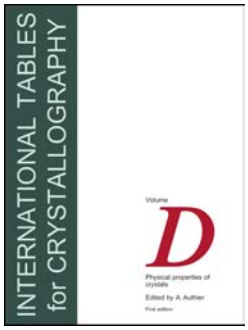

GI ⋆ KoBo-1

Group Informatics (release 1)

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Contents

Introduction

We strongly recommend that the reader prints this document and familiarizes themselves with individual points of the program by following this manual while using the program. It is assumed that the reader has an elementary knowledge of group theory but the basic concepts are defined and fundamental statements are given in the following text, as a rule without proofs. The program is designed for crystallographers and material physicists, with special emphasis on structural phase transitions and the analysis of domains, domain pairs and domain twins.

The information is structured in the following manner:

1. Information relevant to geometric classes.
2. Information relevant to specific groups of these classes.
3. Information relevant to symmetry descents (group–subgroup relations).
4. Information relevant to domain pairs.

The program provides general information of a group-theoretical nature about the crystallographic point groups and their representations such as class structure, class multiplication, character tables and Kronecker products of irreducible representations. An explicit and standardized form of irreducible representations (ireps) is used throughout as is appropriate for their use in the theory of phase transitions and related problems. The application of ireps is facilitated by the use of so-called "typical variables", which represent variables of all possible transformation properties under the action of crystallographic groups. The idea is simple and similar to the *"symbolic method"* of the old invariant theory (Weitzenböck, 1923). Tables of Clebsch–Gordan products are presented which enable the calculation of "tensorial" and "polynomial covariants", where the word "covariant", used with this meaning for the first time by Weyl (1946), replaces the more customary terms *"symmetry-adapted bases"* or *"form-invariant bases"*. Tables of tensorial covariants and of the "extended integrity bases" are provided, which form a versatile basis for calculation of tensor characteristics of domains as well as of various interactions.

The central part of the program contains extensive information about all possible symmetry descents within the classical crystallographic point groups. This information is given in a standardized form; the set of subgroups of each crystallographic group in a standard orientation is displayed in the form of the "lattice" of its subgroups, which serves as a menu for the choice of descents. For each symmetry descent the form of tensors up to fourth rank for the parent group is given and each is followed by information about onsetting components of these tensors in the first domain state. "Principal tensor parameters" which transform like the *"primary"* (*"proper"*, *"full"*) order parameter of an equitranslational transition and "secondary" (*"improper"*, *"partial"*) tensor parameters are distinguished in this description. The principal parameters can be considered in a certain sense as the "cause" of the symmetry descent while secondary parameters are its "consequence". For each symmetry descent a list of polynomials in typical variables is given which serves for constructing the correct form of the Landau potential, invariant under the parent symmetry. The list contains four items:

(i) Integrity bases: Polynomials in components of the primary order parameter from which the main part of the Landau potential is constructed as an invariant function in these components.
(ii) Faint interactions: Coupling of secondary order parameters with the primary parameter.
(iii) Electric switching interactions: Coupling of all onsetting parameters with an external electric field.
(iv) Elastic switching interactions: Coupling of all onsetting parameters with an external stress.

The tables of symmetry descents provide the background for a complete tensorial analysis of nonmagnetic "ferroic" phase transitions including tensor distinction of domain states. In the case of "completely transposable pairs", the distinction of two domain states is clearly seen directly from tables. More general consideration is possible with the use of the method of so-called "Conversion equations" which has been developed during the preparation of this software (Kopský, 2001*b*,*c*,*d*; Kopský & Litvin, 2001). For each symmetry descent information is also provided about the decomposition of the parent group into left, right and double cosets of the ferroic group and about normalizers of this group in the parent group.

This is equivalent to a complete analysis of tensor properties of domain states in "equitranslational" phase transitions where only ferroic domains appear ("antiphase" or "translational" domains are absent). The results are, however, also partially applicable to non-equitranslational ferroic transitions.

To facilitate the consideration of equitranslational phase transitions, the program is supplemented by an option which converts the lattices of subgroups of crystallographic point groups into the lattices of equitranslational subgroups of the space groups.

This manual concludes with seven tabular appendices. Appendix A compares various notations of point-group operations with the standard one used here. In Appendix B the embellished Schönflies and Hermann–Mauguin symbols of oriented groups as used in the software are specified. Isomorphisms which define ireps of groups are given in Appendix C and certain symbols used to abbreviate polynomials are given in Appendix D. Appendix E will be useful to those who wish to extend the results to a complete analysis of domain states. It contains basic conversion equations from which all others can be obtained by substitution of other symbols. A synoptic list of symmetry descents is given in Appendix F. Finally, in Appendix G nonstandard lattice letters which prove to be useful in Hermann–Mauguin symbols of equitranslational subgroups of the space groups are given.

A Software Guide

The following is a brief introductory guide to the software. It is followed by an explanation of the basic concepts, a large fraction of which is either not yet available in group-theoretical textbooks or is to be found under different names. The reader will hopefully find that the unification and standardization of the nomenclature and symbolism is justified by its use. Tables are accompanied by `help` files which will remind the user of the meaning of the information in each table. If in doubt, the user should return to the text of this Manual.

Getting started! The 32 crystallographic geometric classes are the starting point of the program. On opening the program, a panel appears with the names of the crystallographic systems under the heading "Geometric classes". Clicking on a system displays the geometric classes of the system in a tree form. Geometric classes are denoted by Schönflies, Hermann–Mauguin and Shubnikov symbols. Each of the notations can be activated to replace the current default. Shubnikov symbols are used only at this point for correlation with older Russian literature. If you run across such a symbol in the literature, you may start with it, change the notation and continue your search for further information.

The panel contains an originally empty right-hand part divided into an upper and a lower section. Clicking on a geometric class produces in this part the symbols of all specifically oriented point groups of the class which are used in the software; the upper section contains the symbol of a group in its standard orientation. This is the orientation of the parent point group in the tables of ferroic transitions which constitute the central part of this program. For the majority of cases, one standard orientation is chosen; the reasons why more than one choice is given for six geometric classes are discussed below. Groups of the geometric class in nonstandard orientations are listed in the lower section; these are the groups which appear as subgroups of standard parent groups.

Clicking the left button of the mouse activates the consideration of the group in its standard orientation. A subsequent click of the right button reveals a pull-down menu which offers various types of information. You should either hold down the right button and release it on the desired menu item or release it while outside the menu and choose the item with a click of the left button. The menu contains the following items:

Basic info: Displays a table with basic information about the geometric class the group belongs to, including specification of the standard orientations.

Group elements: Displays the Group Calculator, which lists the group elements as symbols of the keys either in standard or spectroscopic notation. The calculator performs the calculation of products (strings) of up to ten group elements *via* left or right multiplication.

These two options are available for groups in standard and nonstandard orientations. Further options are available only for groups in the standard orientation.

Correlation Stnd./Spectro.: Displays tables which correlate the standard symbols of groups, group elements, classes of ireps (irreducible representations) and conjugacy classes (for non-Abelian groups) with spectroscopic symbols.

Class structure: Displays classes of conjugate elements and defines their symbols.

Class mult. table: Displays a class multiplication table.

Character table: Displays characters of irreducible representations.

Kronecker products: Displays Kronecker products of characters.

In the last four menu items it is possible to switch between standard and spectroscopic notation. In the following menu items, the spectroscopic symbols appear only as auxiliary reference symbols.

Ireps and standard variables:

brief: Displays the matrices of group generators for the matrix ireps of the group and defines symbols of these ireps and the meaning of the standard variables. For groups up to the orthorhombic system, for one-dimensional and for three-dimensional ireps, the choice of matrix ireps and of standard variables is unique. For two-dimensional R-ireps of groups of higher systems there are two options ($cf.$ Standard transformations):

complex: Standard typical variables $(\xi_\alpha, \eta_\alpha)$ are used for the complex form of two-dimensional C-ireps which are reducible in uniaxial and tetrahedral groups.

real: Real standard typical variables (x_α, y_α) for equivalent R-ireps are used.

full: Displays the matrices of all group elements for the matrix ireps of the group and defines symbols of these ireps and the meaning of the standard variables. The information often extends over several pages. Continuation of the table here as well as in other files is indicated by the symbols $\Longrightarrow$ $\Longrightarrow$ at the bottom of one page and (cont.N) at the top of the next page; the last page contains (cont.N/end). One can move forward or backward through these pages using the arrows in the upper bar of the window.

Kernels of ireps are given in both cases (brief and full). Relations between R-ireps and C-ireps are given at the bottom of tables in both cases for point groups of higher than orthorhombic system.

Clebsch–Gordan products: Displays Clebsch–Gordan products of covariants in terms of the standard typical variables. For groups up to the orthorhombic system, one table of Clebsch–Gordan products is produced. For groups of higher systems, two options are given:

complex: in terms of variables $(\xi_\alpha, \eta_\alpha)$,
real: in terms of variables (x_α, y_α).

Tensorial covariants: Displays tensorial covariants for tensors up to rank four.

Subgroups: The choice of this menu item displays an interactive panel which consists of two parts. In the upper part are displayed boxes labelled in front by R-ireps of the group G in spectroscopic notation. Real typical variables representing vectors of the typical carrier spaces are given inside each box. If the R-irep is one-dimensional, the symbol of the respective typical variable is given in the box. If the R-irep is two- or three-dimensional, scrolling through the box reveals all vectors of special symmetry and the general vector of the space belonging to the R-irep.

The lattice of subgroups F of a parent point group G is displayed in the panel either in Schönflies or in Hermann–Mauguin notation. Groups are framed and sets of conjugate subgroups are listed in frames which are stacked like a pile of sheets of paper. Consecutive clicks on the pile brings the next subgroup of the set to the top. This is useful when considering equitranslational subgroups. The pull-down menu Graph provides options for manipulating the lattice. Each subgroup can be selected by holding down the left mouse button and moved to another place, the new arrangement can be recorded as the new default or reset to the original default. The lattice and the boxes serve as a menu for displaying further information.

Direct Landau problem: Clicking on a vector in the box reveals its stabilizer - epikernel of the R-irep; the frame with the subgroup turns into an inverse display: white letters on a black background. This is equivalent to the solution of the direct Landau problem. Clicking on a second vector while keeping the `ctrl` button depressed leads to the intersection of both epikernels.

Integrity bases: This option is available either under the pull-down menu View or directly at the box when the box of an irep is activated by previous choice of any of its vectors. It displays the extended integrity bases of the respective irreducible matrix group in terms of the components of a general vector of the space.

Domain: Clicking on a normal subgroup H or on any of the set of conjugate subgroups F_i activates further options. The option Domain, available either under the pull-down menu View or directly at the subgroup in the case of normal subgroups, produces a table with complete information about tensors of the first domain in a symmetry descent $G \Downarrow H$ or $G \Downarrow F_1$ and about the relevant interactions (integrity basis, faint interactions, electric and elastic switching interactions). In some cases, the information is shown on several pages as described above.

The solution of the *Inverse Landau problem* follows from the table.

