Here, the $\mathfrak{G}$-orbit is generated from $\mathbb{S}_1$ and denoted by $\mathfrak{G} \circ \mathbb{S}_1$ and the symmetry group $\mathfrak{H}$ of the fixed SDS $\mathbb{S}_1$ is a subgroup of $\mathfrak{G}$.

$$\mathfrak{G} \circ \mathbb{S}_1 = \{\mathbb{S}_1, \mathbb{S}_2, \cdots, \mathbb{S}_n\} \tag{1}$$

$$\mathbb{S}_j = g_j \circ \mathbb{S}_1 \tag{2}$$

$$\mathfrak{H}_j = \{g \in \mathfrak{G} \mid g \circ \mathbb{S}_j = \mathbb{S}_j\} = g_j * \mathfrak{H} * g_j^{-1} \tag{3}$$

$$\mathfrak{G} = \sum_{g_j \in \mathbf{G:H}} g_j * \mathfrak{H} \tag{4}$$

Since each pair of SDS's, say $\mathbb{S}_1$ and $\mathbb{S}_j$, is related by an operation $g_j \in \mathfrak{G}$ such that $\mathbb{S}_j = g_j \circ \mathbb{S}_1$, their symmetry groups $\mathfrak{H}$ and $\mathfrak{H}_j$ are conjugate subgroups of the parent space group $\mathfrak{G}$ (see (3)). Moreover, all SDS's, say $\mathbb{S}_1, \mathbb{S}_2, \cdots, \mathbb{S}_k$, that have the *same* symmetry group $\mathfrak{H}$ can be labelled by representatives of the decomposition of the normalizer $\mathbf{N}_G(H)$ into $\mathfrak{H}$-left cosets where $k = \mid \mathbf{N}_G(H):\mathfrak{H} \mid$ is valid. The number n

of SDS's equals the number of left cosets in the decomposition of $\mathfrak{G}$ with respect to $\mathfrak{H}$ is called the index of $\mathfrak{H}$ in $\mathfrak{G}$ and given by $n = |\mathfrak{G}:\mathfrak{H}|$. Actually, space group elements of the parent space group $\mathfrak{G}$, briefly written as g, are labelled by a double index (s, a). If necessary we identify $g = g_{sa} = (R_s|\mathbf{w}_s + \mathbf{t}_a)$ where $\mathbf{w}_s$ denotes the *fractional* translation that is uniquely assigned to the point group operation $R_s \in \mathfrak{P}$ and where $\mathbf{t}_a \in \mathfrak{T}$ denotes the translational part of the space group element $g = g_{sa}$ respectively. The group $\mathfrak{P}$ is called the *point* group and $\mathfrak{T}$ the *translation* group of the parent space group $\mathfrak{G}$. In practice, the SDS's $\mathbb{S}_j$ are regarded as special vectors of an *order parameter space* and the action of the space group elements onto the SDS's, formally written as $g \circ \mathbb{S}_j = \mathbb{S}_k$, can be seen as linear operators, like matrices, acting on the vectors of this space [4], [7].

Group-theoretical subdivision of the set of single domain states: In a general case, the group $\mathfrak{H}$ forms a *general* subgroup of the parent space group $\mathfrak{G}$. This means that not only $\mathfrak{S} \subset \mathfrak{T}$ but also $\mathfrak{R} \subset \mathfrak{P}$ is satisfied where $\mathfrak{S}$ denotes the translation group and $\mathfrak{R}$ the point group of the space group $\mathfrak{H}$. Thus, there must exist an *intermediate* group $\mathfrak{M}$ with $\mathfrak{T}$ as its translation group and $\mathfrak{R}$ as its point group which is a *translationsgleiche* subgroup of $\mathfrak{G}$ and simultaneously a *klassengleiche* supergroup of $\mathfrak{H}$. By virtue of $\mathfrak{H} \subset \mathfrak{M} \subset \mathfrak{G}$, the coset decomposition of $\mathfrak{G}$ into left cosets of $\mathfrak{H}$ can be carried out in two steps, namely first to decompose $\mathfrak{G}$ into $\mathfrak{M}$-left cosets, and then to decompose $\mathfrak{M}$ into $\mathfrak{H}$-left cosets. For if $|\mathfrak{G}:\mathfrak{H}| = n$, then it follows from $|\mathfrak{G}:\mathfrak{M}| = |\mathfrak{P}:\mathfrak{R}| = m$ together with $|\mathfrak{M}:\mathfrak{H}| = |\mathfrak{T}:\mathfrak{S}| = d$ that $n = md$ must hold. Let $\mathbf{E}(S)$ be the primitive unit cell of $\mathfrak{S}$, then we take the translations $\mathbf{t}_a \in \mathbf{E}(S) \cap \mathfrak{T}$ as coset representatives for the $\mathfrak{S}$-left cosets in $\mathfrak{T}$. Together with the coset decomposition of $\mathfrak{P}$ with respect to $\mathfrak{R}$ where we take R_s with $s = 1, 2, \cdots, m$ and $R_1 = E$ (identity) as coset representatives, one immediately arrives at the following specified formula for the decomposition of $\mathfrak{G}$ into $\mathfrak{H}$-left cosets.

