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Coset Decompositions of Space Groups: Applications to Domain Structure Analysis

R. Dirl,[a,b]* P. Zeiner,[a,b] B. L. Davies[c] and V. Janovec[d,e]

[a] *Institut für Theoretische Physik, TU Wien, A-1040 Wien, Wiedner Hauptstrasse 8-10, Austria,* [b] *Center for Computational Materials Science, TU Wien, A-1040 Wien, Wiedner Hauptstrasse 8-10, Austria,* [c] *School of Mathematics, University of Wales, Bangor, Gwynedd LL57 1UT, Wales,* [d] *Technical University of Liberec, Hálkova 6, 461 17, Liberec, Czech Republic, and* [e] *Institute of Physics, Academy of Sciences, Na Slovance 2, 180 40 Prague, Czech Republic. E-mail: rdirl@tph.tuwien.ac.at*

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Abstract

Left- and double-coset decompositions of space groups are systematically analysed by putting the emphasis on the introduction of special auxiliary groups. An algorithm is tailored to exploit the specific structure of space groups. The new results are, amongst others, an efficient alternative method to determine for space groups minimal sets of double-coset representatives and a general formula that gives the structure and number of left cosets that are contained in double cosets. Left-coset and double-coset decompositions of space groups are exploited in domain structure analysis.

1. Introductory remarks

The aim of this paper is to investigate left- and double-coset decompositions of space groups with respect to subgroups of finite index. Two approaches are available, either to apply straightforwardly a theorem of Frobenius or, what we describe here in detail, to tailor an alternative procedure that exploits the specific structure of space groups. Both approaches have been implemented in a software package (Davies, Dirl, Zeiner & Janovec, 1993), the details of which will be described elsewhere. The main idea, based on Hermann's theorem (Hermann, 1929), is to split every group–subgroup relation into well defined subgroup chains. The first step is to reduce the group $\mathcal{G}$ to that t intermediate subgroup $\mathcal{M}$, where t is synonymous with *translationsgleich* (Hahn, 1992), whose point-group operations are confined to those of the given subgroup $\mathcal{H}$. The second step is to reduce the group $\mathcal{M}$ to the given subgroup $\mathcal{H}$ by *thinning out* the translations, which implies that $\mathcal{H}$ forms a k subgroup of the former, where k is synonymous with *klassengleich* (Hahn, 1992).

Physical applications of coset and double-coset decompositions of space groups with respect to subspace groups follow the mathematical part. The role of symmetry considerations dealing with group–subgroup relations of space groups in structural phase transitions is widely accepted. Symmetry specifies transformation properties of the order parameter and determines the form of the Landau thermodynamic potential (Izyumov & Syromyatnikov, 1990; Stokes & Hatch, 1988; Tolédano & Tolédano, 1987). Whereas the order parameter is specified by symmetry operations preserved at the transitions, for domain structures, lost operations are significant. The number and the relations between domain states and domain pairs can be found by grouping the lost operations into left and double cosets. Different types of domain states can be related to subgroups retaining characteristic domain properties. For more details, the reader is referred to Janovec (1972), Van Tendeloo & Amelinckx (1974), Janovec (1976), Janovec & Dvořáková (1974), Janovec, Dvořáková, Wike & Litvin (1989), Izyumov & Syromyatnikov (1990), Janovec, Litvin & Fuksa (1995) where many other aspects are likewise treated and examples are discussed at length. Here we discuss also an example to demonstrate the usefulness of coset and double-coset decompositions in the analysis of domain structures.

2. Double cosets of space groups

2.1. *Notations and conventions adopted for space groups*

Every space group $\mathcal{G}$ is fixed by its translation group $\mathcal{T}$, its point group $\mathcal{P}$, and its setting. In other words, we assume $\mathcal{G} = \{\mathcal{T}, \mathcal{P}|o, \mathbf{w}_P\}$, where o denotes its origin and $\mathbf{w}_P = \{\mathbf{w}_j|R_j \in \mathcal{P}\}$ its set of *fractional* translations. The setting of space groups can be changed by shifts of the origin and/or reorientation operations. We say a space group is in a standard setting if it coincides with the settings given by Cracknell, Davies, Miller & Love (1979), which in almost all cases are identical with the first standard choices given in Hahn (1992) (see Stokes & Hatch, 1988). Recall that to describe space groups one can use either the algebraic approach (Ascher & Janner, 1965, 1968/69, Mozrzymas, 1975) or the geometric approach (Hahn, 1992). In detail, the group elements of the space group $\mathcal{G}$ are symbolized by $G \in \mathcal{G}$, where $G = (R_j|\mathbf{w}_j + \mathbf{t}_a)$. The entries $\mathbf{t}_a \in \mathcal{T}$ denote

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arbitrary elements of the translation group $\mathcal{T}$, which are integral linear combinations of a fixed set of primitive basis translations $\{\mathbf{t}_1, \mathbf{t}_2, \mathbf{t}_3\}$. The entries $\mathbf{w}_j$ are *fractional* translations that are uniquely associated with the rotational parts R_j of $G \in \mathcal{G}$, and the symbols $R_j \in \mathcal{P}$ are the elements of the point group $\mathcal{P}$. We adopt the convention $\mathbf{w}_j \in \mathbf{E}(\mathcal{T})$, where $\mathbf{E}(\mathcal{T})$ denotes the primitive cell of $\mathcal{T}$. The composition law of $\mathcal{G}$ reads

$$(R_j|\mathbf{w}_j + \mathbf{t}_a)(R_k|\mathbf{w}_k + \mathbf{t}_b) = (R_{jk}|\mathbf{w}_{jk} + \mathbf{t}_{jk} + \mathbf{t}_a + R_j\mathbf{t}_b), \tag{1}$$

where the fractional translations $\mathbf{w}_{jk} \in \mathbf{E}(\mathcal{T})$ are assigned to $R_{jk} = R_jR_k$, respectively. Note that for the special translations $\mathbf{t}_{jk} = \mathbf{w}_j + R_j\mathbf{w}_k - \mathbf{w}_{jk} \in \mathcal{T}$ must hold.

2.2. *General remarks on coset and double-coset decompositions*

Here, the problem consists of decomposing a given space group $\mathcal{G}$ into double cosets with respect to a given g subgroup $\mathcal{H}$, where g is synonymous with *general* subgroup. The subgroup $\mathcal{H}$ is determined by its translation group $\mathcal{S}$, its point group $\mathcal{R}$, and its setting that is partly fixed by the setting of $\mathcal{G}$. In other words, we have $\mathcal{H} = \{\mathcal{S}, \mathcal{R}|o', \mathbf{z}_R\}$, where o' denotes its origin and $\mathbf{z}_R = \{\mathbf{z}_m|S_m \in \mathcal{R}\}$ its set of fractional translations. In detail, we have $\mathbf{z}_m = \mathbf{w}_m + \mathbf{t}^H_m$ for all $S_m \in \mathcal{R}$, where $\mathbf{t}^H_m \in \mathcal{T}$ together with $\mathbf{s}_{mn} = \mathbf{z}_m + S_m\mathbf{z}_n - \mathbf{z}_{mn} \in \mathcal{S}$ for all $S_m, S_n \in \mathcal{R}$ must be satisfied. Recall that the subgroup relations $\mathcal{S} \subset \mathcal{T}$ and $\mathcal{R} \subset \mathcal{P}$ are only necessary conditions to establish group–subgroup relations between space groups (Senechal, 1980; Dirl & Davies, 1993). Note that in general the subgroup $\mathcal{H}$ refers to a different origin o' and hence need not necessarily be in a standard setting although the space group $\mathcal{G}$ is assumed to be a in a standard setting. However, here we do not deal with the problem of identifying g subgroups with their image-space groups in standard settings, which is a problem in its own right (Hatch & Stokes, 1985; Stokes & Hatch, 1988). Here, the group elements of the subgroup $\mathcal{H}$ are symbolized by $H \in \mathcal{H}$, where $H = (S_k|\mathbf{z}_k + \mathbf{s}_b)$. The entries $\mathbf{s}_b \in \mathcal{S}$ denote arbitrary elements of the subgroup $\mathcal{S}$, which are integral linear combinations of a fixed set of primitive basis translations $\{\mathbf{s}_1, \mathbf{s}_2, \mathbf{s}_3\}$. We assume

$$\mathbf{s} = \mathbf{t}\,\mathbb{N}, \tag{2}$$

where $\mathbf{t} = (\mathbf{t}_1, \mathbf{t}_2, \mathbf{t}_3)$ and $\mathbf{s} = (\mathbf{s}_1, \mathbf{s}_2, \mathbf{s}_3)$ are formally written as row vectors. Thus, the elements of the basis $\{\mathbf{s}_1, \mathbf{s}_2, \mathbf{s}_3\}$ are correlated with the elements of the basis $\{\mathbf{t}_1, \mathbf{t}_2, \mathbf{t}_3\}$ by a non-singular integral matrix $\mathbb{N}$ whose determinant is greater than one if $\mathcal{S}$ is a proper sublattice of $\mathcal{T}$. Recall that the entries $\mathbf{z}_k \in \mathbf{E}(\mathcal{S})$ are fractional translations that are uniquely associated with the rotational parts S_k of $H \in \mathcal{H}$, where $\mathbf{E}(\mathcal{S})$ denotes the primitive cell of $\mathcal{S}$ and the symbols $S_k \in \mathcal{R}$ are the elements of the subgroup $\mathcal{R}$.

Left- and double-coset decompositions of the space group $\mathcal{G}$ with respect to the fixed subgroup $\mathcal{H}$ are written symbolically as follows:

$$\mathcal{G} = \bigcup_{G \in \underline{\mathcal{G}}(\mathcal{H})} G * \mathcal{H} \tag{3}$$

$$\mathcal{G} = \bigcup_{G \in \underline{\Delta\mathcal{G}}(\mathcal{H})} \mathcal{H} * G * \mathcal{H}, \tag{4}$$

where the asterisk $*$ indicates set multiplication. The entries $\underline{\mathcal{G}}(\mathcal{H})$ denote sets of coset representatives of $\mathcal{G}$ with respect to $\mathcal{H}$ while the entries $\underline{\Delta\mathcal{G}}(\mathcal{H})$ denote sets of double-coset representatives of $\mathcal{G}$ with respect to $\mathcal{H}$. Once a left-coset decomposition of $\mathcal{G}$ with respect to $\mathcal{H}$ is determined, the task is to find an admissible minimal subset $\underline{\Delta\mathcal{G}}(\mathcal{H}) \subseteq \underline{\mathcal{G}}(\mathcal{H})$ such that (4) holds. Every double coset $\mathcal{H} * G * \mathcal{H}$ must contain left cosets $G'G * \mathcal{H}$ as a whole entity. This entails that $\mathcal{H} * G * \mathcal{H}$ must be representable as a union of mutually disjoint left cosets $G'G * \mathcal{H}$, where $G' \in \mathcal{G}$. Let $\mathcal{H}(G) = \mathcal{H} \cap G * \mathcal{H} * G^{-1}$, then we may state the well known theorem.