Twinning: This option is available in the pull-down menu View for the first group of the set of conjugate subgroups and also directly at the frame in the case of a normal subgroup. It displays a table which contains the following information: (i) the set of consecutive normalizers of conjugate subgroups; (ii) left, right and double coset resolutions with respect to the first group F_1 of the set; and (iii) twinning group to each double coset.

Equitranslational subgroups of space groups: The pull-down menu Groups contains two options: Point and Space. The second option leads to a complete description of the lattices of equitranslational subgroups of space groups, the first option returns to the lattice of point groups. In this description we use the fact that lattices of equitranslational subgroups are isomorphic to lattices of their respective point groups.

On choosing the option Space, a new panel appears on the screen. In the right-hand part of this panel is a box with all the Hermann–Mauguin symbols of space groups which correspond to the original point group. If one picks up one of these symbols, the specification of space-group type by its sequential number, by its oriented Schönflies symbol and by setting and/or cell choice where applicable appears in the left-hand part of the panel. At the same time, the symbols of the point groups in the lattice, whether they are in Schönflies or in Hermann–Mauguin symbols, are replaced by Schönflies symbols of the respective oriented space-group types.

This is not yet a complete specification of the subgroups, although it is already more informative than the original lattices given by Ascher (1968). The parent group is, however, completely specified by the chosen Hermann–Mauguin symbol. To get the complete specification of an individual subgroup, it is sufficient to click on the frame containing its Schönflies symbol. The information which completely specifies the subgroup appears in the lower bar of the panel, reserved for this information. This consists of the Hermann–Mauguin symbol followed by an origin shift. In cases where the original conventional basis does not coincide with the conventional basis of the subgroup, the lattice letter in the Hermann–Mauguin symbol is embellished and its meaning is expressed on the same line. The reader can consult the last section of this file to familiarize themselves with the logic of this symbolism.

Part A: Groups and their representations

Terminology and physical models: With the exception of the information about subgroups, where lattices of equitranslational subgroups of space groups are given in parallel with the lattices of the point groups with which they are isomorphic, all information is given in terms of the crystallographic point groups and tensor components. The point groups are considered as groups acting on the three-dimensional orthogonal space $V(3)$; this action also defines the action of the point groups on tensorial and polynomial spaces.

Crystals and other materials are, however, objects in the three-dimensional Euclidean space $E(3)$. A detailed description of crystal symmetries and their changes in structural phase transitions should therefore be based on space groups and relations between them. Since the tensorial properties depend only on the point group of a crystal and their changes are also associated only with the change of this point group, a description using the space $V(3)$ is permissible and can be connected with two physical models:

1. The model of infinitely small crystal: This is a model which corresponds to many experimental arrangements. The crystal can be viewed as a point P in $E(3)$ and its symmetry as the site point group G_P. In this model we disregard the internal structure of the crystal (or other material) as well as its finite size.

2. The continuum model of the crystal: In this model we consider the crystal as an infinite homogeneous anisotropic medium which has the same properties at each of its points. Again we disregard here the internal, discrete structure of the crystal and its finite size. The symmetry of such a medium is a subgroup of the Euclidean group $\mathcal{E}(3)$ which contains all translations and has the same site symmetry at each of its points. Such group is a "space group" with a continuous translation subgroup for which we coin the name point-like space group (Kopský, 1993*a*,*b*). There are 32 crystallographic space-group types of such groups and we denote them by symbols VG in analogy with Hermann–Mauguin symbols for the discrete space groups – V stands for the lattice which coincides with the vector space $V(3)$, G for the point group. Thus the symbol $Vm\overline{3}m$ means the space symmetry of any crystal of the geometric class $m\overline{3}m$ in the continuum model.

In this case we can again use the point groups when considering tensor properties, taking into account that each point of the crystal has the same site point symmetry and that the tensorial properties are the same at each point. The information about tensors and their changes at structural phase transitions can again be given in terms of the point groups and tensor components.

Both interpretations can be used as long as we are interested in only one domain state. The second interpretation is necessary when considering domain walls or twin boundaries where tensor properties are homogeneous in planes parallel with the boundary but exhibit a spatial change on a path across the boundary.

Orthogonal operators and isometries: The point groups are subgroups of the full orthogonal group $\mathcal{O}(3)$ which acts on the vector space $V(3)$. The elements of this group are orthogonal operators on $V(3)$ and they are expressed by orthogonal matrices of the matrix group $\mathsf{O}(3)$ in any orthonormal basis $(\mathbf{e}_x, \mathbf{e}_y, \mathbf{e}_z)$ of $V(3)$. The choice of a point P in the corresponding Euclidean space $E(3)$ and this orthonormal basis complete the choice of a Cartesian coordinate system $(P; \mathbf{e}_x, \mathbf{e}_y, \mathbf{e}_z)$ in $E(3)$. To each operator $g \in \mathcal{O}(3)$ there corresponds an isometry $\{g|\mathbf{0}\}_P$ of $E(3)$ and all such isometries constitute a group $\mathcal{O}_P(3)$ – this is the group of all proper and improper rotations of the space $E(3)$ which

leave the point P invariant. To any subgroup $G \subseteq \mathcal{O}(3)$ there corresponds a subgroup $G_P \subseteq \mathcal{O}_P(3)$ and *vice versa*. It is therefore admissible to use the usual language in which orthogonal operators are called by the names of corresponding rotations and we shall follow this custom including the name *"group of rotations"* for the group $\mathcal{O}(3)$.

Geometric classes: The set of groups that are conjugate subgroups of $\mathcal{O}(3)$ is called the "geometric class" (of point groups). Groups of the same geometric class differ only in their orientation in the space. Indeed, if the group F is expressed by certain matrices in the basis $(\mathbf{e}_x, \mathbf{e}_y, \mathbf{e}_z)$, then its conjugate group gFg^{-1} is expressed by the same matrices in the basis $(g\mathbf{e}_x, g\mathbf{e}_y, g\mathbf{e}_z)$.

Remark 1: The concept of geometric class extends to Euclidean groups; a Euclidean group is said to belong to a certain geometric class if its point group belongs to it. Thus we have geometric classes of space groups, layer groups, rod groups and of the site point groups.

Group elements: To present all the information we want, it is sufficient to consider only the subgroups of specifically oriented groups of the geometric classes O_h and D_{6h}. For the group O_h, we choose the natural orientation where the fourfold axes are oriented along the basis vectors $(\mathbf{e}_x, \mathbf{e}_y, \mathbf{e}_z)$ of the Cartesian system. For the group D_{6h}, we choose one of the twofold axes along the vector $\mathbf{e}_x$ and the hexagonal axis along the vector $\mathbf{e}_z$. Since there is no possibility of misunderstanding, we shall use for these quite specific groups and for some of their subgroups (see below) the same symbols as for the corresponding geometric classes. Let us observe that the two groups in these orientations have in common exactly the group D_{2h} for which we again use the same symbol as for the whole geometric class.

The elements of these two groups are denoted by symbols which shall be further referred to as the Standard notation. The principle of this notation is quite commonly used in the literature and it also coincides with the principle on which the recent proposal of a nomenclature in higher dimensions (Janssen *et al.*, 1999) is based. Rotations about axes of angles π, $2\pi/3$, $\pi/2$, $\pi/3$ in a counterclockwise direction are denoted by numbers 2, 3, 4 and 6 with subscripts indicating a positive direction of the axis according to the following correspondence:

Orientations in the cubic group

x	y	z	xy	$x\overline{y}$	yz	$y\overline{z}$	zx	$z\overline{x}$	p	q	r	s
[100]	[010]	[001]	[110]	[$\overline{1}$10]	[011]	[0$\overline{1}$1]	[101]	[10$\overline{1}$]	[111]	[$\overline{1}\overline{1}$1]	[1$\overline{1}$1]	[$\overline{1}$1$\overline{1}$]

Orientations in the hexagonal group

x	x'	x''	y	y'	y''	z
[100]	[010]	[$\overline{1}\overline{1}$0]	[120]	[$\overline{2}$10]	[1$\overline{1}$0]	[001]

The use of subscripts is also specified in Fig. 1. Mirrors are denoted by a common symbol m with a subscript of the twofold axis orthogonal to them. An overbar on the numbers $\overline{3}$, $\overline{4}$ and $\overline{6}$ means the rotoinversion, *i.e.* the combination of the rotation with space inversion; the subscript again denotes the positive direction of the axis. The correlation of this notation with other selected notations used in the literature is given in Appendix A where the relation between powers of the elements is also given. Note that

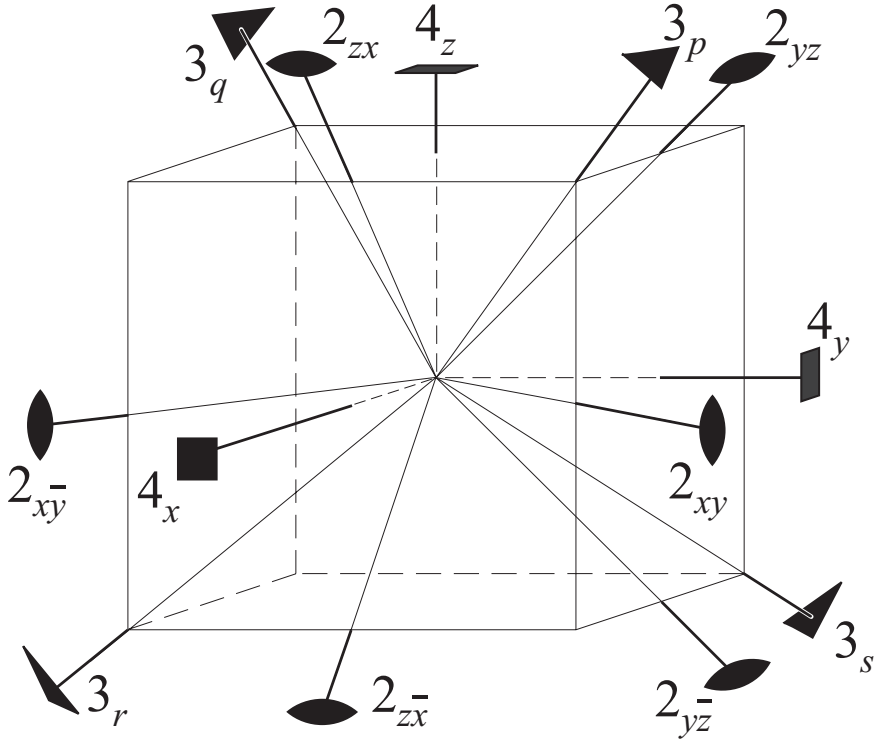


Figure 1a. Symbols for the symmetry axes of the cubic group

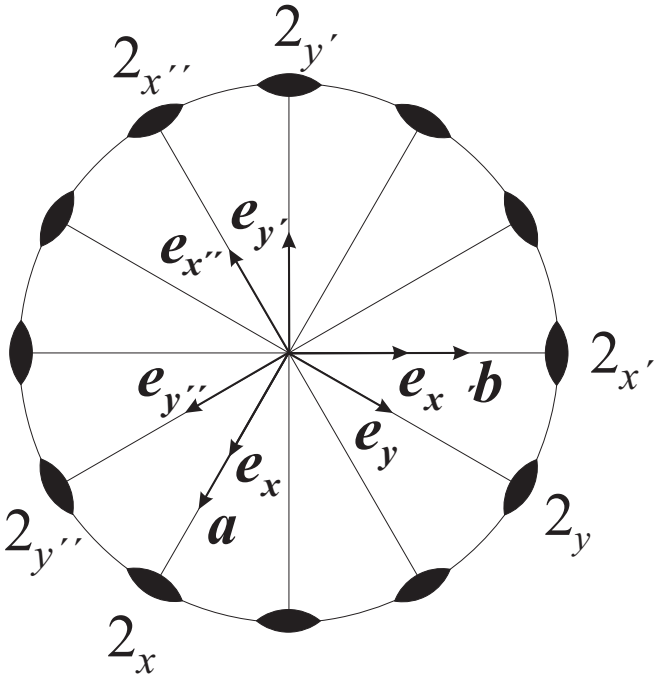


Figure 1b. Symbols for symmetry axes of the hexagonal group

we use the symbol e for the unit element and i for the inversion (symbols 1 and $\overline{1}$ are not acceptable in view of the clash with their meaning in Hermann–Mauguin symbols).