$$\mathfrak{G} = \sum_{R_s \in \mathbf{P}:\mathbf{R}} \sum_{\mathbf{t}_a \in \mathbf{E}(S) \cap \mathbf{T}} \big((R_s|\mathbf{w}_s)(E|\mathbf{t}_a)\big) * \mathfrak{H} \tag{5}$$

Thus, the set of all $\mathfrak{H}$-left cosets which consists of $n = md$ cosets can be partitioned into m subsets where each subset contains d $\mathfrak{H}$-left cosets. From this we infer that the n SDS's of the $\mathfrak{G}$-orbit $\mathfrak{G} \circ \mathbb{S}_1$ can be subdivided into m subsets where each consists of d SDS's respectively. Hence it follows that the SDS's of the subset $\mathfrak{M} \circ \mathbb{S}_1 = \{(E|\mathbf{t}_a) \circ \mathbb{S}_1 \mid \mathbf{t}_a \in \mathfrak{T}:\mathfrak{S}\}$ can be related by pure translations which are lost at the transition from the parent space group $\mathfrak{G}$ to the subgroup $\mathfrak{H}$. Hence each other subset of equivalent type, namely $\big((R_s|\mathbf{w}_s) * \mathfrak{M}\big) \circ \mathbb{S}_1 = \{(R_s|\mathbf{w}_s)(E|\mathbf{t}_a) \circ \mathbb{S}_1 \mid \mathbf{t}_a \in \mathfrak{T}:\mathfrak{S}\}$ with fixed $R_s \in \mathfrak{P}:\mathfrak{R}$ consists of d SDS's. Each such subset of SDS's comprises all SDS's with the same macroscopic *tensorial* properties. Obviously, the intermediate group $\mathfrak{M}$ can be regarded as the stabilizer of $\mathfrak{M} \circ \mathbb{S}_1$ and the remaining subsets of equivalent type, namely $\big((R_s|\mathbf{w}_s) * \mathfrak{M}\big) \circ \mathbb{S}_1$, are obtained by space group operations which label the $\mathfrak{M}$-left cosets in the parent space group $\mathfrak{G}$. The subsets $\big((R_s|\mathbf{w}_s) * \mathfrak{M}\big) \circ \mathbb{S}_1$ are called *ferroic* (*orientational*, *tensorial*) SDS's and the order d of these subsets is called *translational degeneracy* of the ferroic domain states. Finally, we point out that other subdivisions of the set of all SDS's $\mathfrak{G} \circ \mathbb{S}_1$ have been discussed in detail elsewhere [8], [9].

Double cosets and $\mathfrak{G}$-orbits of domain pairs: It is commonly accepted that structures of SDS's can coexist in a domain structure where the latter consists of domains (connected regions with homogeneous bulk structures of SDS's) and of domain walls (boundaries between neighbouring domains). In order to study systematically possible relations between structures of two domains the concept of *domain pairs* has been introduced [1]. Domain pairs are essential in discussing domain distinction and domain walls (for more details see, e.g. [5], [6], [10]). For this purpose one defines the product set

$$(\mathfrak{G} \circ \mathbb{S}_1) \times (\mathfrak{G} \circ \mathbb{S}_1) = \{(\mathbb{S}_j, \mathbb{S}_k) \mid \mathbb{S}_j, \mathbb{S}_k \in \mathfrak{G} \circ \mathbb{S}_1\} \tag{6}$$

which by definition consists of n^2 ordered pairs. Its elements $(\mathbb{S}_j, \mathbb{S}_k)$ are called *ordered domain pairs* (ODP's). There are n ODP's with $\mathbb{S}_k = \mathbb{S}_j$ which are trivial and are irrelevant for the further discussion. Thus, there are $n(n-1)$ non-trivial ODP's. An ODP with a reversed order of SDS's is called a *transposed* ordered domain pair. Two ODP's $(\mathbb{S}_i, \mathbb{S}_j)$ and $(\mathbb{S}_k, \mathbb{S}_\ell)$ are called *crystallographically equivalent* with