Theorem: Let $\mathcal{H} * G * \mathcal{H}$ be a double coset of $\mathcal{G}$ with respect to the given subgroup $\mathcal{H}$ and $\mathcal{H} = \bigcup_A A * \mathcal{H}(G)$ a left-coset decomposition of $\mathcal{H}$ with respect to the intersection group $\mathcal{H}(G)$, where $\underline{\mathcal{H}}[\mathcal{H}(G)] = \{A\}$ denotes a set of left-coset representatives, then we have

$$\mathcal{H} * G * \mathcal{H} = \bigcup_A AG * \mathcal{H}. \tag{5}$$

From this, the theorem of Frobenius, it follows immediately that the number of the left cosets $AG * \mathcal{H}$ contained in the double coset $\mathcal{H} * G * \mathcal{H}$ is identical to the index of the intersection group $\mathcal{H}(G)$ with respect to the subgroup $\mathcal{H}$ of $\mathcal{G}$. For more details or some other aspects concerning double-coset decompositions, the reader is referred to standard references (Frobenius, 1895*a*,*b*; Bradley & Cracknell, 1972; Speiser, 1937; Hall, 1959; Kurosh, 1960; Huppert, 1967; Scott, 1964; Kochendörffer, 1966). Symbolically, we write

$$|\mathcal{H} * G * \mathcal{H} : AG * \mathcal{H}| = |\mathcal{H} : \mathcal{H}(G)|, \tag{6}$$

which we especially employ in the case of space groups since the double and left cosets that we consider are infinite (countable) sets whose relative indexes are assumed to be finite. We show that the construction of intersection groups $\mathcal{H}(G)$ and the coset decompositions of $\mathcal{H}$ with respect to the various $\mathcal{H}(G)$ can be circumvented when decomposing $\mathcal{G}$ into $\mathcal{H}$ double cosets. We also give the $\mathcal{H}$ left-coset decompositions of $\mathcal{H}$ double cosets $\mathcal{H} * G * \mathcal{H}$ without using the Frobenius theorem but compare the results with the Frobenius theorem in the case of t and k subgroups.

2.3. *Double-coset decomposition with respect to t subgroups*

Let $\mathcal{G}$ be a space group and $\mathcal{H}$ a fixed t subgroup, which implies $\mathcal{S} = \mathcal{T}$ and $\mathcal{R} \subset \mathcal{P}$, respectively. Once we know a double-coset decomposition of $\mathcal{P}$ with respect to $\mathcal{R}$, namely

$$\mathcal{P} = \bigcup_{B_d \in \underline{\Delta\mathcal{P}}(\mathcal{R})} \mathcal{R} * B_d * \mathcal{R}, \qquad (7)$$

where $B_d \in \underline{\mathcal{P}}(\mathcal{R})$ symbolizes its left-coset representatives and $\underline{\Delta\mathcal{P}}(\mathcal{R}) \subseteq \underline{\mathcal{P}}(\mathcal{R})$ a minimal set of double-coset representatives, then the corresponding double-coset decomposition of $\mathcal{G}$ with respect to the t subgroup $\mathcal{H}$ reads as follows:

$$\mathcal{G} = \bigcup_{B_d \in \underline{\Delta\mathcal{P}}(\mathcal{R})} \mathcal{H} * (B_d|\mathbf{w}_d) * \mathcal{H}. \qquad (8)$$

Here, the entries $\mathbf{w}_d$ are the fractional translations that are uniquely assigned to the rotational parts $B_d \in \underline{\mathcal{P}}(\mathcal{R})$. Though trivial, we also state for the sake of completeness the decomposition of the $\mathcal{H}$ double cosets into $\mathcal{H}$ left cosets. We have

$$\mathcal{H} * (B_d|\mathbf{w}_d) * \mathcal{H} = \bigcup_{S_l \in \underline{\mathcal{R}}[\mathcal{R}(B_d)]} (S_l|\mathbf{w}_l)(B_d|\mathbf{w}_d) * \mathcal{H}, \qquad (9)$$

where $S_l \in \underline{\mathcal{R}}[\mathcal{R}(B_d)]$ are left-coset representatives of $\mathcal{R}$ with respect to $\mathcal{R}(B_d)$. This result is in one-to-one correspondence with the Frobenius theorem (5) since the intersection group $\mathcal{H} \cap (B_d|\mathbf{w}_d) * \mathcal{H} * (B_d|\mathbf{w}_d)^{-1}$ reduces to a space group whose point group is confined to the intersection group $\mathcal{R}(B_d) = \mathcal{R} \cap B_d * \mathcal{R} * B_d^{-1}$.

2.4. *Double-coset decomposition with respect to k subgroups*

Now let $\mathcal{G}$ be a space group and $\mathcal{H}$ a k subgroup. This implies not only that $\mathcal{S} \subset \mathcal{T}$ and $\mathcal{R} = \mathcal{P}$ has to be satisfied but also that the sets of fractional $\mathbf{w}_P$ and $\mathbf{z}_P$ are compatible in the previously stated sense. To deduce a coset decomposition of $\mathcal{G}$ with respect to its k subgoup $\mathcal{H}$, we state at first coset decompositions of $\mathcal{G}$ and of $\mathcal{H}$ with respect to their translation groups. In detail, we use the expressions $\mathcal{G} = \bigcup_{R_j \in \mathcal{P}} (R_j|\mathbf{w}_j) * \mathcal{T}$ and likewise $\mathcal{H} = \bigcup_{R_j \in \mathcal{P}} (R_j|\mathbf{z}_j) * \mathcal{S}$. Next, we employ the coset decomposition of $\mathcal{T}$ with respect to $\mathcal{S}$, namely $\mathcal{T} = \bigcup_{\mathbf{t}_c} (E|\mathbf{t}_c) * \mathcal{S}$, which entails

$$\mathcal{G} = \bigcup_{\mathbf{t}_c} (E|\mathbf{t}_c) * \mathcal{H} \qquad (10)$$

with $\mathbf{t}_c \in \mathbf{W}(\mathcal{S}) \cap \mathcal{T}$, where $\mathbf{W}(\mathcal{S})$ denotes the Wigner–Seitz cell of the sublattice $\mathcal{S}$.

Because of $\mathcal{H} * (E|\mathbf{t}_c) * \mathcal{H} = \mathcal{H} * (E|R_j\mathbf{t}_c) * \mathcal{H}$, we infer that $\mathcal{H} * (E|R_j\mathbf{t}_c) * \mathcal{H}$ contains all cosets $(E|R_j\mathbf{t}_c) * \mathcal{H}$, where $R_j \in \mathcal{P}$ varies over the whole point group. Moreover, let $\mathcal{P}(\mathbf{t}_c) = \{R_j \in \mathcal{P} | R_j\mathbf{t}_c = \mathbf{t}_c + \mathbf{t}(R_j)\}$ be the group of the $\mathbf{t}_c$ vector, where $\mathbf{t}(R_j) \in \mathcal{S}$ is assumed. Then, every double coset $\mathcal{H} * (E|\mathbf{t}_c) * \mathcal{H}$ can be expressed by

$$\mathcal{H} * (E|\mathbf{t}_c) * \mathcal{H} = \bigcup_{R_k \in \underline{\mathcal{P}}[\mathcal{P}(\mathbf{t}_c)]} (E|R_k\mathbf{t}_c) * \mathcal{H}, \qquad (11)$$

where $\underline{\mathcal{P}}[\mathcal{P}(\mathbf{t}_c)]$ denotes a set of coset representatives of $\mathcal{P}$ with respect to $\mathcal{P}(\mathbf{t}_c)$. We define for every $\mathbf{t}_c \in \mathbf{W}(\mathcal{S}) \cap \mathcal{T}$ its left-coset decomposition of $\mathcal{P}$ with respect to the corresponding $\mathcal{P}(\mathbf{t}_c)$, which allows one to fix subsets $\Delta\mathbf{W}(\mathcal{S}) \subseteq \mathbf{W}(\mathcal{S})$, hereafter called *representation domains*, that contain from each $\mathbf{t}_c$ star $\mathbf{S}(\mathbf{t}_c|\mathcal{P})$ one and only one element. Following the usual conventions, we denote by $\mathbf{S}(\mathbf{t}_c|\mathcal{P}) = \{\mathbf{t}_a \in \mathcal{T} | \mathbf{t}_a = R_k\mathbf{t}_c, R_k \in \mathcal{P}\}$ the $\mathbf{t}_c$ star where $\mathbf{t}_c \in \Delta\mathbf{W}(\mathcal{S}) \cap \mathcal{T}$. Thus, we arrive at

$$\mathcal{G} = \bigcup_{\mathbf{t}_c \in \Delta\mathbf{W}(\mathcal{S}) \cap \mathcal{T}} \mathcal{H} * (E|\mathbf{t}_c) * \mathcal{H}, \qquad (12)$$

which represents the desired double-coset decomposition of $\mathcal{G}$ with respect to the k subgroup $\mathcal{H}$. The proof of (12) is straightforward. Recall that the decompositions of $\mathcal{H}$ double cosets into $\mathcal{H}$ left cosets is given by (11). To prove their one-to-one correspondence with the Frobenius theorem (5), one merely has to verify that every intersection group $\mathcal{H} \cap (E|\mathbf{t}_c) * \mathcal{H} * (E|\mathbf{t}_c)^{-1}$ coincides with that t subgroup of $\mathcal{H}$ whose point is restricted to $\mathcal{P}(\mathbf{t}_c)$.