To facilitate correlation with spectroscopic literature we also use, up to a certain point in this software, the Spectroscopic notation. The spectroscopic symbols for the elements of the point groups are taken from the tables by Altmann & Herzig (1994) and Bradley & Cracknell (1972). However, the spectroscopic notation is not internally compatible, so symbols of the same operations differ in different specific groups and even the two books do not have completely identical nomenclature. In addition, some of the symbols clash with Schönflies symbols for the groups. The type of notation which we describe here as the standard one is also used in the literature. From the comparative tables of notations (Tables A1 and A2 of Appendix A) one can really see the need for us introduce our own, internally compatible standard notation. Correlation between the two notations used here is also given in the files Correlation Stnd./Spectro.

Standard orientations: Material properties which are homogeneous but not isotropic and experimental measurements of such properties are conveniently referred to a certain Cartesian basis. Once such properties are specified with reference to one Cartesian basis, it is possible to express them with reference to any other basis using appropriate linear transformations. The symmetry group of a material implies certain "selection rules" – some linear combinations of tensor components are forbidden or, in other words, must identically vanish. Analogously, the form of interactions between various parameters ("faint interactions") and of interactions between parameters and external fields ("switching interactions") is determined by the symmetry. The allowed form of a material tensor as well as the expressions for tensorial and polynomial covariants (see below) depend, however, not only on the symmetry of the material but also on the choice of the Cartesian system and on the orientation of the symmetry group with reference to this system.

It is therefore necessary and sufficient to choose just one specifically oriented group from each geometric class if we want to describe the allowed tensorial properties of a material with the symmetry of any given geometric class, including the description of symmetry descents and of relevant interactions. We introduce, however, three standard orientations for the monoclinic geometric classes C_{2h}, C_2, C_s, three for the orthorhombic geometric class C_{2v} and two standard orientations for groups of geometric classes D_{2d}, D_3, C_{3v}, D_{3d}, and D_{3h}. There are two reasons for extending the choice:

(i) Standard orientations of space groups of these geometric classes correspond to several standard orientations of their point groups.

(ii) In systematic tensor calculus, it is suitable to consider equally all groups of the same oriented Laue class (see below the tables of tensorial covariants).

Remark 2: To each Euclidean group there corresponds a point group of a certain orientation. Hence we can classify the space, layer, rod and site point groups into oriented geometric classes.

Nonstandard orientations: When considering structural phase transitions, which constitute the main application of our information scheme, we are interested in the change of the parent symmetry to a low phase symmetry and in the change of tensorial properties at the transition. The parent symmetry can be always chosen as a group in the standard orientation. The symmetry of the low phase is always a subgroup of the parent symmetry. We must therefore also take into consideration the subgroups of chosen specific groups. Groups in nonstandard orientations appear as subgroups of groups in standard orienta-

tions. The Schönflies and Hermann–Mauguin symbols of all specific groups which are used in this program are given in Appendix B. The groups are divided into three rows which correspond to subgroups of the groups O_h, D_{6h}, and to their common subgroups which are all subgroups of the group $D_{2h} = O_h \cap D_{6h}$. The orientation of groups is indicated by directional subscripts which are omitted in cases when misunderstanding is not expected.

Isomorphisms: Two groups G and $\widetilde{G}$ are said to be isomorphic if there exists a one-to-one mapping (bijection) $a : G \longrightarrow \widetilde{G}$ sending an element $g \in G$ to an element $\widetilde{g} = a(g) \in \widetilde{G}$, called the image of g, and if this mapping sends the product of the elements into the product of their images:

$$a(gh) = a(g)a(h) = \widetilde{g}\widetilde{h}.$$

From this it follows that the mapping also sends the unit element into a unit element and a reciprocal element into the reciprocal element of its image:

$$a(e) = \widetilde{e}, \qquad a(g^{-1}) = a(g)^{-1} = \widetilde{g}^{-1}.$$

The mapping a is called a group isomorphism.

Oriented Laue classes and isomorphisms: Among point groups we distinguish:

(i) Groups of proper rotations.
(ii) Noncentrosymmetric groups which contain improper rotations.
(iii) Centrosymmetric groups.

Groups which belong to the same geometric class are certainly isomorphic because they are conjugate subgroups of the orthogonal group $\mathcal{O}(3)$. There exist 11 geometric crystallographic classes of groups of proper rotations. In eight of these classes we choose one group of proper rotations to be in a standard orientation and in the trigonal class D_3 we choose two groups as follows:

1. Triclinic system: $C_1 - 1$.
2. Monoclinic system: $C_{2z} - 2_z$.
3. Orthorhombic system: $D_2 - 2_x 2_y 2_z$.
4. Tetragonal system: $C_{4z} - 4_z$ and $D_{4z} - 4_z 2_x 2_{xy}$.
5. Trigonal system: $C_3 - 3_z$ and two groups: $D_{3x} - 3_z 2_x$, $D_{3y} - 3_z 2_y$.
6. Hexagonal system: $C_6 - 6_z$ and $D_6 - 6_z 2_x 2_y$.
7. Cubic system: $T - 23$ and $O - 432$.

Each group G of proper rotations generates groups of an "oriented Laue class". We say that the group belongs to an oriented Laue class if it contains all proper rotations of the group G either by themselves or in combination with the space inversion i. Apart from the group of proper rotations G itself, the oriented Laue class always also contains the centrosymmetric group $G_h = G \otimes I$, where $I \approx C_i = \{e, i\}$ is the inversion group. It is a crystallographic tradition to denote a "Laue class" of space groups by the symbol of the centrosymmetric geometric class; accordingly we denote the oriented Laue class (of point groups) by the symbol of the respective centrosymmetric point group G_h. By Laue class of point groups we then understand the collection of all oriented Laue classes characterized by centrosymmetric groups of geometric class G_h.

Remark 3. In theoretical relations we write I for the space inversion group instead of C_i. We also write G_h for the centrosymmetric group to a group G of proper rotations, although $G_h = C_{3i}$ and D_{3d} for $G = C_3$ and D_3.

The noncentrosymmetric groups which contain improper rotations exist if and only if the group of proper rotations has halving subgroups H; actually each halving subgroup defines exactly one such group in the following manner:

The group G can be expressed as $G = H \cup gH$. Replacing elements of the coset gH by their combinations with the space inversion, we obtain the group $H \cup igH$. The inversion i commutes with every proper rotation, so the group $H \cup igH$ is isomorphic with the group of proper rotations G. We choose the isomorphisms in the most natural way: Elements $h \in H$ are mapped onto themselves, elements $igh \in igH$ are mapped onto $gh \in G$. The isomorphisms used in this software are given in Appendix C.

As follows from the preceding reasoning, each Laue class of classical point groups contains groups of two isomorphic types: those isomorphic to the group of proper rotations and the centrosymmetric groups; there is just one centrosymmetric group in each oriented Laue class. Apart from these isomorphisms there exist isomorphisms across Laue classes: The group C_i is isomorphic to C_{2z} and the group C_{2hz} is isomorphic to the group D_2. These isomorphisms are of no importance in our scheme.

Remark 4. Again we can distinguish oriented Laue classes and Laue classes of space, layer, rod and site point groups.

Order of the group: The simplest characteristic of a finite group G is the number of its elements. This number is called the order of the group and usually denoted by $|G|$. Despite its simplicity, the order of the group appears in important relations.

Classes of conjugate elements: We say that two elements $g, g' \in G$ are conjugate elements in G if an element $f \in G$ exists such that $g' = fgf^{-1}$. Conjugation is an operation which subdivides all elements of a group into classes because it has the three properties required for a class:

1. Symmetry: Each element is conjugate with itself: $g \sim g$.
2. Reflexivity: If f is conjugate with g, then g is conjugate with f and *vice versa*: $g \sim f \Leftrightarrow f \sim g$.
3. Transitivity: If f is conjugate with g and h is conjugate with f then h is conjugate with g or: $f \sim g$ and $h \sim f \Rightarrow h \sim g$.

If the group is Abelian, requesting the class structure results in the statement: Abelian group: Each element constitutes its own class being displayed on the screen. In other cases, the table describing the class structure of all groups belonging to the same oriented Laue class is displayed. Noncentrosymmetric groups have the same class structure as the group of proper rotations which is listed first. Classes are denoted by letters K_i and the subscript 1 is reserved for the class which contains the identity so that it is always the case that $K_1 = \{e\}$. The elements of other classes correspond to the elements of classes in the group of proper rotations and contain the same proper rotations or their combination with the inversion i.

The inversion i commutes with all other point-group elements. Hence the number of classes of the respective centrosymmetric group is twice the number of classes of the group of proper rotations and a class contains either only proper rotations or only improper rotations. We denote by K_i^+ the class of those elements which are contained in the class K_i of the proper rotation group, by K_i^- the class of the same elements combined with the inversion i. It is therefore always the case that $K_1^+ = \{e\}$ and $K_1^- = \{i\}$. It is possible to switch between tables of class structures in terms of standard or spectroscopic

notation of the elements and the correlation between the symbols of classes is again given in Correlation Stnd./Spectro. files.