respect to $\mathfrak{G}$ if a space group element $g \in \mathfrak{G}$ exists such that $(\mathbb{S}_k, \mathbb{S}_l) = (g \circ \mathbb{S}_i, g \circ \mathbb{S}_j)$ is satisfied. ODP's can be classified in the following manner. An ODP $(\mathbb{S}_i, \mathbb{S}_j)$ is called *transposable* (*ambivalent*) if it is crystallographically equivalent with its transposed ODP $(\mathbb{S}_j, \mathbb{S}_i)$. In other words, there exists an element $g \in \mathfrak{G}$ such that $(\mathbb{S}_j, \mathbb{S}_i) = (g \circ \mathbb{S}_i, g \circ \mathbb{S}_j)$ is valid. If this condition cannot be fulfilled, then the ODP is called *non-transposable* (*polar*). Then the ODP and the transposed ODP are called *complementary* ODP's. The basic result is that the previously defined crystallographical equivalence subdivides the set of all ODP's $(\mathfrak{G} \circ \mathbb{S}_1) \times (\mathfrak{G} \circ \mathbb{S}_1)$ into $\mathfrak{G}^{[2]}$-orbits $\mathfrak{G}^{[2]} \circ (\mathbb{S}_i, \mathbb{S}_j)$ where the superscript [2] occurring in $\mathfrak{G}^{[2]} \circ (\mathbb{S}_i, \mathbb{S}_j)$ should indicate that $\mathfrak{G} \sim \mathfrak{G} \boxtimes \mathfrak{G}$ actually acts as Kronecker-product group on the ODP's. From the previous discussion it is obvious that as *representative* ODP's of the orbits $\mathfrak{G}^{[2]} \circ (\mathbb{S}_i, \mathbb{S}_j)$ can be always chosen in such a way that the first SDS is $\mathbb{S}_1$, i.e. a representative ODP has the form $(\mathbb{S}_1, \mathbb{S}_k)$.

The attributes *transposable* (*ambivalent*), *non-transposable* (*polar*) and *complementary* are class properties, i.e. ODP's in an $\mathfrak{G}^{[2]}$-orbit are either all transposable or all non-transposable and all transposed ODP's of a non-transposable orbit constitute another disjoint complementary non-transposable orbit. The group-theoretical analogue of $\mathfrak{G}^{[2]}$-orbits $\mathfrak{G}^{[2]} \circ (\mathbb{S}_i, \mathbb{S}_j)$ are double cosets of the form $\mathfrak{H} * g_k * \mathfrak{H}$ since each representative ODP $(\mathbb{S}_1, \mathbb{S}_k)$ can be written in the form $(\mathbb{S}_1, g_k \circ \mathbb{S}_1)$. Recall, every space group $\mathfrak{G}$ can always be decomposed into mutually disjoint double cosets of its subgroup $\mathfrak{H}$.

$$\mathfrak{G} = \sum_{g_k \in \Delta G:H} \mathfrak{H} * g_k * \mathfrak{H} \qquad k = 1, 2, \cdots, q \tag{7}$$

An inverse $(\mathfrak{H} * g_k * \mathfrak{H})^{-1} = \mathfrak{H} * g_k^{-1} * \mathfrak{H}$ of the double coset $\mathfrak{H} * g_k * \mathfrak{H}$ is either identical with $\mathfrak{H} * g_k * \mathfrak{H}$ or forms another double coset disjoint with $\mathfrak{H} * g_k * \mathfrak{H}$. We shall call the former type of double cosets *self-inverse* (ambivalent) double cosets and disjoint double cosets *complementary* double cosets. This establishes the one-to-one correspondence between the double cosets $\mathfrak{H} * g_k * \mathfrak{H}$ of the decomposition (7) and the corresponding $\mathfrak{G}^{[2]}$-orbits of ODP's [1]. This enables one to find from the double coset decomposition (7) the number q of ODP orbits, their type (transposable or complementary non-transposable), and the representative ODP's for all $\mathfrak{G}^{[2]}$-orbits of ODP's.

The ODP's from different $\mathfrak{G}^{[2]}$-orbits differ in at least some inherent properties, whereas ODP's from the same orbit have *essentially equal* properties, i.e. after performing an operation $g \in \mathfrak{G}$ their structures can be brought into coincidence. The double coset decomposition thus reduces the task of examining $n(n-1)$ ODP's to a considerably lower (especially for large n) number q of double coset representatives. Properties significant for the whole orbit of ODP's (e.g. tensor distinction of domains [9]) can be found by examining the representative ODP's of the orbits. Some conclusions can be drawn already from the type of the double coset, e.g. a necessary condition for the appearance of an incommensurate phase connected with Lifshitz invariants is the existence of a complementary double cosets in the decomposition (7).