2.5. *Double-coset decomposition with respect to g subgroups*

Finally, let $\mathcal{G}$ be a given space group and $\mathcal{H}$ an admissible g subgroup, which implies not only that $\mathcal{S} \subset \mathcal{T}$ and $\mathcal{R} \subset \mathcal{P}$ simultaneously but also that the corresponding sets of fractional translations $\mathbf{w}_P$ and $\mathbf{z}_R$ are compatible. Remember the straightforward approach consists of applying directly the Frobenius theorem by passing over immediately to the g subgroup $\mathcal{H}$ without invoking any intermediate step. This would require the analysis of the structure of the intersection groups $\mathcal{H}(G) = \mathcal{H} \cap G * \mathcal{H} * G^{-1}$, where $G = (R_j|\mathbf{w}_j + \mathbf{t}_a) \in \mathcal{G}$ and to decompose $\mathcal{H}$ into left cosets with respect to the various $\mathcal{H}(G)$ to eliminate redundant double cosets.

However, we prefer to describe our combined approach. The first step of this approach is to reduce $\mathcal{G}$ to its corresponding t subgroup $\mathcal{M}$. The second step consists of reducing $\mathcal{M}$ to the given subgroup $\mathcal{H}$, which by definition forms a k subgroup of the former (see, for instance, Wondratschek & Jeitschko, 1976). First, we comment on the decomposition of $\mathcal{G}$ into $\mathcal{H}$ left cosets. The corresponding left-coset decompositions read

$$\mathcal{G} = \bigcup_{B_d \in \underline{\mathcal{P}}(\mathcal{R})} (B_d|\mathbf{w}_d) * \mathcal{M} \qquad (13)$$

$$\mathcal{M} = \bigcup_{\mathbf{t}_c \in \mathbf{W}(\mathcal{S}) \cap \mathcal{T}} (E|\mathbf{t}_c) * \mathcal{H} \tag{14}$$

$$\mathcal{G} = \bigcup_{B_d} \bigcup_{\mathbf{t}_c} (B_d|\mathbf{w}_d)(E|\mathbf{t}_c) * \mathcal{H}, \tag{15}$$

where the last one is due to the sequence $\mathcal{G} \downarrow \mathcal{M} \downarrow \mathcal{H}$. To fix our conventions, we use exclusively the form $(B_d|\mathbf{w}_d)(E|\mathbf{t}_c)$ for the left-coset representatives of $\mathcal{G}$ with respect to $\mathcal{H}$. Their labelling is unique by fixing $B_d \in \underline{\mathcal{P}}(\mathcal{R})$ and likewise $\mathbf{t}_c \in \mathbf{W}(\mathcal{S}) \cap \mathcal{T}$. Note in passing that the index of $\mathcal{H}$ in $\mathcal{G}$ can be expressed by $|\mathcal{G} : \mathcal{H}| = |\underline{\mathcal{P}}(\mathcal{R})||\mathbf{W}(\mathcal{S}) \cap \mathcal{T}|$.

2.5.1. *Decomposition of $\mathcal{G}$ into $\mathcal{M}$ double cosets.* Since $\mathcal{M}$ always exists and by definition presents a t subgroup of $\mathcal{G}$, we merely have to apply (8) to express $\mathcal{G}$ in terms of $\mathcal{M}$ double cosets.

$$\mathcal{G} = \bigcup_{B_d \in \underline{\Delta\mathcal{P}}(\mathcal{R})} \mathcal{M} * (B_d|\mathbf{w}_d) * \mathcal{M}, \tag{16}$$

where $B_d \in \underline{\mathcal{P}}(\mathcal{R})$ varies over the minimal subset $\underline{\Delta\mathcal{P}}(\mathcal{R}) \subseteq \underline{\mathcal{P}}(\mathcal{R})$ of left-coset representatives that define the corresponding double-coset decomposition of $\mathcal{P}$ with respect to $\mathcal{R}$. Thus, the remaining task consists of expressing every $\mathcal{M}$ double coset $\mathcal{M} * (B_d|\mathbf{w}_d) * \mathcal{M}$ in terms of $\mathcal{H}$ double cosets.

2.5.2. *Decomposition of $\mathcal{M}$ double cosets into $\mathcal{H}$ double cosets.* Here, we discuss all features of $\mathcal{M}$ double cosets $\mathcal{M} * (B_d|\mathbf{w}_d) * \mathcal{M}$ expressed by $\mathcal{M}$ double cosets, which are independent whether $\mathcal{H}$ is a symmorphic or a non-symmorphic space group. By virtue of (14), we arrive at

$$\mathcal{M} * (B_d|\mathbf{w}_d) * \mathcal{M} = \bigcup_{\mathbf{t}_c \in \mathbf{W}(\mathcal{S}) \cap \mathcal{T}} \mathcal{H} * (B_d|\mathbf{w}_d)(E|\mathbf{t}_c) * \mathcal{H} \tag{17}$$

since every translation vector satisfying $\mathbf{t}_c + B_d\mathbf{t}_e = \mathbf{s}_a \in \mathcal{S}$, where $\mathbf{t}_c, \mathbf{t}_e \in \mathbf{W}(\mathcal{S}) \cap \mathcal{T}$ can be re-absorbed into $\mathcal{H}$. Accordingly, the remaining task is to reduce $\mathbf{W}(\mathcal{S})$ to minimal sets $\Delta\mathbf{W}(B_d, \mathcal{S}) \subseteq \mathbf{W}(\mathcal{S})$ such that $\mathcal{H} * (B_d|\mathbf{w}_d)(E|\mathbf{t}_c) * \mathcal{H} \cap \mathcal{H} * (B_d|\mathbf{w}_d)(E|\mathbf{t}_e) * \mathcal{H} = \emptyset$ for every pair of translations $\mathbf{t}_c, \mathbf{t}_e \in \Delta\mathbf{W}(B_d, \mathcal{S}) \cap \mathcal{T}$. Note in particular that the subsets $\Delta\mathbf{W}(B_d, \mathcal{S}) \subseteq \mathbf{W}(\mathcal{S})$ in general depend explicitly on $B_d \in \underline{\Delta\mathcal{P}}(\mathcal{R})$.

The first restriction of $\mathbf{W}(\mathcal{S})$ to smaller subsets comes from the invariance of the double cosets $\mathcal{H} * (B_d|\mathbf{w}_d)(E|\mathbf{t}_c) * \mathcal{H}$ with respect to arbitrary elements $\mathbf{s}_a, \mathbf{s}_b \in \mathcal{S}$, which can be written as

$$\begin{aligned}&\mathcal{H} * (B_d|\mathbf{w}_d)(E|\mathbf{t}_c) * \mathcal{H}\\&\quad = \mathcal{H} * (B_d|\mathbf{w}_d)(E|\mathbf{t}_c + B_d^{-1}\mathbf{s}_a + \mathbf{s}_b) * \mathcal{H}.\end{aligned} \tag{18}$$

By virtue of the invariance relation (18), which must hold for all $\mathbf{s}_a, \mathbf{s}_b \in \mathcal{S}$, we infer that whenever $\mathbf{t}_c = B_d^{-1}\mathbf{s}_a + \mathbf{s}_b \in \mathbf{W}(\mathcal{S}) \cap \mathcal{T}$ is realized, then $\mathcal{H} * (B_d|\mathbf{w}_d)(E|\mathbf{t}_c) * \mathcal{H} = \mathcal{H} * (B_d|\mathbf{w}_d) * \mathcal{H}$ must be valid since every $\mathbf{t}_c = B_d^{-1}\mathbf{s}_a + \mathbf{s}_b$ can be re-absorbed. Note in particular that, for every fixed $B_d \in \underline{\Delta\mathcal{P}}(\mathcal{R})$, the sets of translations defined by

$$\mathcal{S}(B_d) = \{\mathbf{t} \in \mathcal{T}|\mathbf{t} = B_d^{-1}\mathbf{s}_a + \mathbf{s}_b, \mathbf{s}_a, \mathbf{s}_b \in \mathcal{S}\} = \mathcal{S} \uplus B_d^{-1}\mathcal{S} \tag{19}$$

form subgroups of the translation group $\mathcal{T}$, which may contain $\mathcal{S}$ itself as a proper subgroup. In other words, $\mathcal{S} \subseteq \mathcal{S}(B_d) \subseteq \mathcal{T}$, which implies that we must have $\mathcal{S} \cap B_d\mathcal{S} \subseteq \mathcal{S}$ and likewise $\mathcal{S} \uplus B_d^{-1}\mathcal{S} \subseteq \mathcal{T}$, whereas the union sets $\mathcal{S} \cup B_d^{-1}\mathcal{S}$ in general do not form groups though $\mathcal{S}$ and $B_d^{-1}\mathcal{S}$ are proper subsets of $\mathcal{T}$. Apart from this, it follows from (17) and (18) that

$$\mathcal{M} * (B_d|\mathbf{w}_d) * \mathcal{M} = \bigcup_{\mathbf{t}_c \in \mathbf{W}[\mathcal{S}(B_d)] \cap \mathcal{T}} \mathcal{H} * (B_d|\mathbf{w}_d)(E|\mathbf{t}_c) * \mathcal{H}, \tag{20}$$

where $\mathbf{W}[\mathcal{S}(B_d)]$ denotes the Wigner–Seitz cell of the intermediate lattice $\mathcal{S}(B_d)$, which apart from special cases are proper subwedges of $\mathbf{W}(\mathcal{S})$, *i.e.* $\mathbf{W}[\mathcal{S}(B_d)] \subset \mathbf{W}(\mathcal{S})$ since in general $\mathcal{S}(B_d)$ contains $\mathcal{S}$ as a proper subgroup. After these preliminary restrictions of $\mathbf{W}(\mathcal{S})$ to smaller subsets, which do not rely upon the specific structure of symmorphic or of non-symmorphic k subgroup $\mathcal{H}$, we consider separately in the following the implications coming from symmorphic and from non-symmorphic space groups.