Class multiplication: We denote by lower-case k_i the number of elements in the conjugacy class K_i. If we take all products $g_i g_j$ of group elements where $g_i \in K_i$ and $g_j \in K_j$, we obtain a set of elements, the number of which is the product $k_i k_j$ of the numbers of elements in the two classes. An element may occur in this product set several times, in which case all elements of the class to which it belongs appear in the set the same number of times. This is expressed by the class multiplication formula:

$$K_i K_j = \sum_{l}^{|K|} c_{ij,l} K_l,$$

where the coefficients $c_{ij,l}$, called the class multiplication coefficients, express the number of times every element of a class K_l occurs in the set $K_i K_j$. These numbers are related to the order of the group by the evident relation

$$|G|^2 = \sum_{i,j=1}^{|K|} k_i k_j = \sum_{i,j,l}^{|K|} c_{ij,l} k_l.$$

Class multiplication is given in the form of tables analogous to the multiplication table of the group and coincide with it in the case of Abelian groups. If the group is Abelian, requesting class multiplication results in the statement: Abelian group: Class multiplication table is identical with the multiplication table of elements. In the case of noncentrosymmetric groups, the class multiplication table is displayed with the title Isomorphism type G, with Schönflies and Hermann–Mauguin symbols for the group of proper rotations G. In the case of a centrosymmetric group, the table is displayed with the title Centrosymmetric group G_h, with Schönflies and Hermann–Mauguin symbols for G_h.

Subgroups

This section reviews the basic facts about subgroups needed in the theory of representations. A more advanced consideration of lattices of subgroups and their connection with representation spaces is given at the start of Part B.

Subgroups: A set H of elements h of G is called a subgroup of G if it is itself a group under the same multiplication law. Each group G contains at least two subgroups:

(i) The group G itself.

(ii) The group C_1 consisting only of the unit element e.

These subgroups are usually called the trivial subgroups. The cyclic groups of prime order contain only these two subgroups.

Cosets and coset resolution: Let $F = \{e, f_2, \ldots, f_p\}$ be a subgroup of G, consisting of $p = |F|$ elements f_i. We shall always list the unit element first, because it is contained in any subgroup; the unit element therefore always corresponds to the suppressed subscript 1; *i.e.* $f_1 = e$. Let us now choose an element g of G and construct two sets by multiplication of the elements of F by g either from the left or from the right: $gF = \{g, gf_2, \ldots, gf_p\}$ and $Fg = \{g, f_2 g, \ldots, f_p g\}$. If $g \in F$ then $gF = Fg = F$. The elements in each such set

are distinct and their number is therefore $p = |F|$ = the order of the group F. The set gF is called a left coset of F in G, the set Fg is called a right coset of F in G.

We now compare two left cosets g_iF and g_jF to show that they are either disjoint or identical. If $g_if = g_j\widetilde{f}$, where $f, \widetilde{f} \in F$ is an element which the two cosets have in common, then $g_i = g_j\widetilde{f}f^{-1}$ belongs to g_jF because $\widetilde{f}f^{-1} = f_k$ is an element of F. Hence every element g_if_m, $m = 1, 2, \ldots, p$ is also an element $g_jf_kf_m$ of g_jF because f_kf_m is certainly in F. On the other hand, each element g_jf_m of g_jF is an element $g_if_k^{-1}f_m$ of g_iF because $g_j = g_if_k^{-1} = g_if\widetilde{f}^{-1}$ and $f_k^{-1}f_m$ is certainly an element of F. Analogously, we can prove that right cosets Fg_i and Fg_j are either disjoint or identical.

Corollary: (i) It is possible to express the group G as a union of left cosets of its subgroup F:

$$G = F \cup g_2F \cup \ldots \cup g_qF.$$

This expression is called the left coset resolution of G with respect to its subgroup F or the decomposition of the group G into the left cosets of its subgroup F.

(ii) It is possible to express the group G as a union of right cosets of its subgroup F:

$$G = F \cup Fg_2' \cup \ldots \cup Fg_q'.$$

This expression is called the right coset resolution of G with respect to its subgroup F or the decomposition of the group G into the right cosets of its subgroup F.

(iii) Lagrange theorem: The number q of left cosets of a subgroup is equal to the number of right cosets and it is a divisor of the order of the group G.

This number is denoted by $q = [G : F]$ and is called the index of the subgroup F in the group G. Since $p = |F|$ is also the number of elements in each coset, the product $pq = |G|$ equals the order of the group G.

The elements g_i or g_j' in a particular left or right coset resolution are called the coset representatives. Any element of either the left or right coset can be chosen as its representative. If a sequence of elements $\{e, f_2, \ldots, f_p\}$ in the subgroup F is chosen, then the change of the choice of a representative of a coset changes the sequence of the elements in the coset.

It is important to realize that the representatives of left cosets are generally different from the representatives of right cosets. However, it is always possible to choose the right coset representatives as the inverses $g_i' = g_i^{-1}$ of the left coset representatives. The set of elements inverse to elements of a left coset g_iF is identical with a right coset Fg_i^{-1} and *vice versa*: the set of elements inverse to elements of a right coset Fg_j is identical with the left coset $g_j^{-1}F$.

Double cosets: The set of all distinct elements of the form f_igf_j, where $f_i, f_j \in F$ and g is an element of G, is called the double coset of F in G and denoted by FgF. The element g, called the double coset representative, belongs to FgF and the double coset does not change if g is replaced by another of its elements, so any element may be chosen as a representative.

The set of elements $(FgF)^{-1} = Fg^{-1}F$ contains all elements inverse to the elements of a double coset FgF. It is itself a double coset with representative g^{-1} and it is called the inverse double coset to FgF.

A double coset FgF is called ambivalent if it is identical with its own inverse. This means that the coset contains with each element also its inverse. It is, however, sufficient that the double coset contains an inverse to one of its elements in order that it be ambivalent.

If a double coset does not contain an inverse to one of its elements, then it cannot contain an inverse to any of its elements. The intersection of the double coset with its inverse is then empty:

$$FgF \cap (FgF)^{-1} = \emptyset$$

and the double coset is called polar. Polar double cosets exist in pairs FgF and $Fg^{-1}F$ which are called complementary double cosets.

A double coset FgF consists of whole left cosets as well as of whole right cosets. Indeed, if we take $f_i = e$, we get $gF \subseteq FgF$, while if we take $f_j = e$, we get $Fg \subseteq FgF$.

If a left coset gF is identical with the right coset Fg, then it also coincides with the double coset FgF. Such cosets will be distinguished as simple double cosets while double cosets consisting of several left cosets and hence of the same number of right cosets will be called multiple double cosets.

If elements of the subgroup F are arranged in a certain sequence $F = \{e, f_2, \ldots, f_p\}$, then the choice of a representative element g determines the sequences of elements $gF = \{g, gf_2, \ldots, gf_p\}$, $Fg = \{g, f_2g, \ldots, f_pg\}$ in the left as well as in the right coset. These sequences are not necessarily identical even if $gF = Fg$. However, the choice of the representative g does not determine the sequence of elements in the multiple double coset FgF. The number of products of the form f_igf_j is p^2, but not all of them are distinct.

Conjugate subgroups: Again we consider a subgroup F of G. We choose an element $g \in G$ and construct the set of elements $gFg^{-1} = \{e, gf_2g^{-1}, \ldots, gf_pg^{-1}\}$. This set is also a subgroup of the group G, isomorphic to the group F. Indeed, we define a mapping $\varphi_g : F \longrightarrow gFg^{-1} : f_i \longrightarrow \varphi_g(f_i) = gf_ig^{-1}$. This mapping is an isomorphism, because

$$\varphi_g(f_if_j) = gf_if_jg^{-1} = gf_ig^{-1}.gf_jg^{-1} = \varphi_g(f_i)\varphi_g(f_j).$$

The group gFg^{-1} is called a conjugate subgroup to the subgroup F.

Normal subgroups: If a subgroup H of the group G has the property that $gHg^{-1} = H$ for any element $g \in G$, then the subgroup H is called a normal subgroup of G (an older logical name is the self-conjugate subgroup).

A normal subgroup H of the group G has the property that the left and right coset resolutions of G with respect to its subgroup H are identical. In other words, each left coset gH contains the same elements as the right coset Hg. Indeed, for an element $gh \in gH$ we find an element $ghg^{-1} = \widetilde{h} \in H$ and it is $gh = \widetilde{h}g$. In the case of cosets of a normal subgroup we do not need to distinguish the left and right cosets; we still have to distinguish the left and right representatives; while the cosets g_iH and Hg_i contain the same elements of G, they generally appear in a different order.

Cosets of a normal subgroup have another important property: If we take an arbitrary element $g_ih_1 \in g_iH$ and an arbitrary element $g_jh_2 \in g_jH$, then the product $g_ih_1g_jh_2$ always belongs to the same coset g_kH, where g_k can be chosen as $g_k = g_ig_j$. Indeed, if g_i, g_j and hence also g_k are fixed, then an arbitrary choice of the two elements means that $h_1, h_2 \in H$ are arbitrary. However, $h_1g_j = g_j\widetilde{h}_1$ where $\widetilde{h}_1 \in H$ and hence $g_ih_1g_jh_2 = g_ig_j\widetilde{h}_1h_2 = g_k\widetilde{h}_1h_2$. Since $\widetilde{h}_1h_2 \in H$, we have proved that the product of any elements from two cosets g_iH and g_jH always lies in the coset g_kH, where g_ig_j is one of the possible representatives g_k.

Factor groups: From the preceding, it follows that the set of cosets $\gamma_i = g_iH = Hg_i$ can be itself considered as a group with the multiplication law defined as follows: $\gamma_i\gamma_j = \gamma_k$ if

$g_i g_j = g_k$ where $g_i \in \gamma_i$, $g_j \in \gamma_j$, $g_k \in \gamma_k$. The group of cosets with this multiplication law is called the factor group of the group G with respect to its normal subgroup H and is denoted by G/H. The subgroup H plays the role of the unit element $\varepsilon = H$ in the factor group.

Normalizers: Again, let G be a group and F a subgroup of G. The set of all elements $g \in G$, for which $gFg^{-1} = F$, constitutes a subgroup of G, called the first normalizer of F in G and denoted by $N_G^{(1)}(F)$. This normalizer is the largest subgroup of G in which F is normal. Hence all double cosets of F in the decomposition of $N_G^{(1)}(F)$ are the simple double cosets. *Vice versa*, the collection of all simple double cosets of F in the coset resolution of G constitutes the first normalizer $N_G^{(1)}(F)$.

If $N_G^{(1)}(F) = G$, then the subgroup F is normal in G. If $N_G^{(1)}(F) = F$, the subgroup F is called a self-normalizer (in G). If $F \subset N_G^{(1)}(F) \subset G$, so that F is neither normal nor a self-normalizer, then we consider the normalizer of the group $N_G^{(1)}(F)$ in G. The resulting group is denoted by $N_G^{(2)}(F)$ and is called the second normalizer of F in G. It is again either $N_G^{(2)}(F) = G$, so that $N_G^{(1)}(F)$ is normal in G, or $N_G^{(2)}(F) = N_G^{(1)}(F)$, so that the first normalizer $N_G^{(1)}(F)$ is a self normalizer, or $F \subset N_G^{(1)}(F) \subset N_G^{(2)}(F) \subset G$. In the latter case we consider again the next normalizer.

Continuing the procedure, we get a set of consecutive normalizers, which are important in considering the fine structure of domain states (Kopský, 1982, 1983). If the subgroup is of finite index, the chain of consecutive normalizers is finite. The following statements hold for finite groups:

1. A maximal subgroup of the group G is always normal or it is a self-normalizer.
2. The set of consecutive normalizers terminates either with the group G itself or with a self-normalizer.