Intersection of conjugate subgroups and symmetries of domain pairs: Obviously, the symmetry group of an ordered domain pair, say $(\mathbb{S}_1, \mathbb{S}_j)$ must coincide with the intersection group $\mathfrak{H}_{1j}$ of the symmetry groups $\mathfrak{H}$ and $\mathfrak{H}_j$ of the corresponding SDS's $\mathbb{S}_1$ and $\mathbb{S}_j$ respectively. Likewise, we introduce the concept of *unordered* domain pairs (UDP's) which, in a loose way of speaking, can be seen as *symmetrized* product states within the framework of the order parameter space if the latter is consistently extended to a product space. Actually, we assume that if there exists an operation $g^{\#} \in \mathfrak{G}$ such that $(\mathbb{S}_j, \mathbb{S}_1) = (g^{\#} \circ \mathbb{S}_1, g^{\#} \circ \mathbb{S}_j)$ is valid, then we consider the subset $\{(\mathbb{S}_1, \mathbb{S}_j), (\mathbb{S}_j, \mathbb{S}_1)\}$ as an UDP. Its symmetry group $\mathfrak{J}_{1j}$ contains $\mathfrak{H}_{1j}$ as subgroup of index two.

$$\mathfrak{H}_{1j} = \mathfrak{H} \cap \mathfrak{H}_j \tag{8}$$

$$\mathfrak{J}_{1j} = \mathfrak{H}_{1j} \cup g^{\#} * \mathfrak{H}_{1j} \tag{9}$$

The obvious consequence is that the symmetry groups of ODP's $(g \circ \mathbb{S}_1, g \circ \mathbb{S}_j)$ which by definition belong to the *same* $\mathfrak{G}^{[2]}$-orbit are conjugate subgroups of the parent space group $\mathfrak{G}$. For if $\mathfrak{H}_{1j}$ is the stabilizer of the ODP $(\mathbb{S}_1, \mathbb{S}_j)$, then $g * \mathfrak{H}_{1j} * g^{-1}$ is the symmetry group of $(g \circ \mathbb{S}_1, g \circ \mathbb{S}_j)$ respectively. Clearly, each ODP $(\mathbb{S}_1, \mathbb{S}_k)$ that is *non-transposable* does not allow one to define an UDP and hence its symmetry group remains $\mathfrak{H}_{1k}$ respectively.

2 Software support in the symmetry analysis of domain states

To illustrate the procedure of finding double and left coset resolutions and their significance in domain structure analysis let us consider the triply commensurate charge-density-wave domain states in 2*H* polytype *TaSe*$_2$ [11], [12], [13]. The *parent* phase has $\mathfrak{G} = P6_3/mmc$ (#194) symmetry and the *distorted* commensurate phase exhibits $\mathfrak{H} = Cmcm$ (#63) symmetry with tripled primitive translations along two hexagonal primitive lattice translations which implies $(\mathbf{s}_1, \mathbf{s}_2, \mathbf{s}_3) = (3\mathbf{t}_1, 3\mathbf{t}_2, \mathbf{t}_3)$ where $\mathbf{s}_1, \mathbf{s}_2, \mathbf{s}_3$ denotes the primitive translations of the sublattice $\mathfrak{S}$. The group $\mathfrak{H}$ is therefore a *general* subgroup with reduced point group symmetry $\mathfrak{R} \subset \mathfrak{P}$ and reduced translation symmetry $\mathfrak{S} \subset \mathfrak{T}$. Accordingly, there are $m = |6/mmm{:}mmm| = 24 : 8 = 3$ ferroic (orientational) SDS's and within each of them $d = 9$ SDS's related by lost translations may exist. Thus in all there are $n = 3 \cdot 9 = 27$ SDS's which can be labelled by the index pair (s, a) of the space group operations $g = g_{sa}$ where $s = 1, 2, 3$ and $a = 1, 2, \cdots, 9$ are their range of variations.

Using Ref. [14], we find that $\mathfrak{M} = Cmcm$ (#63) with *primitive* lattice translations $\mathbf{t}_1, \mathbf{t}_2, \mathbf{t}_3$ identical with that of the group $\mathfrak{G}$. The left coset decomposition of $\mathfrak{G}$ with respect to $\mathfrak{M}$ is determined by the software which finds the representatives (1|0), (3|0), and $(3^2|0)$ for which we choose the number of ferroic domain states $s = 1, 2, 3$ respectively. Nine representative translations $\{\mathbf{t}_a \mid a = 1, 2, \cdots, 9\}$ of the decomposition of $\mathfrak{M}$ into $\mathfrak{H}$-left cosets can be seen from Fig.1 which displays examples of several SDS's where the latter are graphically represented by their corresponding *conventional* unit cells.