Symmorphic $\mathcal{H}$: decomposition of $\mathcal{M}$ double cosets into $\mathcal{H}$ double cosets: First we assume that $\mathcal{H}$ forms a symmorphic k subgroup of $\mathcal{M}$, which represents the simpler situation. Let $\mathcal{H} * (B_d|\mathbf{w}_d)(E|\mathbf{t}_c) * \mathcal{H}$ be a given $\mathcal{H}$ double coset, where $B_d \in \underline{\Delta\mathcal{P}}(\mathcal{R})$ and $\mathbf{t}_c \in \mathbf{W}[\mathcal{S}(B_d)] \cap \mathcal{T}$, then $\mathcal{H} * (B_d|\mathbf{w}_d)(E|\mathbf{t}_c) * \mathcal{H} = \mathcal{H} * (S_jB_dS_k^{-1}|\mathbf{w}_d + \mathbf{v}_{jd})(E|S_k\mathbf{t}_c) * \mathcal{H}$ for all $S_j, S_k \in \mathcal{R}$ and where $\mathbf{v}_{jd} = S_j\mathbf{w}_d - \mathbf{w}_d$ can be interpreted as a B_d-dependent shift of the origin. This implies that all elements $(S_jB_dS_k^{-1}|\mathbf{w}_d + \mathbf{v}_{jd})(E|S_j\mathbf{t}_c)$ are likewise contained in the $\mathcal{H}$ double cosets $\mathcal{H} * (B_d|\mathbf{w}_d)(E|\mathbf{t}_c) * \mathcal{H}$, respectively. To prove this, one has to use the composition law of $\mathcal{G}$ and in addition that $\mathbf{z}_j = \mathbf{w}_j = \mathbf{0}$ for all $S_j \in \mathcal{R}$ since the g subgroup $\mathcal{H}$ is assumed to be symmorphic and $\mathcal{G}$ in a standard setting. Here it is worth emphasizing that the space-group elements $(S_jB_dS_k^{-1}|\mathbf{w}_d+\mathbf{v}_{jd})$ cannot be factorized since in general neither $(S_jB_dS_k^{-1}|\mathbf{w}_d) \in \mathcal{G}$ nor $(E|\mathbf{v}_{jd}) \in \mathcal{G}$ holds true. However, if we take $S_j = B_dQ_jB_d^{-1} \in \mathcal{R}(B_d)$ with some $Q_j \in \mathcal{R}$ and in particular $S_k^{-1} = B_d^{-1}S_j^{-1}B_d = Q_j^{-1}$, then the coset representative $B_d \in \underline{\Delta\mathcal{P}}(\mathcal{R})$ is mapped onto itself and one arrives at the identities $\mathcal{H} * (B_d|\mathbf{w}_d)$-$(E|\mathbf{t}_c) * \mathcal{H} = \mathcal{H} * (B_d|\mathbf{w}_d)(E|B_d^{-1}\mathbf{v}_{jd} + S_k\mathbf{t}_c) * \mathcal{H}$, which hold for all $S_j, S_k \in \mathcal{R}$. Moreover, note that $\mathbf{v}_{jd} \in \mathcal{T}$ must hold for all $S_j \in \mathcal{R}(B_d)$, which implies that $\mathbf{v}_{jd}$ can be interpreted as a trivial shift of the origin. If we take some $S_j \in \mathcal{R}|\mathcal{R}(B_d)$ together with $S_k = E$, then $B_d \in \underline{\Delta\mathcal{P}}(\mathcal{R})$ is mapped onto some equivalent element of the same $\underline{\mathcal{P}}(\mathcal{R}; B_d)$ orbit $\underline{\mathcal{P}}(\mathcal{R}; B_d) = \{B_e \in \underline{\mathcal{P}}(\mathcal{R})|B_e =$

$S_e B_d$, $S_e \in \underline{\mathcal{R}}[\mathcal{R}(B_d)]\}$ and hence must lead to an equivalent but different $\mathcal{H}$ double coset.

For this reason, we restrict the range of variation of the point-group elements to the intersection group $\mathcal{R}(B_d)$ in order to ensure that the respective $B_d \in \underline{\Delta \mathcal{P}}(\mathcal{R})$ remains unchanged. Next, we have to analyse for fixed B_d and any given translation $\mathbf{t}_c \in \mathbf{W}[\mathcal{S}(B_d)]$ the following set of translations $\mathbf{S}[\mathbf{t}_c|\mathcal{R}(B_d)] = \{\mathbf{t}_a \in \mathcal{T}|\mathbf{t}_a = Q_j\mathbf{t}_c + \mathbf{v}_{jd}^{\sharp}\}$, where $Q_j \in \mathcal{R}(B_d)$ and the special translations $\mathbf{v}_{jd}^{\sharp} = Q_j B_d^{-1}\mathbf{w}_d - B_d^{-1}\mathbf{w}_d$ have to be taken into account. For obvious reasons, every set $\mathbf{S}[\mathbf{t}_c|\mathcal{R}(B_d)]$ is called a generalized $\mathcal{R}(B_d)$ star since it may contain a shift of the origin in the case of non-symmorphic space groups $\mathcal{G}$. Of course, if the space group $\mathcal{G}$ is symmorphic then all $\mathcal{P}(\underline{\mathcal{R}})$ stars reduce to ordinary stars. However, if $\mathcal{G}$ is non-symmorphic then at least one generalized $\mathcal{R}(B_d)$ star must be investigated. Now, if we take from each $\mathcal{R}(B_d)$ star one and only one element, then the corresponding subset $\Delta\mathbf{W}[\mathcal{S}(B_d)] \subseteq \mathbf{W}[\mathcal{S}(B_d)]$ contains a minimal set of coset representatives. Hence, we arrive at the final expressions

$$\mathcal{M} * (B_d|\mathbf{w}_d) * \mathcal{M} = \bigcup_{\mathbf{t}_c \in \Delta\mathbf{W}[\mathcal{S}(B_d)] \cap \mathcal{T}} \mathcal{H} * (B_d|\mathbf{w}_d)(E|\mathbf{t}_c) * \mathcal{H} \tag{21}$$

$$\mathcal{G} = \bigcup_{B_d \in \underline{\Delta\mathcal{P}}(\mathcal{R})} \bigcup_{\mathbf{t}_c \in \Delta\mathbf{W}[\mathcal{S}(B_d)] \cap \mathcal{T}} \mathcal{H} * (B_d|\mathbf{w}_d)(E|\mathbf{t}_c) * \mathcal{H}, \tag{22}$$

where the first formula represents the desired double-coset decomposition of every $\mathcal{M}$ double coset into its corresponding $\mathcal{H}$ double cosets and where the second formula is straightforwardly obtained by combining (16) and (21) in consecutive order.

To summarize (22) presents the double-coset decomposition of the space group $\mathcal{G}$ in terms of the symmorphic g subgroup $\mathcal{H}$. For convenience, we recapitulate the basic steps of our approach to determine systematically double-coset decompositions of given space groups into double cosets of symmorphic g subgroups. In detail, one has to determine (i) the minimal set $\underline{\Delta\mathcal{P}}(\mathcal{R}) \subseteq \underline{\mathcal{P}}(\mathcal{R})$, (ii) the auxiliary translation groups $\mathcal{S}(B_d) = \mathcal{S} \uplus B_d^{-1}\mathcal{S} \subseteq \mathcal{T}$, (iii) the Wigner–Seitz cells $\mathbf{W}[\mathcal{S}(B_d)] \subseteq \mathbf{W}(\mathcal{S})$, (iv) the $\mathcal{R}(B_d)$ stars $\mathbf{S}[\mathbf{t}_c|\mathcal{R}(B_d)]$, and (v) the corresponding representation domains $\Delta\mathbf{W}[\mathcal{S}(B_d)] \subseteq \mathbf{W}[\mathcal{S}(B_d)]$, in order to be able to write down the double-coset decompositions (22) where only in step (iv) does the symmorphic structure of the g subgroup enter essentially.

Non-symmorphic $\mathcal{H}$: decomposition of $\mathcal{M}$ double cosets into $\mathcal{H}$ double cosets: Here we assume that $\mathcal{H}$ forms a non-symmorphic g subgroup of the space group $\mathcal{G}$. It is immediate from the preceding discussion that up to (20) the reduction steps are identical since they do not depend on the peculiarities of symmorphic or non-symmorphic space groups. Thus, we may start from (20) where the translations $\mathbf{t}_c \in \mathbf{W}(\mathcal{S}) \cap \mathcal{T}$ again are restricted to the sets $\mathbf{W}[\mathcal{S}(B_d)] \cap \mathcal{T}$ that refer to the corresponding intermediate translation groups $\mathcal{S}(B_d)$, which have been defined in (19). Recall that since $\mathcal{H}$ is non-symmorphic we have $\mathbf{z}_j = \mathbf{w}_j + \mathbf{t}_j^H$, which must hold for all $S_j \in \mathcal{R}$, where, due to the conventions $\mathbf{t}_j^H \in \mathbf{E}(\mathcal{S}) \cap \mathcal{T}$, the special translations $\mathbf{t}_j^H$ are uniquely determined. By the same arguments, which now are more involved, one ends up with the following identities:

$$\begin{aligned}\mathcal{H} &* (B_d|\mathbf{w}_d)(E|\mathbf{t}_c) * \mathcal{H}\\ &= \mathcal{H} * (B_d|\mathbf{w}_d)(E|Q_j\mathbf{t}_c + \mathbf{y}_j + \mathbf{t}_j^d) * \mathcal{H},\end{aligned} \tag{23}$$

where the extra symbols $\mathbf{y}_j = \mathbf{v}_{jd}^{\sharp} + \mathbf{x}_j$, $\mathbf{v}_{jd}^{\sharp} = Q_j B_d^{-1}\mathbf{w}_d - B_d^{-1}\mathbf{w}_d$, $\mathbf{x}_j = B_d^{-1}\mathbf{w}_j^d - \mathbf{w}_j$, $\mathbf{t}_j^d = B_d^{-1}\mathbf{t}_j^{Hd} - \mathbf{t}_j^H$ are introduced as shorthand notations, and where $Q_j \in \mathcal{R}(B_d)$ is assumed. Recall that the fractional translations $\mathbf{w}_d$ and $\mathbf{w}_j^d$ are assigned to B_d and to $B_d Q_j B_d^{-1}$, and the primitive translations $\mathbf{t}_j^H$ and $\mathbf{t}_j^{Hd}$ are assigned to Q_j and to $B_d Q_j B_d^{-1}$. We define generalized $\mathcal{R}(B_d)$ stars as follows: $\mathbf{S}_{ns}[\mathbf{t}_c|\mathcal{R}(B_d)] = \{\mathbf{t}_a \in \mathcal{T}|\mathbf{t}_a = Q_j\mathbf{t}_c + \mathbf{y}_j + \mathbf{t}_j^d\}$, where $\mathbf{v}_{jd}^{\sharp}$ define some shift of the origin, but $\mathbf{x}_j$, apart from $\mathbf{t}_j^d \in \mathcal{T}$, some non-trivial transformations. If we ignore these subtleties, it allows us to define representation domains $\Delta\mathbf{W}_{ns}[\mathcal{S}(B_d)] \subseteq \mathbf{W}[\mathcal{S}(B_d)]$ by taking from each $\mathcal{R}(B_d)$ star $\mathbf{S}_{ns}[\mathbf{t}_c|\mathcal{R}(B_d)]$ one and only one element. Thus, we arrive at