In the case of subgroups of the crystallographic point groups only the following cases occur:

(i) $F = H$ is a normal subgroup.

(ii) $N_G^{(1)}(F) = H$ is a normal subgroup of G. The group $F = F_1$ belongs to the set of conjugate subgroups F_i of which H is a common normalizer.

(iii) $F = F_1$ is a self-normalizer. The groups F_i then constitute a set of conjugate self-normalizers.

(iv) The first normalizer $N_G^{(1)}(F)$ is a self-normalizer.

(v) The second normalizer $N_G^{(2)}(F)$ is a self-normalizer.

Homomorphism: A mapping $a : G \longrightarrow \mathcal{G}$ of a group G into a group $\mathcal{G}$ which sends the element $g \in G$ to an element $\widetilde{g} = a(g) \in \mathcal{G}$, called the image of g, is called a group homomorphism if this mapping sends the product of elements into the product of their images:

$$a(gh) = a(g)a(h) = \widetilde{g}\widetilde{h}.$$

An isomorphism is therefore a particular case of a homomorphism; a homomorphism is an isomorphism if it is a one-to-one mapping. Note also that a homomorphism is defined as a mapping into a group $\mathcal{G}$.

Kernels and images: Those elements of the group G that are mapped by the homomorphism a onto the unit element $\widetilde{e}$ of $\mathcal{G}$ form a subgroup H of the group G called the kernel of the homomorphism a, written as $H = \mathrm{Ker}\ a$. This subgroup is normal in G and elements of each coset g_iH are mapped by the homomorphism a onto the same element $\widetilde{\gamma}_i = a(g_iH)$. The set of these elements forms a group $\mathcal{H} = \{\widetilde{e}, \widetilde{\gamma_2}, \ldots, \widetilde{\gamma_q}\}$ called the image of the homomorphism a and denoted by $\mathcal{H} = \mathrm{Im}\ a$. This group is isomorphic to the factor group G/H.

Note that we distinguished the elements of the image and of the factor group only by a tilde to emphasize the isomorphism of G/H and $\mathcal{H}$. Technically, the factor group G/H is the group of cosets of a normal subgroup while the image of a homomorphism may have different meanings. It is also important to see that every homomorphism defines a normal subgroup – its kernel – and hence a factor group. On the other hand, each normal subgroup defines a certain homomorphism – the natural homomorphism onto the factor group. Any other homomorphism is obtained as an isomorphism of a specific group with this factor group.

Representations

Introduction. Quite generally, the term representation is used for various homomorphisms of the group G into some general groups of specific mathematical objects. The most useful, in physical applications, are representations of groups by linear operators where elements of the group act on linear spaces (or modules) and by permutations where elements of the group act on a (finite) set. The choice of the basis of the linear space or the choice of numerical labels of the elements of the set then leads to representations of the group by matrices.

Representations by linear operators: There exist many types of linear spaces (or modules) and, accordingly, many types of representations. If V is such a space and $\mathcal{G}V$ the general group of linear operators acting on this space, then a representation of the group G by operators on V is a homomorphism $U : G \longrightarrow \mathcal{G}V$ which maps each element $g \in G$ onto an operator $U(g) \in \mathcal{G}V$. This homomorphism has a certain kernel $H = \mathrm{Ker}\ U$ which is defined as the group of all those elements of G for which $U(g) = I$ – the unit element of $\mathcal{G}V$. It has also a certain image $\mathcal{H} = \mathrm{Im}\ U$ which consists of operators $U_i = U(g_iH) = U(Hg_i)$. The kernel is a normal subgroup of G and the image is isomorphic to the factor group G/H; a representation assigns the same operator to all elements of the coset $g_iH = Hg_i$.

Matrix representations: These are defined as homomorphisms of the group G into certain groups of matrices. Though independent consideration of matrix groups is possible, the actual gist of applications of representation theory lies in the connection of operator with matrix representations. Indeed, if we choose a basis of the space V, then each operator of $\mathcal{G}V$ is defined by its matrix and all these matrices form a certain matrix group $\mathsf{G}V$. Specification of a basis of V defines an isomorphism $\Sigma : \mathcal{G}V \longrightarrow \mathsf{G}V$. The operator representation U of the group G then defines its matrix representation $D^{(V)} : G \longrightarrow \mathsf{G}V$ which assigns to each element $g \in G$ that matrix $D^{(V)}(g)$ which the isomorphism Σ assigns to the operator $U(g)$. The matrix representation is therefore the result of consecutive application of the homomorphism U followed by isomorphism Σ and this isomorphism depends on the choice of the basis of V.

This approach, suitable for a general study of representation theory, is used in some textbooks, for example, in the textbook by Lyubarskii (1960). It can be simplified by the introduction of the concept of group action.

The group action: We say that the group G acts on a set $\mathcal{S}$ if to each element $g \in G$ and to each element $s \in \mathcal{S}$ there is assigned an element $gs \in \mathcal{S}$. This is the most general formulation, which applies to representations by linear operators as well as by permutations. We simply bypass the symbol $U(g)$ for an operator which represents the element $g \in G$, using the symbol g itself for the operator on the space V.

A representation of a group is called faithful if it is an isomorphism. From this viewpoint, each point group is its own faithful representation by operators of $\mathcal{O}(3)$ which act on the ordinary vector space $V(3)$; this is the so-called vector representation. This representation defines the action of the point group on spaces of tensors and of polynomials, which are our main concern. The dimension of tensorial and polynomial spaces grows quickly with the order and as a result it would be complicated to describe the transformation properties of tensors and of polynomials. The theory of irreducible representations facilitates the description of these properties. We shall describe below a method of "typical carrier spaces", and "typical bases, variables and covariants", developed more than twenty years ago (Kopský, 1975, 1976*a*) and tailored specifically for the consideration of tensorial properties and their changes at structural phase transitions, and for the construction of thermodynamic potential. All representations which we need in this program are real orthogonal representations. However, the most important theorem of the representation theory, known as Schur's lemma, is valid only in the field of complex numbers. The deviations from its consequences, which appear with reference to some irreducible representations of crystallographic point groups, have a simple standard character explained below (*cf.* Standard transformations).

The vector representation: The point groups are defined as groups of real orthogonal operators $g \in \mathcal{O}(3)$ acting on the three-dimensional vector space $V(3) = V(\mathbf{e}_x, \mathbf{e}_y, \mathbf{e}_z)$. We can say that each point group is its own faithful representation, which is called the "vector representation". Corresponding matrices of vector representations in the Cartesian (orthonormal) basis $\{\mathbf{e}_x, \mathbf{e}_y, \mathbf{e}_z\}$ will be denoted by $D^{(V)}(g)$. For the purposes of tensor calculus and formulae with summations we also use alternative labelling of vectors and their components by numbers as follows:

$$\mathbf{x} = x\mathbf{e}_x + y\mathbf{e}_y + z\mathbf{e}_z = \sum_{i=1}^{3} x_i \mathbf{e}_i,$$

where

$$x = x_1,\ y = x_2,\ z = x_3 \quad \mathbf{e}_x = \mathbf{e}_1,\ \mathbf{e}_y = \mathbf{e}_2,\ \mathbf{e}_z = \mathbf{e}_3.$$

The action of the point group $G \subseteq \mathcal{O}(3)$ on the space $V(3)$ is defined by:

$$g\mathbf{e}_i = \sum_{j=1}^{3} D^{(V)}_{ji}(g)\mathbf{e}_j.$$

If $\mathbf{x} \in V(3)$, then the operator $g \in \mathcal{O}(3)$ sends it to a vector $g\mathbf{x} = \sum_{i=1}^{3} x_i g\mathbf{e}_i = \sum_{i=1}^{3}\sum_{j=1}^{3} D^{(V)}_{ji}(g) x_i \mathbf{e}_j = \sum_{i=1}^{3} x'_j \mathbf{e}_j$, so that the coordinates of the new vector in the old basis are

$$x'_i = (g\mathbf{x})_i = \sum_{j=1}^{3} D^{(V)}_{ij}(g) x_j.$$

This corresponds to the convention by which operators are expressed by square matrices, vectors by column matrices and the action of an operator g on vector $\mathbf{x}$ resulting in vector $\mathbf{x}'$ with coordinates $x'_i = (g\mathbf{x})_i$ is expressed in matrix form by

$$\begin{pmatrix} D^{(V)}_{11}(g) & D^{(V)}_{12}(g) & D^{(V)}_{13}(g) \\ D^{(V)}_{21}(g) & D^{(V)}_{22}(g) & D^{(V)}_{23}(g) \\ D^{(V)}_{31}(g) & D^{(V)}_{32}(g) & D^{(V)}_{33}(g) \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} x' \\ y' \\ z' \end{pmatrix}.$$

The action of the point group $G \subseteq \mathcal{O}(3)$ on the space $V(3)$ also defines the action of this group on spaces of tensors and their components, on polynomials or, more generally, functions of a vector $\mathbf{x} \in V(3)$ or even on polynomials or functions of tensors expressed in their components.

Tensor representations: The vector representation defines tensor representations as follows: We introduce a space $V^n(3)$, the basis vectors of which are formally written as:

$$\mathbf{e}_{i_1,i_2,\ldots i_n} = \mathbf{e}_{i_1}\mathbf{e}_{i_2}\ldots\mathbf{e}_{i_n}.$$

A general element of this space is therefore

$$\mathbf{u} = \sum_{i_1,i_2,\ldots,i_n} u_{i_1,i_2,\ldots i_n}\mathbf{e}_{i_1,i_2,\ldots i_n}.$$

Such an element is called the tensor of rank n and the space $V^n(3)$ is called the tensor space. The action of the group G and actually also of the whole orthogonal group $\mathcal{O}(3)$ on this space is defined by the action of its elements on the basis according to

$$g\mathbf{e}_{i_1,i_2,\ldots i_n} = D^{(u)}_{j_1j_2\ldots j_n,i_1i_2\ldots i_n}(g)\mathbf{e}_{j_1,j_2,\ldots j_n} = D^{(V)}_{j_1i_1}(g)D^{(V)}_{j_2i_2}(g)\ldots D^{(V)}_{j_ni_n}(g)\mathbf{e}_{j_1,j_2,\ldots j_n},$$

so that the matrices of tensor representation are expressed through matrices of vector representation as follows:

$$D^{(u)}_{j_1j_2\ldots j_n,i_1i_2\ldots i_n}(g) = D^{(V)}_{j_1i_1}(g)D^{(V)}_{j_2i_2}(g)\ldots D^{(V)}_{j_ni_n}(g).$$

Apart from this, we can define an operation of the symmetric group S_n on this space as the group of permutations of indices $i_1, i_2, \ldots, i_n$. On this basis we can construct tensors of various symmetries with reference to permutation of indices – the so-called intrinsic symmetries. According to a general theorem, tensors of a defined intrinsic symmetry constitute a space which is invariant under the action of the group $\mathcal{O}(3)$ and hence under the point groups $G \subseteq \mathcal{O}(3)$. We define below some tensor spaces of lower orders with symmetrized indices which are used in physics.