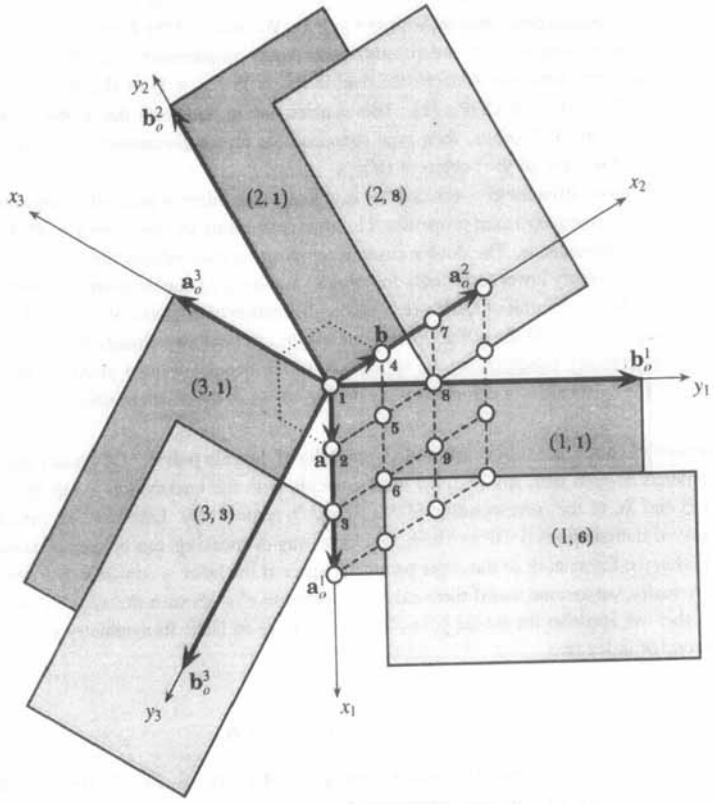

Fig 1: Domain states labelled by (s, a)

Here, as already pointed out, we only sketch some features of the software where the space group $\mathfrak{G} = P6_3/mmc$ in standard setting [14], [15] is taken as the supergroup and $\mathfrak{H} = Cmcm$ as fixed subgroup of

the former. To be more specific, we have $\mathfrak{P} = 6/mmm = \{1, 2, \cdots, 24\}$ as the point group of $\mathfrak{G}$ and take $\mathfrak{R} = mmm = \{1, 4, 7, 10, 13, 16, 19, 22\}$ as the point group of $\mathfrak{H}$ where our notation concerning the point group operations has to be understood as follows.

Table 1: *Labels for symmetry operations of* 6/*mmm*

HM	CDML	HM	CDML	HM	CDML	HM	CDML	HM	CDML	HM	CDML
1	1	$\bar{1}$	13	6	2	$\bar{6}$	14	$2_{1\bar{1}}$	9	$m_{1\bar{1}}$	21
3	3	$\bar{3}$	15	6^5	6	$\bar{6}^5$	18	2_{12}	10	m_{01}	22
3^2	5	$\bar{3}^5$	17	2_{10}	7	$m_{2\bar{1}}$	19	$2_{2\bar{1}}$	8	$m_{\bar{1}0}$	20
2_z	4	m_z	16	2_{01}	11	$m_{\bar{1}2}$	23	$2_{1\bar{1}}$	12	m_{11}	24

Our notation is derived from the International (Hermann-Mauguin (**HM**)) symbols for point group symmetry operations. Positive directions of the primary, secondary and tertiary symmetry axes are chosen according to the Table 2.4.1. of International Tables for Crystallography, Vol. A [14]. The **CDML**-notation (number) refers to Ref. [15].

(i) The symmetry groups or stabilizers $\mathfrak{H}_j$, $j = 1, 2, \cdots, 27$ of all domain states $\mathbb{S}_j = g_j \circ \mathbb{S}_1$ (where g_j is a left coset representative of $\mathfrak{H}$ in $\mathfrak{G}$) are given by $\mathfrak{H}_j = g_j * \mathfrak{H} * g_j^{-1}$ and form a conjugate subgroup stratum. The software outputs the stratum in algebraic (or parametric) form in three sections below corresponding to the three distinct orientations of the *orthorhombic C* sublattice which are in 1-1 correspondence with the left cosets (represented by R_j) of the point group $\mathfrak{R}$ of $\mathfrak{H}$ in the point group $\mathfrak{P}$ of the parent phase group $\mathfrak{G}$. The conventional unit cell vectors $\mathbf{a}', \mathbf{b}', \mathbf{c}'$ of each sublattice are expressed as linear combinations of the conventional unit cell vectors $\mathbf{a}, \mathbf{b}, \mathbf{c}$ of the hexagonal lattice of the parent phase.