$$\mathcal{M} * (B_d|\mathbf{w}_d) * \mathcal{M} = \bigcup_{\mathbf{t}_c \in \Delta\mathbf{W}_{ns}[\mathcal{S}(B_d)] \cap \mathcal{T}} \mathcal{H} * (B_d|\mathbf{w}_d)(E|\mathbf{t}_c) * \mathcal{H}, \tag{24}$$

which looks identical to (21) but in fact differs essentially in the definition of the generalized $\mathcal{R}(B_d)$ star $\mathbf{S}_{ns}[\mathbf{t}_c|\mathcal{R}(B_d)]$ and their corresponding *representation domains* $\Delta\mathbf{W}_{ns}[\mathcal{S}(B_d)]$. Once the representation domains $\Delta\mathbf{W}_{ns}[\mathcal{S}(B_d)]$ are determined, the last step consists of combining (16) with (24) to arrive at

$$\mathcal{G} = \bigcup_{B_d \in \underline{\Delta\mathcal{P}}(\mathcal{R})} \bigcup_{\mathbf{t}_c \in \Delta\mathbf{W}_{ns}[\mathcal{S}(B_d)] \cap \mathcal{T}} \mathcal{H} * (B_d|\mathbf{w}_d)(E|\mathbf{t}_c) * \mathcal{H}, \tag{25}$$

which represents the desired double-coset decomposition of the superspace group $\mathcal{G}$ into a minimal number of $\mathcal{H}$ double cosets. As in the symmorphic case, we may summarize the procedure: In detail, one has to determine (i) the minimal set $\underline{\Delta\mathcal{P}}(\mathcal{R}) \subseteq \underline{\mathcal{P}}(\mathcal{R})$, (ii) the auxiliary translation groups $\mathcal{S}(B_d) = \mathcal{S} \uplus \mathcal{R}^{-1}\mathcal{S} \subseteq \mathcal{T}$, (iii) the Wigner–Seitz cells $\mathbf{W}[\mathcal{S}(B_d)] \subseteq \mathbf{W}(\mathcal{S})$, (iv) the $\mathcal{R}(B_d)$ stars $\mathbf{S}_{ns}[\mathbf{t}_c|\mathcal{R}(B_d)]$ and (v) the corresponding representation domains $\Delta\mathbf{W}_{ns}[\mathcal{S}(B_d)] \subseteq \mathbf{W}[\mathcal{S}(B_d)]$ in order to be able to write down the double-coset decompositions (25) where only in step (iv) does the non-symmorphic structure of the g subgroup enter essentially into the discussion.

2.6. *Decomposition of double cosets into left cosets*

The remaining task is to decompose the $\mathcal{H}$ double cosets $\mathcal{H} * (B_d|\mathbf{w}_d)(E|\mathbf{t}_c) * \mathcal{H}$ that occur in (22) and (25) into their corresponding left cosets $(B_l|\mathbf{w}_l)(E|\mathbf{t}_a) * \mathcal{H}$. This can be done simultaneously for both types of subgroups. The most natural strategy is use the decomposition of $\mathcal{H}$ into $\mathcal{N}_d$ left cosets, where the auxiliary subgroups $\mathcal{N}_d$ of $\mathcal{H}$ are determined by restricting in $\mathcal{H}$ the point group $\mathcal{R}$ to the corresponding intersection groups $\mathcal{R}(B_d)$ with $B_d \in \underline{\Delta\mathcal{P}}(\mathcal{R})$.

$$\mathcal{H} = \bigcup_{S_l \in \underline{\mathcal{R}}[\mathcal{R}(B_d)]} (S_l|\mathbf{z}_l) * \mathcal{N}_d. \tag{26}$$

This implies that when acting from the left on the coset $(B_d|\mathbf{w}_d)(E|\mathbf{t}_c) * \mathcal{H}$ in order to determine the distinct $\mathcal{H}$ left cosets, we take for the $\mathcal{H}$ space-group elements the sequential order $(S_l|\mathbf{z}_l)(E|\mathbf{s}_a)(R_j|\mathbf{z}_j)$, where $R_j = B_d Q_j B_d^{-1} \in \mathcal{R}(B_d)$ and $\mathbf{s}_a \in \mathcal{S}$, and finally $S_l \in \underline{\mathcal{R}}[\mathcal{R}(B_d)]$ is assumed. The idea is that $(R_j|\mathbf{z}_j)$ and likewise $(E|\mathbf{s}_a)$ do not change $(B_d|\mathbf{w}_d)$, whereas only the last step, namely the application of every $(S_l|\mathbf{w}_l)$ transforms $(B_d|\mathbf{w}_d)$ into different elements $(B_l|\mathbf{w}_l)$ mod $\mathcal{H}$.

The elements $(S_j|\mathbf{z}_j)(E|\mathbf{s}_a)(R_j|\mathbf{z}_j)$ are applied to the $\mathcal{H}$ left cosets $(B_d|\mathbf{w}_d)(E|\mathbf{t}_c) * \mathcal{H}$ in consecutive order. The first step consists of proving $(R_j|\mathbf{z}_j)(B_d|\mathbf{w}_d)(E|\mathbf{t}_c) * \mathcal{H} = (B_d|\mathbf{w}_d)(E|\hat{\mathbf{t}}_j) * \mathcal{H}$, where $R_j = B_d Q_j B_d^{-1} \in \mathcal{R}(B_d)$ has to be taken into account. A straightforward manipulation yields for the corresponding translations $\hat{\mathbf{t}}_j \in \mathcal{T}$ the expressions $\hat{\mathbf{t}}_j = Q_j \mathbf{t}_c + \mathbf{t}_j^d + \mathbf{y}_j$, which are in coincidence with the definition of the generalized $\mathcal{R}(B_d)$ stars.

To label for fixed $B_d \in \underline{\Delta\mathcal{P}}(\mathcal{R})$ and given $\mathbf{t}_c \in \Delta\mathbf{W}[\mathcal{S}(B_d)] \cap \mathcal{T}$, the translational part $\hat{\mathbf{t}}_j$ of the corresponding left-coset representatives that come from the application of $(B_d Q_j B_d^{-1}|\mathbf{z}_j)$ with varying $Q_j \in \mathcal{R}(B_d)$, we proceed as follows: For a given $\mathbf{t}_c \in \Delta\mathbf{W}[\mathcal{S}(B_d)] \cap \mathcal{T}$, we construct its corresponding *stabilizer group* $\mathcal{R}(\mathbf{t}_c|B_d) = \{Q_j \in \mathcal{R}(B_d) | Q_j \mathbf{t}_c \equiv \mathbf{t}_c\}$ and likewise determine a set $\{F_j\}$ of left-coset representatives of $\mathcal{R}(B_d)$ with respect to $\mathcal{R}(\mathbf{t}_c|B_d)$. Accordingly, we define for $\mathbf{t}_c$ the elements of the corresponding $\mathcal{R}(B_d)$ orbits according to the following conventions: $\hat{\mathbf{t}}_{cj} = F_j \mathbf{t}_c + \mathbf{t}_j^d + \mathbf{y}_j$, where $F_j \in \mathcal{R}(B_d) : \mathcal{R}(\mathbf{t}_c|B_d)$ is assumed. Thus, for fixed B_d, fixed $\mathbf{t}_c$ and varying Q_j, the number of different $\mathcal{H}$ left cosets coincides with the order $|\mathbf{S}[\mathbf{t}_c|\mathcal{R}(B_d)]|$ of the corresponding $\mathcal{R}(B_d)$ star.

The second step consists of applying $(E|\mathbf{s}_a)$ to the left cosets $(B_d|\mathbf{w}_d)(E|\hat{\mathbf{t}}_{cj}) * \mathcal{H}$, where in particular $\mathbf{t}_{cj} \in \mathbf{S}[\mathbf{t}_c|\mathcal{R}(B_d)]$ and $\mathbf{s}_a \in \mathcal{S}$ is assumed. A straightforward application of the composition law of $\mathcal{G}$ yields $(E|\mathbf{s}_a)(B_d|\mathbf{w}_d)(E|\hat{\mathbf{t}}_{cj}) = (B_d|\mathbf{w}_d)(E|\hat{\mathbf{t}}_{cj} + B_d^{-1}\mathbf{s}_a)$. Accordingly, if the translations $\mathbf{s}_a = \mathbf{s}_k \in \mathcal{S}$ are chosen such that $B_d^{-1}\mathbf{s}_k = \mathbf{s}_k^\sharp \in \mathcal{S}(B_d) : \mathcal{S}$ are the (left) coset representatives of $\mathcal{S}(B_d)$ with respect to $\mathcal{S}$, then

$$(E|\mathbf{s}_k)(B_d|\mathbf{w}_d)(E|\hat{\mathbf{t}}_{cj}) * \mathcal{H} = (B_d|\mathbf{w}_d)(E|\hat{\mathbf{t}}_{cj} + \mathbf{s}_k^\sharp) * \mathcal{H} \tag{27}$$

defines additional mutually disjoint $\mathcal{H}$ left cosets that are contained in the original $\mathcal{H}$ double coset $\mathcal{H} * (B_d|\mathbf{w}_d)(E|\mathbf{t}_c) * \mathcal{H}$. Thus, for fixed $\hat{\mathbf{t}}_{cj} \in \mathbf{S}[\mathbf{t}_c|\mathcal{R}(B_d)]$, the number of different $\mathcal{H}$ left cosets coincides with $|\mathcal{S}(B_d) : \mathcal{S}|$, which is the index of $\mathcal{S}$ in $\mathcal{S}(B_d)$.