The tensor space is just another linear (orthogonalized) space on which the group $\mathcal{O}(3)$ and its subgroups act. Let us denote a tensor of a certain intrinsic symmetry by $\mathbf{A}$, the space of such tensors by $V^{(A)}$ and its basis by $\{\mathbf{e}^{(A)}_i\}_{i\in I(A)}$, where i runs through a certain set of indices $I(A)$. Each index set $I(A)$ is therefore part of the definition of the basis of the tensor space $V^{(A)}$ with reference to which we express the tensor components. There exist standard choices of index sets for tensors of material physics which relate the tensor to a Cartesian coordinate system $(P; \mathbf{e}_x, \mathbf{e}_y, \mathbf{e}_z)$ of the Euclidean space $E(3)$ and hence to an orthonormal (Cartesian) basis $(\mathbf{e}_x, \mathbf{e}_y, \mathbf{e}_z)$ of vector space $V(3)$; corresponding bases $\{\mathbf{e}^{(A)}_i\}_{i\in I(A)}$ will be referred to as Cartesian bases of tensor spaces $V^{(A)}$. The general tensor of the space $V^{(A)}$ is expressed as

$$\mathbf{A} = \sum_{i\in I(A)} A_i\mathbf{e}^{(A)}_i,$$

where A_i are the Cartesian tensor components. The action of the group $\mathcal{O}(3)$ and of its subgroups G on the space $V^{(A)}$ is given by

$$g\mathbf{A} = \sum_{i\in I(A)} A_i g\mathbf{e}_i^{(A)} = \sum_{i,j\in I(A)} A_i D_{ji}^{(A)}(g)\mathbf{e}_j^{(A)},$$

so that the transformation properties of tensor components are given by

$$(g\mathbf{A})_i = \sum_{i\in I(A)} D_{ij}^{(A)}(g)A_j,$$

where $D_{ij}^{(A)}(g)$ are the matrices of tensor representation in the basis $\{\mathbf{e}_i^{(A)}\}_{i\in I(A)}$. The calculation of these matrices is in fact exactly the procedure we want to avoid.

Why? Well, they are $n \times n$ matrices, where n is the dimension of $V^{(A)}$ and the dimensions are unpleasantly high; for example $n = 6$ for the permittivity or deformation tensor, $n = 18$ for the piezoelectric tensor and $n = 21$ for the elastic stiffness tensor.

How? The answer is given by the theory of irreducible representations, which shows how to find the bases in which the action of the group is expressed in the simplest manner.

Polynomial and functional representations: In the previous section we defined tensor spaces related to the ordinary vector space $V(3)$; this corresponds to tensors of material physics which are our main concern. To find the invariant form of various interactions under the action of point groups, it is useful to develop methods for the determination of transformation properties of polynomials and ultimately of functions of tensors. Here we begin with a tensor space $V^{(u)}(n)$, where n now means its dimension. We denote the basis vectors by $\{\mathbf{e}_1, \mathbf{e}_2, \ldots, \mathbf{e}_n\}$; this can be achieved by relabelling the symmetrized indices $i_1, i_2, \ldots, i_n$, in other words by defining the index set $I(u)$ as the mapping of numbers from 1 to n onto the set of symmetrized indices. The general tensor of the space $V^{(u)}(n)$ is then expressed as $\mathbf{u} = \sum_{i=1}^n u_i\mathbf{e}_i$. The action of the elements of $G \subseteq \mathcal{O}(3)$ on this basis and transformation of tensor components are expressed in the standard manner:

$$g\mathbf{e}_i = \sum_{j=1}^n D_{ji}^{(u)}(g)\mathbf{e}_j, \quad (g\mathbf{u})_i = \sum_{j=1}^n D_{ij}^{(u)}(g)u_j.$$

Although these relations have formally the same form as the action of the elements $g \in \mathcal{O}(3)$ on the basis or on vectors of $V(3)$, there is a principal difference: Each transformation of the orthonormal basis of $V(3)$ can be interpreted as a result of an action of a certain orthogonal operator $g \in \mathcal{O}(3)$. Each operation g on the tensor space may be interpreted as a transformation of this space while not every transformation can be interpreted as an operator g on the tensor space $V^{(u)}(n)$.

If $f(\mathbf{u})$ is a function of the tensor $\mathbf{u}$, we define the transformed function $gf(\mathbf{u}) = f_g(\mathbf{u})$ as that function which has the same values for a transformed tensor $g\mathbf{u}$ as the original function has for the tensor $\mathbf{u}$. From this we get the relation $f_g(g\mathbf{u}) = f(\mathbf{u})$ or, finally, $f_g(\mathbf{u}) = f(g^{-1}u)$.

Let us now assume that the functions we have in mind are the components of the tensor, so that $f_i(\mathbf{u}) = u_i$. Then the transformed functions are $f_{gi}(\mathbf{u}) = f_i(g^{-1}\mathbf{u})$. But it is $g^{-1}\mathbf{u} = \sum_{i,j=1}^n D_{ij}(g^{-1})u_j\mathbf{e}_i$ of which the ith component is $\sum_{j=1}^n D_{ji}^t(g^{-1})u_j = \sum_{j=1}^n \widetilde{D}_{ji}(g)u_j$, where $\widetilde{D}_{ji}(g) = [D_{ji}^t]^{-1}(g) = [D_{ji}^{-1}]^t(g)$ denotes the matrix which is reciprocal and transposed to the original matrix $D_{ij}(g)$ – the so-called adjoint matrix.

We come therefore to a conclusion that the tensor coordinates, considered as functions of the tensor (they are the linear functions of a tensor), transform by matrices of an adjoint

representation to that by which the basis vectors of the tensor space transform. If the original matrices are real orthogonal, then $D^t(g) = D^{-1}(g)$ and hence $\widetilde{D}(g) = D(g)$; from the fact that the inverse matrix to an orthogonal is equal to its transpose, it follows that the adjoint matrix to an orthogonal is identical with it. In general physical applications the unitary representations are used for which the inverse matrix is equal to its complex conjugate. We shall use below complex variables only for the purposes of completeness, because a skilled reader can also use our results for quantum-mechanical problems. For our main purposes we can state that the transformation properties of tensor coordinates and of tensor bases are identical.

Linear functions of a tensor $\mathbf{u}$ are a particular case of polynomials in components of $\mathbf{u}$. The space of all polynomials in components of $\mathbf{u}$ splits into subspaces $\mathcal{P}_k(\mathbf{u})$ of homogeneous polynomials of the same order k in these components and each of these subspaces is invariant under the action of point groups $G \subseteq \mathcal{O}(3)$. Finally, the linear envelope $\mathcal{P}(\mathbf{u}) = \oplus_k \mathcal{P}_k(\mathbf{u})$ of all these spaces contains various spaces $\mathcal{F}(\mathbf{u})$ of functions; of interest is the space of smooth functions of tensor $\mathbf{u}$, *i.e.* those functions which have all derivatives. The use of the extended integrity bases, described below, enables us to classify even such functions as these by their transformation properties. However, in practice we use, as a rule, only the polynomial expansion.

Explicit work with tensor and polynomial representations in their general form is very complicated because the dimension of the matrices involved grows quickly with rank or order. The matrices inform us about the transformation properties of tensor components and of their functions. The theory of irreducible representations facilitates procedures with such components and functions. It shows how to choose more suitable bases in which the matrices have the simplest possible form. In addition, the classification of bases by irreducible representations selects physical states belonging to the same energies.

Irreducible representations

Reducibility/Irreducibility/Decomposability: Now we consider the action of a group G on a general linear space $V(n)$ which may be one of the tensor or polynomial spaces. We say that the space $V(n)$ is reducible under the action of the group G if the space contains a proper G-invariant subspace $V(m_1)$, otherwise we say that the space is irreducible. We say that the space $V(n)$ is decomposable under the action of the group G if it splits into a direct sum $V(n) = V(m_1) \oplus V(m_2)$ of G-invariant subspaces $V(m_1)$ and $V(m_2)$, so that each vector $\mathbf{x} \in V(n)$ is uniquely expressible as a sum $\mathbf{x} = \mathbf{x}_1 + \mathbf{x}_2$ of vectors $\mathbf{x}_1 \in V(m_1)$, $\mathbf{x}_2 \in V(m_2)$ and each element $g \in G$ sends a vector $\mathbf{x}_1 \in V(m_1)$ to a vector $g\mathbf{x}_1 \in V(m_1)$ and a vector $\mathbf{x}_2 \in V(m_2)$ to a vector $g\mathbf{x}_2 \in V(m_2)$. If we now choose a basis of the space $V(n)$ in such a manner that m_1 of its vectors $\{\mathbf{e}_1^{(1)}, \ldots, \mathbf{e}_{m_1}^{(1)}\}$ constitute a basis of $V(m_1)$, m_2 of its vectors $\{\mathbf{e}_1^{(2)}, \ldots, \mathbf{e}_{m_2}^{(2)}\}$ constitute a basis of $V(m_2)$, then the matrix form of the action of all elements $g \in G$ will be quasidiagonal:

$$D^{(V)}(g) = \begin{pmatrix} D^{(V_1)}(g) & 0 \\ 0 & D^{(V_2)}(g) \end{pmatrix}$$

Decomposability is a stronger property than reducibility. However, if the groups are finite, as all crystallographic groups are, and if the subject on which the group acts is a linear space, then reducibility implies decomposability. This is why in textbooks we usually only find the concept of reducibility, which is handled as if it is decomposability.

The spaces $V(m_1)$, $V(m_2)$ can be themselves again reducible and we can continue the procedure of reducing them further. Eventually we arrive at a direct sum $\oplus_{i=1}^{k} V(m_i)$ of k G-invariant irreducible subspaces $V_1 = V(m_1)$, $V_2 = V(m_2)$,..., $V_k = V(m_k)$ of dimensions m_i, $i = 1, 2, \ldots, k$ with bases $\{\mathbf{e}_1^{(1)}, \ldots, \mathbf{e}_{m_1}^{(1)}\}$, $\{\mathbf{e}_1^{(2)}, \ldots, \mathbf{e}_{m_2}^{(2)}\}$, $\{\mathbf{e}_1^{(k)}, \ldots, \mathbf{e}_{m_k}^{(k)}\}$ in which the matrices of all elements $g \in G$ will have the quasidiagonal form:

$$D^{(V)}(g) = \begin{pmatrix} D^{(V_1)}(g) & 0 & 0 \\ 0 & D^{(V_2)}(g) & 0 \\ \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots & & \\ 0 & 0 & D^{(V_k)}(g) \end{pmatrix}. \tag{1}$$

Classes of representations and characters: If a group G acts on the space $V(n)$, then the matrices $D^{(V)}(g)$ which represent the action of individual elements $g \in G$ depend on the choice of the basis $\{\mathbf{e}_1, \ldots, \mathbf{e}_n\}$. A transformation $\mathbf{e}'_i = \sum_j^n S_{ji}\mathbf{e}_j$ to another basis $\{\mathbf{e}'_1, \ldots, \mathbf{e}'_n\}$ leads to new matrices $D^{(V)'}(g) = S^{-1}D^{(V)}(g)S$. Two matrix representations related by this similarity transformation are called "equivalent". Matrix representations of a group G constitute therefore "classes of equivalent representations". To each class of equivalent representations we assign a function on the group G by $\chi(g) = \mathrm{Tr}\ D^{(V)}(g)$, where Tr means the trace of the matrix, *i.e.* the sum of its diagonal elements (another symbol in use is Sp from German word *Spur*). This function is called the "character" of the representation $D^{(V)}(g)$ and has the following properties:

1. It does not depend on the choice of the basis of $V(n)$ and hence on the particular matrix form of the representation because $\mathrm{Tr}\ D(g) = \mathrm{Tr}\ S^{-1}D(g)S$.