The conjugating element $g_j = (R_j | \mathbf{w}_j)(E | \mathbf{t})$ where $\mathbf{w}_j$ denotes the fractional translation assigned to R_j in $\mathfrak{G}$, and $\mathbf{t} = s\mathbf{t}_1 + t\mathbf{t}_2$ with $s, t = 0, 1, 2$, and $\mathbf{t}_1 = \mathbf{a}$, $\mathbf{t}_2 = \mathbf{b}$, $\mathbf{t}_3 = \mathbf{c}$. Only the generating elements of $\mathfrak{H}_j$ are given to save space where the point group symbols are given in the notation of Ref. [15]. For each generating element $R_k \in \mathfrak{R}$, the generating element $(R_k | \mathbf{w}_k + \mathbf{T}_k)$ of $\mathfrak{H}_j$ is given where $\mathbf{w}_k$ denotes the fractional translation assigned to R_k in $\mathfrak{G}$, and $\mathbf{T}_k$ denotes the primitive vector of $\mathfrak{T}$ (but fractional in $\mathfrak{G}$) assigned to R_k in $\mathfrak{H}_j$. The coordinates of $\mathbf{T}_k$ are expressed with respect to the primitive vectors $\mathbf{t}_1, \mathbf{t}_2, \mathbf{t}_3$ of $\mathfrak{G}$ above.

Table 2: *Symmetry groups of single domain states*

LCR	symmetry group	conv. lat. trans.	generating elements
$R_1 = 1$	$\mathfrak{H}_{(1,a)} = Cmcm$ (#63)	$\mathbf{a}' = \mathbf{a}_o^1 = +3\mathbf{a}$	$(4\|(0, 0, 1/2) + (2s, 2t, 0))$
		$\mathbf{b}' = \mathbf{b}_o^1 = +3\mathbf{a} + 6\mathbf{b}$	$(7\|(0, 0, 0) + (t, 2t, 0))$
		$\mathbf{c}' = \mathbf{c}_o^1 = +\mathbf{c}$	$(13\|(0, 0, 0) + (2s, 2t, 0))$
$R_2 = 3$	$\mathfrak{H}_{(2,a)} = Cmcm$ (#63)	$\mathbf{a}' = \mathbf{a}_o^2 = +3\mathbf{b}$	$(4\|(0, 0, 1/2) + (2s, 2t, 0))$
		$\mathbf{b}' = \mathbf{b}_o^2 = -6\mathbf{a} - 3\mathbf{b}$	$(11\|(0, 0, 0) + (2s, s, 0))$
		$\mathbf{c}' = \mathbf{c}_o^2 = +\mathbf{c}$	$(13\|(0, 0, 0) + (2s, 2t, 0))$
$R_3 = 5$	$\mathfrak{H}_{(3,a)} = Cmcm$ (#63)	$\mathbf{a}' = \mathbf{a}_o^3 = -3\mathbf{a} - 3\mathbf{b}$	$(4\|(0, 0, 1/2) + (2s, 2t, 0))$
		$\mathbf{b}' = \mathbf{b}_o^3 = +3\mathbf{a} - 3\mathbf{b}$	$(9\|(0, 0, 0) + (s - t, -s + t, 0))$
		$\mathbf{c}' = \mathbf{c}_o^3 = +\mathbf{c}$	$(13\|(0, 0, 0) + (2s, 2t, 0))$

Note for each left coset representative $R_j \in \mathfrak{P}:\mathfrak{R}$ there exist exactly 9 distinct conjugate subgroups which is due to $s, t = 0, 1, 2$ where the intersection groups $\mathfrak{H}_{1j}$ are denoted by $\mathfrak{H}_{(s,a)}$ respectively. We see that all $\mathfrak{H}_j$, $j = 1, 2, \cdots, 27$ are distinct conjugate subgroups which implies that the normalizer $\mathbf{N}_G(H)$ of $\mathfrak{H}$ in $\mathfrak{G}$ is identical to $\mathfrak{H}$; no two distinct domain states possess the same symmetry group.

(ii) It is clear that the elements in the complex $\mathfrak{C}_{kj} = g_k * \mathfrak{H} * g_j^{-1}$ and only these elements transform the left coset $g_j * \mathfrak{H}$ into the left coset $g_k * \mathfrak{H}$ and therefore transform the domain state $\mathbb{S}_j$ into the domain state $\mathbb{S}_k$. Furthermore, with $g_{kj} = g_k g_j^{-1}$ then $\mathfrak{C}_{kj} = g_{kj} * \mathfrak{H}_j$ so that $\mathfrak{C}_{kj}$ is a left coset of $\mathfrak{H}_j$ in $\mathfrak{G}$. Therefore, once all the stabilizers $\mathfrak{H}_j$ are known from (i), all operations that transform a given domain state into another domain state are known.