The final step consists of applying the left-coset representatives $(S_l|\mathbf{z}_l)$ to the left cosets $(B_d|\mathbf{w}_d)(E|\hat{\mathbf{t}}_{cj} + \mathbf{s}_k^\sharp) * \mathcal{H}$, where $S_l \in \underline{\mathcal{R}}[\mathcal{R}(B_d)]$, in order to determine the remaining associated $\mathcal{H}$ left cosets. We adopt the conventions $R_l = S_l B_d$ in order to fix the left-coset representatives that refer to $\underline{\Delta\mathcal{P}}(\mathcal{R})$. Again, simple manipulations yield the following identities: $(S_l|\mathbf{z}_l)(B_d|\mathbf{w}_d)(E|\hat{\mathbf{t}}_{cj} + \mathbf{s}_k^\sharp) = (R_l|\mathbf{w}_l)(E|\hat{\mathbf{t}}_{cj} + \mathbf{s}_k^\sharp + \mathbf{T}_l)$ with $\mathbf{T}_l = B_d^{-1}[S_l^{-1}(\mathbf{t}_{ld} + \mathbf{t}_l^H)]$ as special translations and where $\mathbf{t}_{ld} = \mathbf{w}_l + R_l \mathbf{w}_d - \mathbf{w}_{ld} \in \mathcal{T}$ has to be taken into account. What remains to be checked is whether the special translations $\mathbf{T}_l$ can be re-absorbed or contribute non-trivially to the translational part of the left-coset representatives. Apart from this technical detail, we arrive at the final formulae

$$\mathcal{H} * (B_d|\mathbf{w}_d)(E|\mathbf{t}_c) * \mathcal{H} = \bigcup_{lkj} (R_l|\mathbf{w}_l)(E|\hat{\mathbf{t}}_{cj} + \mathbf{s}_k^\sharp + \mathbf{T}_l) * \mathcal{H} \tag{28}$$

$$N(B_d|\mathbf{t}_c) = |\mathcal{R} : \mathcal{R}(B_d)||\mathcal{S}(B_d) : \mathcal{S}||\mathcal{R}(B_d) : \mathcal{R}(\mathbf{t}_c|B_d)|, \tag{29}$$

where $N(B_d|\mathbf{t}_c)$ denotes the number of $\mathcal{H}$ left cosets that are contained in the corresponding $\mathcal{H}$ double coset $\mathcal{H} * (B_d|\mathbf{w}_d)(E|\mathbf{t}_c) * \mathcal{H}$. Accordingly, the non-trivial by-product of our analysis is that we can give a closed expression, namely (29), for the number of $\mathcal{H}$ left cosets that are contained in $\mathcal{H}$ double cosets without referring to the Frobenius theorem.

3. Physical applications

3.1. *Left-coset decompositions and single domain states*

Let us consider a structural phase transition accompanied by a symmetry reduction. Then, the space group $\mathcal{H}$ of the ordered (distorted) phase is a proper subgroup of the space group $\mathcal{G}$ of the disordered (parent) phase, $\mathcal{H} \subset \mathcal{G}$. Owing to this symmetry reduction, the ordered phase is degenerate: it can appear in several crystallographically equivalent (with respect to $\mathcal{G}$) homogeneous ordered structures that differ only in orientation and/or position with respect to the coordinate system of the disordered phase. These crystallographically equivalent ordered structures are called *single-domain states* (SDS's) or *variants* (Van Tendeloo & Amelinckx, 1974), and will be denoted $\mathbb{S}_1, \mathbb{S}_2, \ldots, \mathbb{S}_n$.

The set of all SDS's forms a $\mathcal{G}$ orbit (we shall further use the term orbit for $\mathcal{G}$ orbit unless mentioned otherwise), $\mathcal{G} \diamond \mathbb{S}_1 = \{\mathbb{S}_1, \mathbb{S}_2, \ldots, \mathbb{S}_n\}$. This means that for any two SDS's $\mathbb{S}_i, \mathbb{S}_j$ there exists an operation $G \in \mathcal{G}$ such that $\mathbb{S}_j = G \diamond \mathbb{S}_i$. The *stabilizer* (isotropy group) $\mathrm{Stab}_G(\mathbb{S}_j)$ of $\mathbb{S}_j$ in $\mathcal{G}$ is the maximal subgroup of $\mathcal{G}$ that leaves $\mathbb{S}_j$ invariant,

$$\mathcal{H}_j = \mathrm{Stab}_G(\mathbb{S}_j) = \{G \in \mathcal{G} | G \diamond \mathbb{S}_j = \mathbb{S}_j\}, j = 1, 2, \ldots, n. \tag{30}$$

The space group $\mathcal{H}_j$ describes the symmetry of the single-domain state $\mathbb{S}_j$. For simplicity and better correspondence with §2, we put $\mathcal{H}_1 \equiv \mathcal{H}$, *i.e.* we choose for $\mathbb{S}_1$ a SDS for which $\mathcal{H}$ is the stabilizer.

There is one-to-one correspondence between the left cosets of $\mathcal{H}$ in the decomposition [compare with (3), now the coset representatives are endowed with subscripts]

$$\mathcal{G} = \bigcup_{G_l \in \underline{\mathcal{G}}(\mathcal{H})} G_l * \mathcal{H} \tag{31}$$

and the single-domain states of the orbit $\mathcal{G} \diamond \mathbb{S}_1$,

$$\mathcal{G} \diamond \mathbb{S}_1 = \{\mathbb{S}_1, \mathbb{S}_2, , \mathbb{S}_n\} \tag{32}$$

with $\mathbb{S}_l = G_l \diamond \mathbb{S}_1$ where G_l, $l = 1, 2, \ldots, n$, are the representatives of the $\mathcal{H}$ left cosets in the decomposition (31) and where for the representative G_1 of the first left coset the identity operation is chosen. The stabilizer of the domain state $\mathbb{S}_l = G_l \diamond \mathbb{S}_1$ is equal to $\mathcal{H}_l = G_l * H * G_l^{-1}$. The number n of SDS's equals the index of $\mathcal{H}$ in $\mathcal{G}$, $n = |\mathcal{G} : \mathcal{H}|$ (see *e.g.* Janovec, 1972; Van Tendeloo & Amelinckx, 1974).

In a general case, $\mathcal{H}$ is a g subgroup of $\mathcal{G}$. Then there always exists an intermediate group $\mathcal{M}$ that is a t subgroup of $\mathcal{G}$ and k supergroup of $\mathcal{H}$ (see §2.5) and the decomposition of $\mathcal{G}$ into left cosets of $\mathcal{H}$ can be performed in two steps: (i) The decomposition of $\mathcal{G}$ into m left cosets of $\mathcal{M}$ [see (13)], $m = |\mathcal{G} : \mathcal{M}| = |\mathcal{P}| : |\mathcal{R}|$, where $\mathcal{P}$ and $\mathcal{R}$ are point groups of $\mathcal{G}$ and $\mathcal{M}$, respectively, and $|\mathcal{P}|$ and $|\mathcal{R}|$ are the order of $\mathcal{P}$ and $\mathcal{R}$, respectively. (ii) The decomposition of $\mathcal{M}$ into d left cosets of $\mathcal{H}$ [see (14)], $d = |\mathcal{M} : \mathcal{H}| = |\mathcal{T} : \mathcal{S}| = |\mathbb{N}| = V_S : V_T$, where $\mathcal{T}$ and $\mathcal{S}$ are translation groups of $\mathcal{M}$ (and of $\mathcal{G}$) and $\mathcal{H}$, respectively, $|\mathbb{N}|$ is the determinant of the matrix $\mathbb{N}$ [see (2)] and V_S and V_T are the volumes of the primitive unit cells of $\mathcal{S}$ and $\mathcal{T}$, respectively.

The set of all $n = md$ left cosets of $\mathcal{H}$ can in this way be partitioned into m subsets each consisting of $d\,\mathcal{H}$ left cosets and, correspondingly, the n single-domain states of the orbit $\mathcal{G} \diamond \mathbb{S}_1$ can be divided into m subsets, each of which comprises d SDS's. From (13) and (14), it follows that the SDS's of the first subset $\{\mathbb{S}_1, \mathbb{S}_2, \ldots, \mathbb{S}_d\}$ can be related by pure translations $(E|\mathbf{t}_c)$ from the set $\mathbf{W}(\mathcal{S}) \cap \mathcal{T}$, which can be identified with translations lost at the transition from $\mathcal{G}$ to $\mathcal{H}$. Every other subset of SDS's consists of other d SDS's that can again be related by (generally other) translations lost at the transition. Thus, each subset comprises all SDS's with the same macroscopic tensorial properties. The stabilizer of the first subset is equal to the group $\mathcal{M}$. From (13), one can deduce that different subsets are related by operations containing rotations or rotoinversions and possess, therefore, different tensor properties. The subsets thus correspond to *ferroic* (*orientational*, *tensorial*) *single-domain states* or *orientational variants*. The number d can be called *translational degeneracy of ferroic domain states*. This partitioning enables one to introduce a convenient labelling of SDS's: The subscript $l = (j, a)$ of a SDS $\mathbb{S}_l = \mathbb{S}_{(j,a)}$ consists of two numbers: the first one, $j = 1, 2, \ldots, m$, specifies the ferroic SDS, the second one, $a = 1, 2, \ldots, d$, specifies the position of each SDS within the subset. This label can also be written in a short form, namely j_a. Other divisions of SDS's, *e.g.* according to their tensor properties, can be performed and is discussed elsewhere (see *e.g.* Janovec, Litvin & Fuksa, 1995; Fuksa & Janovec, 1995).

3.2. *Double cosets and orbits of domain pairs*

Structures of SDS's can coexist in a domain structure that consists of domains (connected regions with homogeneous bulk structures of SDS's) and domain walls (boundaries between neighbouring domains). To study possible relations between structures of two domains, a concept of a pair of domain states, domain pair for short, has been introduced (Janovec, 1972).