2. Characters are functions of conjugacy classes, *i.e.* the elements of the same class K_i have the same character because $\mathrm{Tr}\ D(fgf^{-1}) = \mathrm{Tr}\ D(f)D(g)D(f)^{-1} = \mathrm{Tr}\ D(g)$.

3. The character of the unit element e equals the dimension of the representation: $\chi(e) = \dim\ V(n) = n$. Indeed, the matrix $D(e)$ contains n times number 1 on the diagonal, so that $\mathrm{Tr}\ D(e) = n$.

4. If the representation is reducible, then the trace of each matrix $D^{(V)}(g)$ is the sum of traces of the matrices which appear as blocks in the quasidiagonal form, so that $\chi(g) = \sum_{i=1}^{k} \chi_i(g)$, where $\chi_i(g) = \mathrm{Tr}\ D^{(V_i)}$.

Characters of irreducible representations: If the group G is finite, then the number of equivalence classes of irreducible representations (ireps) is finite and equals the number of conjugacy classes in G, *i.e.* the number we denoted by $|K|$. This means that the number of different character functions for irreducible representations is also finite. We give them certain numerical labels $\alpha = 1, 2, \ldots, |K|$ and denote them by $\chi_\alpha(g)$. The label 1 is always reserved for the character $\chi_1(g) = 1$ of the identity irep. Irreducible characters have certain marvellous properties:

1. They are mutually orthogonal with respect to averaging over the group G, which means that

$$\frac{1}{|G|}\sum_{g\in G} \chi_\alpha(g)\chi^*_\beta(g) = \delta_{\alpha\beta}, \tag{2}$$

where $\delta_{\alpha\beta}$ is the Kronecker delta, which equals 1 if $\alpha = \beta$, 0 if $\alpha \neq \beta$ and the asterisk denotes complex conjugate.

2. Any representation of G with a character $\chi(g)$ is a direct sum of irreducible representations. The character $\chi(g)$ is the sum

$$\chi(g) = \sum_{\alpha=1}^{|K|} n_\alpha \chi_\alpha(g), \tag{3}$$

in which n_α is the "multiplicity" (or frequency) with which an irep of the class χ_α appears in the representation of the class $\chi(g)$. Using formula (2) we find that the multiplicity equals

$$n_\alpha = \frac{1}{|G|} \sum_{g\in G} \chi(g)\chi^*_\alpha(g). \tag{4}$$

3. Hence the irreducible subspaces $V(m_i)$ can be classified by ireps of the group G. We give them accordingly labels α which specify the class of irep by which the subspace transforms and labels $a = 1, 2, \ldots, n_\alpha$ which label individual subspaces belonging to the same class of ireps. The whole space is then a direct sum

$$V(n) = \bigoplus_{\alpha=1}^{|K|} \bigoplus_{a=1}^{n_\alpha} V_{\alpha,a}(d_\alpha) = \bigoplus_{\alpha=1}^{|K|} V_\alpha(n_\alpha d_\alpha), \tag{5}$$

where

$$V_\alpha(n_\alpha d_\alpha) = \bigoplus_{a=1}^{n_\alpha} V_{\alpha,a}(d_\alpha)$$

is the linear envelope of all spaces which transform by the irep of the class χ_α. The subspaces $V_\alpha(n_\alpha d_\alpha)$ are mutually orthogonal, while the subspaces $V_{\alpha a}(d_\alpha)$ can be chosen as orthogonal subspaces but also as non-orthogonal subspaces. The numbers $d_\alpha = \chi_\alpha(e)$ are the dimensions of irreducible subspaces $V_{\alpha a}(d_\alpha)$.

The fundamental theorem on representations

To each class $\chi_\alpha(G)$ of ireps of a specific group G we can choose one certain matrix irep $D^{(\alpha)} : g \longrightarrow D^{(\alpha)}(g)$. Let us consider any space $V(n)$ on which the group G acts as a group of linear operators. If this space splits into G-irreducible subspaces according to relation (5), it is possible to choose the bases $\{\mathbf{e}_{\alpha a,1}, \ldots, \mathbf{e}_{\alpha a,d_\alpha}\}$ of subspaces $V_{\alpha a}$ in such a manner that their vectors transform simultaneously by the same matrix irep $D^{(\alpha)}$, so that

$$g\mathbf{e}_{\alpha a,i} = \sum_{j=1}^{d_\alpha} D^{(\alpha)}_{ji}(g)\mathbf{e}_{\alpha a,j}. \tag{A}$$

If there is only one space $V_\alpha(d_\alpha)$ which transforms by an irep of the class χ_α, then the space is uniquely defined and the choice of the basis $\{\mathbf{e}_{\alpha,1}, \ldots, \mathbf{e}_{\alpha,d_\alpha}\}$ which transforms by matrices of $D^{(\alpha)}$ is unique up to a common factor. In other words, all bases which transform by this irep have the form $b\{\mathbf{e}_{\alpha,1}, \ldots, \mathbf{e}_{\alpha,d_\alpha}\} = \{b\mathbf{e}_{\alpha,1}, \ldots, b\mathbf{e}_{\alpha,d_\alpha}\}$, where b is a constant factor; if bases are to be unitary orthonormal, it must be $|b| = 1$, *i.e.* $b = \mathrm{e}^{i\varphi}$; to keep the basis real orthogonal, we have only the choice $b = \pm 1$. If the number of independent subspaces $V_{\alpha a}(d_\alpha)$ is $a = 1, 2, \ldots, n_\alpha > 1$ and their bases are $\{\mathbf{e}_{\alpha a,1}, \ldots, \mathbf{e}_{\alpha a,d_\alpha}\}$, then there exist alternative choices of subspaces $V_{\alpha b}(d_\alpha)$, $b = 1, 2, \ldots, n_\alpha$ with bases $\{\mathbf{e}_{\alpha b,1}, \ldots, \mathbf{e}_{\alpha b,d_\alpha}\}$, related to bases of subspaces $V_{\alpha a}(d_\alpha)$ by

$$\mathbf{e}_{\alpha b,j} = \sum_{a=1}^{n_\alpha} B_{ab}\mathbf{e}_{\alpha a,j}. \tag{i}$$

The counterpart of equations (A) and (i) for components $x_{\alpha a,i}$ of a vector $\mathbf{x} \in V(n)$ in the basis $\{\mathbf{e}_{\alpha a,1}, \ldots, \mathbf{e}_{\alpha a,d_\alpha}\}$ reads:

$$(g\mathbf{x})_{\alpha a,i} = \sum_{j=1}^{d_\alpha} D^{(\alpha)}_{ij}(g) x_{\alpha a,j}. \tag{B}$$

$$x_{\alpha b,j} = \sum_{a=1}^{n_\alpha} C_{ba} x_{\alpha a,j}, \tag{ii}$$

where $CB = BC = I$ or $C^{-1} = B$, $B^{-1} = C$. The matrices B and C have to be unitary or orthogonal if we want to keep the bases normalized.

Equations (A), (B) and transformations (i), (ii) constitute the basic relations of the theory of irreducible representations. The bases $\{\mathbf{e}_{\alpha a,1}, \ldots, \mathbf{e}_{\alpha a,d_\alpha}\}$ are further called the $D^{(\alpha)}(G)$-bases and the sets of variables $\mathbf{x}^{(\alpha)}_a = (x_{\alpha a,1}, \ldots, x_{\alpha a,d_\alpha})$ are called $D^{(\alpha)}(G)$-covariants. The name covariant is of classical origin (Weyl, 1946) and we use it instead of terms like *symmetry-adapted basis* or *form-invariant basis* which can be found in the literature. If the irep is one-dimensional, the matrices $D^{(\alpha)}(g)$, $g \in G$ are identical with characters $\chi_\alpha(g)$. In this case, a $\chi_\alpha(G)$-covariant takes the form of one variable $x_{\alpha a}$; such covariants are also called relative invariants and if $\chi_1(G)$ is the identity irep they are called invariants. Covariants are compact mathematical entities; we can define linear combinations of $D^{(\alpha)}(G)$-covariants and hence also the linear independence of $D^{(\alpha)}(G)$-covariants. The advantage of $D^{(\alpha)}(G)$-bases and of $D^{(\alpha)}(G)$-covariants is rather obvious. Instead of handling $n \times n$ matrices which express the action of G on the space $V(n)$ we have to work with minimal possible dimensions of irreducible subspaces which are transformed independently. Of course, if we want to use these advantages, we must develop methods for the calculation of $D^{(\alpha)}(G)$-bases and/or of $D^{(\alpha)}(G)$-covariants. This will be done below in the section Tensorial covariants for tensor spaces and in the section on the Extended integrity bases for polynomial spaces.

The content of this section is a consequence of Schur's lemma and it is valid only if we consider representations in the field of complex numbers C; we shall use the abbreviation C-irep or just irep. When considering tensor properties we use representations of real spaces and accordingly we also use the decomposition of these representations into representations which are irreducible over the real field R; sometimes they are called the "physically irreducible representations" or abbreviated as "pireps; we shall use the abbreviation R-irep. Some R-ireps do not reduce when the field is extended to C; to those ireps we can apply all results of the next section; some two-dimensional R-ireps reduce into pairs of complex conjugate C-ireps when the field is extended. The necessary amendment of the consequences is simple and we shall handle it in one standard manner later under the heading The standard transformations.

Remark: In spectroscopy, the consequence of the distinction between R-reducibility and C-reducibility is known as the *"Kramers degeneracy"*. In its general form, the relationship between R-ireps and C-ireps may be quite complicated. In our cases we are handling the simplest possible situation.