(iii) The classes of crystallographically equivalent domain pairs with similar domain distinction are in 1-1 correspondence with the double cosets in the double coset decomposition of $\mathfrak{G}$ with respect to $\mathfrak{H}$. The

software gives this decomposition by listing the left coset representatives of the left cosets which comprise each double coset, and the first in the list is chosen to represent the double coset itself. In addition for each double coset the inverse double coset is identified.

Table 3: *Decompositions of the $\mathfrak{H}$-double cosets into $\mathfrak{H}$-left cosets.*

DC	LCR's	inverse DC	type
1	(1|**0**)(1|000)	1	*self-inverse*
2	(1|**0**)(1|100), (1|**0**)(1|200)	2	*self-inverse*
3	(1|**0**)(1|010), (1|**0**)(1|110), (1|**0**)(1|020), (1|**0**)(1|220)	3	*self-inverse*
4	(1|**0**)(1|210), (1|**0**)(1|120)	4	*self-inverse*
5	(3|**0**)(1|000), (3^2|**0**)(1|000)	5	*self-inverse*
6	(3|**0**)(1|010), (3|**0**)(1|020), (3^2|**0**)(1|110), (3^2|**0**)(1|220)	6	*self-inverse*
7	(3|**0**)(1|210), (3|**0**)(1|120), (3^2|**0**)(1|210), (3^2|**0**)(1|120)	7	*self-inverse*
8	(3|**0**)(1|100), (3|**0**)(1|200), (3^2|**0**)(1|100), (3^2|**0**)(1|200)	9	*complementary*
9	(3|**0**)(1|110), (3|**0**)(1|220), (3^2|**0**)(1|010), (3^2|**0**)(1|020)	8	*polar*

The results are summarized in the Table 3, where each row contains representative operations of all $\mathfrak{H}$-left cosets that form one $\mathfrak{H}$-double coset. The representatives are expressed as products of two operations: The first one is the representative of the $\mathfrak{M}$-left coset in the decomposition of $\mathfrak{G}$ and the second operation is the representative of the $\mathfrak{H}$-left coset in the decomposition of $\mathfrak{M}$. The third column gives the No of the inverse double coset and the last column specifies the type of the double coset (self-inverse (ambivalent) or complementary polar) which specifies also the type of the corresponding domain pairs. We see that all double cosets, except last two, are ambivalent (self-inverse); double cosets 8 and 9 are complementary polar double cosets. Thus $27 \cdot 26 = 702$ non-trivial ODP's is partitioned into 8 orbits and the representatives of these orbits are samples of all significantly different relations between two SDS's. The Table does not contain, except from the trivial one, any ambivalent double coset that would consist just of one left coset. From this it follows that the normalizer of $\mathfrak{H}$ in $\mathfrak{G}$ equals $\mathfrak{H}$. This means that no two single domain states have the same symmmetry group as already remarked in (i) above.

(iv) The symmetry group $\mathfrak{H}_{1j}$ of representative (ODP) $(\mathbb{S}_1, \mathbb{S}_j)$ is the intersection of the stabilizers $\mathfrak{H}$ and $\mathfrak{H}_j$. Let g_j denote the jth double coset representative (DCR) of Table 3 above and consider the 8 non-trivial DCRs in turn. The software results show that five of these groups have the *same* international symbol, namely $\mathfrak{H}_{13}$, $\mathfrak{H}_{16}$, $\mathfrak{H}_{17}$, $\mathfrak{H}_{18}$, and $\mathfrak{H}_{19}$ so that we only list below $\mathfrak{H}_{12}$, $\mathfrak{H}_{13}$, $\mathfrak{H}_{14}$, and $\mathfrak{H}_{15}$. The index of $\mathfrak{H}_{1j}$ in $\mathfrak{G}$, namely $\mid \mathfrak{G}{:}\mathfrak{H}_{1j} \mid = \mid \mathfrak{T}{:}\mathfrak{S}_{1j} \mid * \mid \mathfrak{P}{:}\mathfrak{R}_{1j} \mid$ is given in each case where $\mathfrak{S}_{1j}$ denotes the translation and $\mathfrak{R}_{1j}$ the point group of $\mathfrak{H}_{1j}$ respectively.