An *ordered domain pair* (ODP) consists of the first SDS $\mathbb{S}_i$ and a second SDS $\mathbb{S}_j$, both from the same orbit $\mathcal{G} \diamond \mathbb{S}_1$; such an ODP will be denoted $(\mathbb{S}_i, \mathbb{S}_j)$. An ODP with a reversed order of SDS's is called a *transposed ordered domain pair*, $(\mathbb{S}_j, \mathbb{S}_i) = (\mathbb{S}_i, \mathbb{S}_j)^T$. An ODP $(\mathbb{S}_i, \mathbb{S}_j)$ is unequal to the transposed ODP $(\mathbb{S}_j, \mathbb{S}_i)$ unless $i = j$ (trivial ODP). Two ODP's $(\mathbb{S}_i, \mathbb{S}_j)$ and $(\mathbb{S}_k, \mathbb{S}_l)$ are *crystallographically equivalent* with respect to $\mathcal{G}$ if an operation $G \in \mathcal{G}$ exists such that $(\mathbb{S}_k, \mathbb{S}_l) = (G \diamond \mathbb{S}_i, G \diamond \mathbb{S}_j)$. The ODP's can be classified in the following manner. An ODP $(\mathbb{S}_i, \mathbb{S}_j)$ is *transposable* (*ambivalent*) if it is crystallographically equivalent with the transposed ODP $(\mathbb{S}_j, \mathbb{S}_i)$, *i.e.* if such an operation $G \in \mathcal{G}$ exists that $(\mathbb{S}_j, \mathbb{S}_i) = (G \diamond \mathbb{S}_i, G \diamond \mathbb{S}_j)$. If this condition cannot be fulfilled, the ODP is *non-transposable (polar)*. Then the ODP and the transposed ODP are called *complementary non-transposable ODP's*.

The crystallographical equivalence divides the set of all ODP's that can be formed from $\mathcal{G} \diamond \mathbb{S}_1$ into orbits (classes of crystallographically equivalent ODP's) $\mathcal{G} \diamond (\mathbb{S}_i, \mathbb{S}_j)$. The representative ODP's of the orbit $\mathcal{G} \diamond (\mathbb{S}_i, \mathbb{S}_j)$ can always be 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 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.

Recall that the group $\mathcal{G}$ can always be decomposed into disjoint double cosets of its subgroup $\mathcal{H}$ [compare with (4)]:

$$\mathcal{G} = \bigcup_{G_l \in \underline{\Delta\mathcal{G}}(\mathcal{H})} \mathcal{H} * G_l * \mathcal{H}, \quad l = 1, \ldots, q, \; q \leq n. \quad (33)$$

An inverse $(\mathcal{H} * G_l * \mathcal{H})^{-1} = \mathcal{H} * G_l^{-1} * \mathcal{H}$ of the double coset $\mathcal{H} * G_l * \mathcal{H}$ is either identical with $\mathcal{H} * G_l * \mathcal{H}$ or forms another double coset disjoint with $\mathcal{H} * G_l * \mathcal{H}$. We shall call the former type of double cosets *self-inverse* (*ambivalent*) *double cosets* and disjoint double cosets $\mathcal{H} * G_l * \mathcal{H}$ and $\mathcal{H} * G_l^{-1} * \mathcal{H}$ *complementary polar double cosets*. Then, a relation between double cosets $\mathcal{H} * G_l * \mathcal{H}$ of the decomposition (33) and all possible orbits of ODP's formed from the orbit $\mathcal{G} \diamond \mathbb{S}_1$ is expressed by the following theorem (Janovec, 1972):

Theorem: There is a one-to-one correspondence between self-inverse (ambivalent) and complementary polar double cosets of the decomposition (33) and transposable (ambivalent) and complementary non-transposable orbits of ODP's. The representative ODP's of these orbits can be found in the form $(\mathbb{S}_1, G_l \diamond \mathbb{S}_1)$, where $G_l \in \mathcal{G}$ are representatives of the double-coset decomposition (33).

This theorem enables one to find from the double-coset decomposition (33) the number q of ODP orbits, their type (transposable or complementary non-transposable) and the representative ODP's for all orbits of ODP's. The ODP's from different 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 $G_l \in \mathcal{G}$ their structures can be brought into coincidence. The division of ODP's into orbits thus reduces the task of examining $n(n-1)$ ODP's to a considerably lower (especially for large n) number q of representative ODP's. Properties significant for the whole orbit of ODP's [*e.g.* tensor distinction of domains (Janovec, Litvin & Fuksa, 1995)] 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 a Lifshitz invariant is the existence of a complementary double coset in the decomposition (33) (Janovec & Dvořák, 1986). Finally, we note that in the described analysis of orbits of ODP's the only input data are just two space groups $\mathcal{H} \subset \mathcal{G}$ and no further information, *e.g.* crystal structures of both phases, is needed.

3.3. *Example*

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 the $2H$ polytype of $TaSe_2$ (Dvořák & Janovec, 1985). The ordered phase has $\mathcal{G} = P6_3/mmc$ (No. 194) symmetry and the disordered commensurate phase exhibits $\mathcal{H} = Cmcm$ (No. 63) symmetry with tripled primitive translations along two hexagonal primitive lattice translations, hence

$$\mathbb{N} = \begin{bmatrix} 3 & 0 & 0 \\ 0 & 3 & 0 \\ 0 & 0 & 1 \end{bmatrix}. \quad (34)$$

The group $\mathcal{H}$ is, therefore, a g subgroup with reduced point-group symmetry $\mathcal{R} \subset \mathcal{P}$ and reduced translation symmetry $\mathcal{S} \subset \mathcal{T}$. There are $m = |6/mmm : mmm| = 24 : 8 = 3$ ferroic (orientational) SDS's and within each of them $d = |\mathbb{N}| = 9$ SDS's related by lost translations may exist. Thus, in all there are $n = 3.9 = 27$ SDS's. We shall perform the coset resolutions of $\mathcal{G}$ with respect to $\mathcal{H}$ following the procedure consisting in three steps described in §2.5 and 2.6.

Step 1: Determination of the *translationsgleiche* subgroup $\mathcal{M}$ of $\mathcal{G}$ and double-coset decomposition of $\mathcal{G}$ with respect to $\mathcal{M}$. In Hahn (1992), we find that $\mathcal{M} = Cmcm$ (No. 64) with *primitive* lattice translations $\mathbf{t}_1, \mathbf{t}_2, \mathbf{t}_3$ identical with that of the group $\mathcal{G}$. The double-coset decomposition of $\mathcal{G}$ with respect to $\mathcal{M}$ is determined by double-coset decomposition of the corresponding point group $\mathcal{P}$ with respect to $\mathcal{R}$. Since $|\mathcal{P} : \mathcal{R}| = 3$, $\mathcal{P}$ consists of three left cosets of $\mathcal{R}$. We choose the operation 6 (rotation of 60° around the sixfold axis) as the representative of the second left coset. The intersection group $\mathcal{R}(6) = 2_z/m_z$, hence from the Frobenius theorem it follows that the non-trivial double coset comprises two left cosets and the rotation 6 can be chosen as the representative of this double coset. The corresponding operation of the space group $\mathcal{G}$ is $(6|\frac{1}{2}\mathbf{t}_3)$ and the decomposition of $\mathcal{G}$ is

$$\mathcal{G} = \mathcal{M} \cup \mathcal{M} * (6|\tfrac{1}{2}\mathbf{t}_3) * \mathcal{M}. \quad (35)$$

Step 2: Decomposition of $\mathcal{M}$ double cosets into $\mathcal{H}$ double cosets. The left coset decomposition of $\mathcal{M}$ with respect to $\mathcal{H}$ is

$$\mathcal{M} = \bigcup_{n_1, n_2 = 0,1,2} (1|n_1\mathbf{t}_1 + n_2\mathbf{t}_2) * \mathcal{H}. \quad (36)$$

The *union* translation groups [defined by (19)] are $\mathcal{S}(1) = \mathcal{S}(6) = \mathcal{S}$ since the point-group operation 6 leaves the sublattice $\mathcal{S}$ invariant. The next task consists of determining generalized $\mathbf{S}[\mathbf{t}_c|\mathcal{R}(B_d)]$ stars, which are abbreviated by $\mathbf{S}(\mathbf{t}_c|B_d)$:

$$\mathbf{S}(\mathbf{t}_c|B_d) = \{\mathbf{t}_a \in \mathcal{T} | \mathbf{t}_a = Q_k\mathbf{t}_c + \mathbf{y}_k + \mathbf{t}_k^d\}, \quad (37)$$

where $Q_k \in \mathcal{R}(B_d)$ and the translations $\mathbf{t}_c$ are elements of the corresponding Wigner–Seitz cell $\mathbf{W}[\mathcal{S}(B_d)]$ that can be likewise replaced by corresponding primitive cell $\mathbf{E}[\mathcal{S}(B_d)]$. One can prove that $\mathbf{y}_k = \mathbf{t}_k^d = \mathbf{0}$ for all $Q_k \in \mathcal{R}(B_d)$. Simple manipulations yield

$$\mathbf{S}(\mathbf{0}|1) = \mathbf{S}(\mathbf{0}|6) = \{\mathbf{0}\} \tag{38}$$
$$\mathbf{S}(\mathbf{t}_1|1) = \{\mathbf{t}_1, 2\mathbf{t}_1, \mathbf{t}_1 + \mathbf{t}_2, 2\mathbf{t}_1 + \mathbf{t}_2\} \tag{39}$$
$$\mathbf{S}(\mathbf{t}_2|1) = \mathbf{S}(\mathbf{t}_2|6) = \{\mathbf{t}_2, 2\mathbf{t}_2\} \tag{40}$$
$$\mathbf{S}(\mathbf{t}_1 + 2\mathbf{t}_2|1) = \mathbf{S}(\mathbf{t}_1 + 2\mathbf{t}_2|6) = \{\mathbf{t}_1 + 2\mathbf{t}_2, 2\mathbf{t}_1 + \mathbf{t}_2\} \tag{41}$$
$$\mathbf{S}(\mathbf{t}_1 + \mathbf{t}_2|6) = \{\mathbf{t}_1 + \mathbf{t}_2, 2\mathbf{t}_1 + 2\mathbf{t}_2\}. \tag{42}$$

(To adhere more closely to the international symbols, we have replaced in this example the symbol E of the identity operation by 1.) We can choose as representation domains

$$\Delta\mathbf{W}_{ns}[\mathcal{S}(1)] = \{\mathbf{0}, \mathbf{t}_1, \mathbf{t}_2, \mathbf{t}_1 + 2\mathbf{t}_2\} \tag{43}$$
$$\Delta\mathbf{W}_{ns}[\mathcal{S}(6)] = \{\mathbf{0}, \mathbf{t}_1, \mathbf{t}_2, \mathbf{t}_1 + \mathbf{t}_2, \mathbf{t}_1 + 2\mathbf{t}_2\}, \tag{44}$$

which yields to the following double-coset decompositions:

$$\mathcal{M} = \mathcal{H} \cup \mathcal{H} * (1|\mathbf{t}_1) * \mathcal{H} \cup \mathcal{H} * (1|\mathbf{t}_2) * \mathcal{H} \cup \mathcal{H} * (1|\mathbf{t}_1 + 2\mathbf{t}_2) * \mathcal{H} \tag{45}$$
$$\begin{aligned}\mathcal{M} * 6 * \mathcal{M} = {} & \mathcal{H} * (6|\tfrac{1}{2}\mathbf{t}_3) * \mathcal{H} \cup \mathcal{H} * (6|\tfrac{1}{2}\mathbf{t}_3 + \mathbf{t}_1) * \mathcal{H} \\ & \cup \mathcal{H} * (6|\tfrac{1}{2}\mathbf{t}_3 + \mathbf{t}_2) * \mathcal{H} \cup \\ & \mathcal{H} * (6|\tfrac{1}{2}\mathbf{t}_3 + \mathbf{t}_1 + \mathbf{t}_2) * \mathcal{H} \cup \\ & \mathcal{H} * (6|\tfrac{1}{2}\mathbf{t}_3 + \mathbf{t}_1 + 2\mathbf{t}_2) * \mathcal{H}.\end{aligned} \tag{46}$$

Step 3: Decomposition of the $\mathcal{H}$ double cosets into $\mathcal{H}$ left cosets (see §2.6). First, we determine the auxiliary subgroups $\mathcal{N}_d$ that appear in the decomposition (26). For $B_d = 1$, we get $\mathcal{N}_d = \mathcal{H}$. For $B_d = 6$, the corresponding group $\mathcal{N}_d$ is the *translationsgleiche* subgroup of $\mathcal{H}$ whose point group equals $\mathcal{R}(6) = 2_z/m_z$ and the decomposition (26) is

$$\mathcal{H} = \mathcal{N}_d \cup (2_{10}|\mathbf{0}) * \mathcal{N}_d, \tag{47}$$

where the twofold axis 2_{10} is parallel to $\mathbf{t}_1$. The second task consists of determining the stabilizer groups

$$\mathcal{R}(\mathbf{t}_c|B_d) = \{Q_k \in \mathcal{R}(B_d)|Q_k\mathbf{t}_c \equiv \mathbf{t}_c\}. \tag{48}$$

Straightforward calculations yield

$$\mathcal{R}(\mathbf{0}|1) = \mathcal{R} \tag{49}$$
$$\mathcal{R}(\mathbf{0}|6) = \mathcal{R}(6) \tag{50}$$
$$\begin{aligned}\mathcal{R}(\mathbf{t}_1|1) &= \mathcal{R}(\mathbf{t}_1|6) = \mathcal{R}(\mathbf{t}_2|6) = \mathcal{R}(\mathbf{t}_1 + \mathbf{t}_2|6) \\ &= \mathcal{R}(\mathbf{t}_1 + 2\mathbf{t}_2|6) = \{1, m_z\}\end{aligned} \tag{51}$$
$$\mathcal{R}(\mathbf{t}_2|1) = \{1, 2_{01}, m_z, m_{\bar{1}0}\} \tag{52}$$
$$\mathcal{R}(\mathbf{t}_1 + 2\mathbf{t}_2|1) = \{1, 2_{2\bar{1}}, m_z, m_{\bar{1}2}\}, \tag{53}$$

where the twofold axes along the secondary and tertiary symmetry directions are specified by the first two integer components of a vector along the symmetry axis and mirror planes perpendicular to the secondary and tertiary directions are specified by the first two Miller indices. These stabilizer groups provide the decompositions of the $\mathcal{H}$ double cosets into the $\mathcal{H}$ left cosets.

Table 1. *Decompositions of the $\mathcal{H}$ double cosets into $\mathcal{H}$ left cosets*

Representatives of left cosets	Type
$(1\|\mathbf{0})(1\|\mathbf{0})$	Self-inverse
$(1\|\mathbf{0})(1\|\mathbf{t}_2)$, $(1\|\mathbf{0})(1\|2\mathbf{t}_2)$	Self-inverse
$(1\|\mathbf{0})(1\|\mathbf{t}_1)$, $(1\|\mathbf{0})(1\|\mathbf{t}_1 + \mathbf{t}_2)$, $(1\|\mathbf{0})(1\|2\mathbf{t}_1)$, $(1\|\mathbf{0})(1\|2\mathbf{t}_1 + 2\mathbf{t}_2)$	Self-inverse
$(1\|\mathbf{0})(1\|\mathbf{t}_1 + 2\mathbf{t}_2)$, $(1\|\mathbf{0})(1\|2\mathbf{t}_1 + \mathbf{t}_2)$	Self-inverse
$(6\|\frac{1}{2}\mathbf{t}_3)(1\|\mathbf{0})$, $(3\|\mathbf{0})(1\|\mathbf{0})$	Self-inverse
$(6\|\frac{1}{2}\mathbf{t}_3)(1\|\mathbf{t}_1)$, $(6\|\frac{1}{2}\mathbf{t}_3)(1\|2\mathbf{t}_1)$, $(3\|\mathbf{0})(1\|\mathbf{t}_1 + \mathbf{t}_2)$, $(3\|\mathbf{0})(1\|2\mathbf{t}_1 + 2\mathbf{t}_2)$	Self-inverse
$(6\|\frac{1}{2}\mathbf{t}_3)(1\|\mathbf{t}_1 + 2\mathbf{t}_2)$, $(6\|\frac{1}{2}\mathbf{t}_3)(1\|2\mathbf{t}_1 + \mathbf{t}_2)$, $(3\|\mathbf{0})(1\|\mathbf{t}_1 + 2\mathbf{t}_2)$, $(3\|\mathbf{0})(1\|2\mathbf{t}_1 + \mathbf{t}_2)$	Self-inverse
$(6\|\frac{1}{2}\mathbf{t}_3)(1\|\mathbf{t}_2)$, $(6\|\frac{1}{2}\mathbf{t}_3)(1\|2\mathbf{t}_2)$, $(3\|\mathbf{0})(1\|\mathbf{t}_2)$, $(3\|\mathbf{0})(1\|2\mathbf{t}_2)$	Complementary polar
$(6\|\frac{1}{2}\mathbf{t}_3)(1\|\mathbf{t}_1 + \mathbf{t}_2)$, $(6\|\frac{1}{2}\mathbf{t}_3)(1\|2\mathbf{t}_1 + 2\mathbf{t}_2)$, $(3\|\mathbf{0})(1\|\mathbf{t}_1)$, $(3\|\mathbf{0})(1\|2\mathbf{t}_1)$	Complementary polar

The results are summarized in Table 1, where each row contains representative operations of all $\mathcal{H}$ left cosets that form one $\mathcal{H}$ double coset. The representatives are expressed as products of two operations: The first one is the representative $(B_d|\mathbf{w}_d)$ of the $\mathcal{M}$ left coset in the decomposition of $\mathcal{G}$ [see (13)]. There are three $\mathcal{M}$ left cosets [with the representatives $(1|\mathbf{0})$, $(6|\frac{1}{2}\mathbf{t}_3)$, $(3|\mathbf{0})$], which correspond to the three ferroic (orientational) domain states. The second operation of the product is the representative of the $\mathcal{H}$ left coset in the decomposition of $\mathcal{M}$ [see (14)]. There are nine such $\mathcal{H}$ left cosets [with representatives given in (36)] that correspond to possible locations of the ordered structure in each ferroic domain state. The last column specifies the type of the double coset [self-inverse (ambivalent) or complementary polar].

We see that six non-trivial double cosets are self-inverse (ambivalent), the last two are complementary polar double cosets. Thus, $27 \times 26 = 702$ non-trivial ODP's are partitioned into eight orbits and the representatives of these orbits are samples of all significantly different relations between two SDS's.

Complementary polar double cosets are worthy of further attention since they indicate the possible appearance of incommensurate phases between parent and ordered phases. More detailed analysis (Janovec & Dvořák, 1985) has shown that one of these polar double cosets can generate 54 symmetry-equivalent coherent domain walls with negative energy; from these walls, 9 different symmetry-equivalent incommensurate stripe phases, called block states, can be formed. These block states have equal energy and can, therefore, coexist in the form of blocks that are similar to domains. Rather complicated incommensurate structures consisting of such blocks were observed by electron microscopy (Chen, Gibson & Fleming, 1982).

Finally, we summarize in tabular form the present example together with two other examples in order to demonstrate the obvious importance of software support (Davies, Dirl, Zeiner & Janovec, 1993). Further

Table 2. *Some comparative details of three examples*

Formula	$\mathcal{G}$	$\mathcal{H}$	$\mathbb{N}$	d	m	$n = dm$	$n(n-1)$	$q-1$
$TaSe_2$	$P6_3/mmc$ (No. 194)	$Cmcm$ (No. 63)	$\begin{bmatrix} 3 & 0 & 0 \\ 0 & 3 & 0 \\ 0 & 0 & 1 \end{bmatrix}$	9	3	27	702	8 (1)
Au_5Mn_2	$Fm\bar{3}m$ (No. 225)	$C2/m$ (No. 12)	$\begin{bmatrix} 1 & 2 & 0 \\ -2 & 3 & 0 \\ 0 & 0 & 1 \end{bmatrix}$	7	12	84	6972	9 (1)
IF_7	$Im\bar{3}m$ (No. 229)	$Aba2$ (No. 41)	$\begin{bmatrix} 2 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 2 \end{bmatrix}$	8	12	96	9120	30 (3)

properties of domain pairs are discussed in Fuksa & Janovec (1995), Janovec, Litvin & Fuksa (1995) and Davies, Dirl, Janovec & Zikmund (1997).

Recall that the entries $n(n-1)$ in Table 2 give the number of the non-trivial ODP's, $q-1$ the number of orbits of ODP's, and the numbers in brackets the pairs of non-self-inverse double cosets. The first example is described in detail in Dvořák & Janovec (1985), the second in Van Tendeloo, Wolf & Amelinckx (1977) and the third one in Tomaszewski (1992).

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