Table 4: *Symmetry groups of ordered domain pairs*

LCR	symmetry group	conv. lat. trans.	generating elements	index
g_2 = (1|**0**)(1|100)	$\mathfrak{H}_{12}$ = *C*2*cm* (#40)	**a′** = +3**a** **b′** = +3**a** + 6**b** **c′** = +**c**	(7|(0, 0, 0) + (0, 0, 0)) (16|(0, 0, 1/2) + (0, 0, 0))	54
g_3 = (1|**0**)(1|010)	$\mathfrak{H}_{13}$ = *Pm* (#6)	**a′** = +3**a** **b′** = +3**b** **c′** = +**c**	(16|(0, 0, 1/2) + (0, 0, 0))	108
g_4 = (1|**0**)(1|210)	$\mathfrak{H}_{14}$ = *Cm*2*m* (#38)	**a′** = +3**a** **b′** = +3**a** + 6**b** **c′** = +**c**	(10|(0, 0, 1/2) + (0, 0, 0)) (16|(0, 0, 1/2) + (0, 0, 0))	54
g_5 = (3|**0**)(1|000)	$\mathfrak{H}_{15}$ = $P2_1/m$ (#11)	**a′** = +3**a** **b′** = +3**b** **c′** = +**c**	(4|(0, 0, 1/2) + (0, 0, 0)) (16|(0, 0, 1/2) + (0, 0, 0))	54

The symmetry group of the UDP $\{(\mathbb{S}_1, \mathbb{S}_j), (\mathbb{S}_j, \mathbb{S}_1)\}$ associated with the ODP $(\mathbb{S}_1, \mathbb{S}_j)$ is denoted by $\mathfrak{J}_{1j}$ respectively. The symmetry groups of ODP's and UDP's for the *transposable* ODP's are listed in Table 5 below.

Table 5: *Symmetry groups of un-ordered domain pairs*

LCR	symmetry group	conv. lat. trans.	generating elements	index
$g_2 = (1\|\mathbf{0})(1\|100)$	$\mathfrak{J}_{12} = Cmcm$ (#63)	$\mathbf{a}' = +3\mathbf{a}$ $\mathbf{b}' = +3\mathbf{a} + 6\mathbf{b}$ $\mathbf{c}' = +\mathbf{c}$	(4|(0, 0, 1/2) + (1, 0, 0)) (7|(0, 0, 0) + (0, 0, 0)) (16|(0, 0, 1/2) + (0, 0, 0))	27
$g_3 = (1\|\mathbf{0})(1\|010)$	$\mathfrak{J}_{13} = P2_1/m$ (#11)	$\mathbf{a}' = +3\mathbf{a}$ $\mathbf{b}' = +3\mathbf{b}$ $\mathbf{c}' = +\mathbf{c}$	(4|(0, 0, 1/2) + (0, 1, 0)) (16|(0, 0, 1/2) + (0, 0, 0))	54
$g_4 = (1\|\mathbf{0})(1\|210)$	$\mathfrak{J}_{14} = Cmcm$ (#63)	$\mathbf{a}' = +3\mathbf{a}$ $\mathbf{b}' = +3\mathbf{a} + 6\mathbf{b}$ $\mathbf{c}' = +\mathbf{c}$	(4|(0, 0, 1/2) + (2, 1, 0)) (7|(0, 0, 0) + (2, 1, 0)) (16|(0, 0, 1/2) + (0, 0, 0))	27
$g_5 = (3\|\mathbf{0})(1\|000)$	$\mathfrak{J}_{15} = Cmcm$ (#63)	$\mathbf{a}' = -3\mathbf{a} - 3\mathbf{b}$ $\mathbf{b}' = +3\mathbf{a} - 3\mathbf{b}$ $\mathbf{c}' = +\mathbf{c}$	(4|(0, 0, 1/2) + (0, 0, 0)) (9|(0, 0, 0) + (0, 0, 0)) (16|(0, 0, 1/2) + (0, 0, 0))	27
$g_6 = (3\|\mathbf{0})(1\|010)$	$\mathfrak{J}_{16} = Cm2m$ (#38)	$\mathbf{a}' = -3\mathbf{a} - 3\mathbf{b}$ $\mathbf{b}' = +3\mathbf{a} - 3\mathbf{b}$ $\mathbf{c}' = +\mathbf{c}$	(12|(0, 0, 1/2) + (2, 2, 0)) (16|(0, 0, 1/2) + (0, 0, 0))	54
$g_7 = (3\|\mathbf{0})(1\|210)$	$\mathfrak{J}_{17} = C2cm$ (#40)	$\mathbf{a}' = -3\mathbf{a} - 3\mathbf{b}$ $\mathbf{b}' = +3\mathbf{a} - 3\mathbf{b}$ $\mathbf{c}' = +\mathbf{c}$	(9|(0, 0, 0) + (2, 1, 0)) (16|(0, 0, 1/2) + (0, 0, 0))	54

Finally it should be noted that most of the symmetry groups of ODP's and UDP's are not in *standard* setting which implies that shifts of the origin and re-orientations have to be carried out to bring them into coincidence with their counterparts tabulated in the International Tables for Crystallography [14]. Both the shifts of the origin and re-orientations are likewise obtained by means of the software.

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