Explicit irreducible representations and typical variables: For the purposes of tabulation it is suitable to introduce rather abstract carrier spaces, bases and variables. The idea is very old and stems from the theory of invariants where an analogous approach is known as the symbolic method (Weitzenböck, 1923). For a given group G we introduce

the typical carrier space $V_o = \oplus_{\alpha=1}^{|K|} V_\alpha$ which contains exactly once a carrier space V_α for each class $\chi_\alpha(G)$ of ireps. In each class $\chi_\alpha(G)$ we choose a certain standard matrix irep $D^{(\alpha)}(G)$ of the group G. To this irep there corresponds a basis $\{\mathbf{e}_{a,1}, \ldots, \mathbf{e}_{\alpha,d_\alpha}\}$ called the typical $D^{(\alpha)}$-basis and a set of variables $\mathbf{x}^{(\alpha)} = (x_{\alpha,1}, \ldots, x_{\alpha,d_\alpha})$, called the typical variables. The whole set $\mathbf{x}^{(\alpha)}$ is called the typical $D^{(\alpha)}$-covariant. The concept has been revived together with the term covariant by the author (Kopský, 1976*a*) for the purposes of suitable recording and handling of transformation properties of tensors and of polynomials. The typical variables are now standardized in comparison with their original labelling; in tables they appear as standard typical variables.

The spectroscopic and standard nomenclature of ireps:

Spectroscopic notation: Again, there does not exist a unique and generally accepted symbolism of classes of ireps of the point groups. The most commonly used spectroscopic notation for classes of ireps uses letters A and B for one-dimensional ireps, E for two-dimensional ireps, and T for three-dimensional ireps [letters F, H, and I are used for the four-, five-, and six-dimensional ireps which appear either as ireps of the icosahedral group or as double-valued ireps of the cubic and icosahedral group; *cf.* Altmann & Herzig (1994) or Bradley & Cracknell (1972)]. The letters, if used more than once, are distinguished either by numerical subscripts or by primes and double primes.

The number of ireps of a centrosymmetric group $G_h = G \otimes I$ is twice the number of ireps of the group of proper rotations G and they are distinguished by parity. To each irep $\chi_\alpha(G)$ of G there correspond two ireps of G_h: $\chi_\alpha^+(G_h)$ of even parity and $\chi_\alpha^-(G_h)$ of odd parity. Matrices (and accordingly also characters) of a proper rotation g and respective improper rotation $ig = gi$ in the group G_h are identical with the matrix (and character) of g in the group G for the even-parity irep χ_α^+; for the odd-parity irep χ_α^- the matrix (and character) of ig has the opposite sign. In spectroscopic notation, these classes of ireps are distinguished by subscripts "g" (German *"gerade" = "even"*) and "u" (German *"ungerade" = "odd"*).

Uniaxial groups and groups T (23) and T_h ($m\overline{3}$) have two-dimensional real ireps which split in the field of complex numbers into two conjugate complex one-dimensional ireps. These one-dimensional ireps are denoted by ${}^1E$ and ${}^2E$ with numerical subscripts when more than one class of such ireps exists (in the case of crystallographic groups the subscripts are maximally 1 and 2) and with subscripts "g" and "u" if parity is to be distinguished. The respective real two-dimensional irep is then denoted by ${}^1E \oplus^2 E$.

Standard notation and standard typical variables: The spectroscopic notation is insufficient for our purposes because it specifies the classes of ireps, while we shall work with the explicit matrix form of ireps and with their respective bases. We developed a special notation for our purposes which is called here the standard notation. One of the advantages of this notation is the transparency of subduction relations which correlate the typical variables (and consequently all variables) for a group with variables for its subgroups. The scheme actually includes all finite groups and is extremely convenient for considering the transformation properties of tensors. First we shall describe the choice of the standard typical variables for groups of proper rotations.

Groups of proper rotations: The standard typical variables for real one-dimensional ireps are denoted by sans-serif letters x_i with numerical subscripts $i = 1, 2, 3, 4$. The index 1 is reserved for that variable which transforms by the identity irep χ_1 so that x_1

is the typical invariant. Other variables x_i are called the typical relative invariants because the actual variables transforming in the same way are usually called relative invariants.

The proper rotation groups D_2 $(2_x2_y2_z)$, D_{4z} $(4_z2_x2_{xy})$ and D_6 $(6_z2_x2_y)$ have four one-dimensional ireps and the labels are chosen so that the subscript 2 corresponds to an irep with kernel C_{2z} (2_z), C_{4z} (4_z) and C_6 (6_z), respectively, while subscript 3 corresponds to ireps with kernels C_{2x} (2_x), D_2 $(2_x2_y2_z)$ and D_{3x} (3_z2_x), subscript 4 to ireps with kernels C_{2y} (2_y), $\widehat{D}_2$ $(2_{xy}2_{x\overline{y}}2_z)$ and D_{3y} (3_z2_y). In other words, index 2 indicates that the variable x_2 does not change sign under rotations about the principal axis, index 3 indicates that the variable x_3 does not change sign under the twofold rotations about axes conjugate with 2_x and index 4 indicates that the variable x_4 does not change sign under the action of the other set of conjugate axes. This rule is extended to noncrystallographic proper rotation groups D_n $(n_z2_{x_1}2_{x_2})$ with even n.

The proper rotation groups D_{3x} (3_z2_x), D_{3y} (3_z2_y) and O (432) have two real one-dimensional ireps and the subscript 2 is used for the nontrivial irep. Hence x_2 is that variable which does not change sign under the rotations about the principal axis and changes sign under the rotation about auxiliary axes [in the case of group O (432) it does not change under the elements of the subgroup T (23) and changes sign under the action of elements from the coset 4_zT $(4_z.23)$]. Again, the same holds for noncrystallographic proper rotation groups D_n (n_z2_x) with odd n.

The subgroups C_{2z} (2_z), C_{4z} (4_z) and C_6 (6_z) have two one-dimensional ireps and the nontrivial irep is assigned the subscript 3. Accordingly, the subduction from the respective dihedral groups sends the variables x_1 and x_2 into x_1, the variables x_3 and x_4 into x_3.

The groups D_n and C_n with $n \geq 3$ have two-dimensional real ireps. These ireps are irreducible over the real field and for groups D_n also in the complex field. For the groups C_n they are reducible in the complex field into a pair of conjugate complex ireps. The variables (x_1, y_1) which appear in all these groups have the meaning of the components of an ordinary vector in the xy plane. The variables (x_2, y_2) which appear in groups D_6 and C_6 (actually, they already appear in the noncrystallographic groups D_5 and C_5) transform under a rotation by an angle φ about the z axis like components of an ordinary vector under a rotation by 2φ about the z axis. Analogously, variables (x_n, y_n), $n \geq 3$ which appear in noncrystallographic groups with higher order of the principal axis transform under a rotation by an angle φ about the z axis like components of an ordinary vector under a rotation by $n\varphi$ about the z axis. The index n of these variables has an informative value; it is equal to the lowest-rank tensor the components of which transform like these variables.

Two-dimensional real ireps also appear for groups T (23) and O (432), where variables are denoted by (x_3, y_3). This irep is irreducible over the complex field for the group O (432) and reducible into a pair of conjugate complex ireps in the group T (23).

The reduction of two-dimensional ireps is considered below on a unified basis for all cases in the section Standard transformations, where complex variables are introduced to complete the scheme and the consequences of the violation of conditions for Schur's lemma are explained.

Three-dimensional ireps appear for groups T (23) and O (432), where variables are denoted by (x_1, y_1, z_1). These variables transform like the components of a vector in the space $V(3)$. To the second three-dimensional irep of the group O (432) we assign variables (x_2, y_2, z_2) which transform like the product $\mathsf{x}_2(x_1, y_1, z_1)$ (see also the Clebsch–Gordan product tables, which are very illustrative for exploring various relations between transformation properties of standard typical variables).

Noncentrosymmetric groups: The standard typical variables for a noncentrosymmetric group $H \cup igH$ are identical to the standard variables of the respective group of proper rotations $G = H \cup gH$. Their transformation properties are defined so that each standard variable transforms under an element of $H \cup igH$ in the same way as under the respective element of the proper rotation group $G = H \cup gH$.

Centrosymmetric groups: A centrosymmetric group $G_h = G \otimes I = G \cup iG$ contains all elements $g \in G$ and of the coset $ig = gi \in iG = Gi$. The number of conjugacy classes is doubled as compared with conjugacy classes of G and the number of ireps and of variables is also doubled. Even and odd ireps are distinguished by superscripts $^+$ and $^-$, respectively; these superscripts indicate the parity of the variable under the action of the space inversion i; variables with the superscript $^+$ do not change sign, variables with the superscript $^-$ change sign under the action of i. Each variable x^+ then transforms in the same way under the action of both elements $g \in G$ and $ig \in iG$ as the variable x transforms under the element $g \in G$, while the variable x^- transforms under an element $g \in G$ in the same way as x and under the action of $ig \in iG$ it transforms in the same way as x under the action of $g \in G$ with an additional change of the sign.

Character and representation tables: Character tables represent historically an important tool for considering selection rules. Thus, in tensor calculus, it is possible to calculate quickly the number of linearly independent components of a tensor which belong to a particular irreducible representation. The number of those which belong to the identity representation is then the number of nonvanishing independent tensor parameters – invariants. Character tables are therefore also provided, although the program enables us to find more explicit results – instead of getting the numbers of tensorial components we can find an exact form of tensor components which transform like the typical variables (see the tables of tensorial covariants). To specify transformation properties of typical variables we have to specify the matrices of the group elements by which they transform.

Character tables are provided in the Standard and Spectroscopic notations, which are compared in the files Correlation Std./Spectro. As a standard notation of one-dimensional real characters we use the letter χ_i, $i = 1, 2, 3, 4$ with the same subscript as that of the respective variables x_i. Characters of two- and three-dimensional ireps are denoted by upper-case $\mathcal{X}_i$, $i = 1, 2, 3$ and characters of pairs of complex conjugate one-dimensional ireps are denoted by χ_{ic} and χ^*_{ic}, $i = 1, 2, 3$. For centrosymmetric groups we add the superscripts $^+$ and $^-$.

In the case of Abelian groups, the elements are also given either in the spectroscopic or standard notation; otherwise the characters are given as functions of conjugacy classes for which we use the same symbols in both cases.

Tables of explicit representations are given in an abbreviated form, where only the matrices of the group generators are presented, and in full where all distinct matrices are given. In these tables we use only the standard form. Characters of one-dimensional ireps coincide with transformation matrices for which we use the same symbols. For matrices of two-dimensional ireps we use the symbols $D^{(\alpha)}_R$ if they are real or $D^{(\alpha)}_C$ if they are complex; the three-dimensional ireps are given only in a real form.

The standard transformations

The action of a rotation by φ around the z axis, denoted as an operator $g(\varphi)$, is expressed in the Cartesian basis ($\mathbf{e}_x$, $\mathbf{e}_y$, $\mathbf{e}_z$) by the equations

$$g(\varphi)\mathbf{e}_x = \mathbf{e}_x.\cos\varphi + \mathbf{e}_y.\sin\varphi,$$

$$g(\varphi)\mathbf{e}_y = -\mathbf{e}_x.\sin\varphi + \mathbf{e}_y.\cos\varphi,$$

$$g(\varphi)\mathbf{e}_z = \mathbf{e}_z,$$

to which there corresponds a matrix

$$D_R^{(1)}[g(\varphi)] = \begin{pmatrix} \cos\varphi & -\sin\varphi & 0 \\ \sin\varphi & \cos\varphi & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

of a real vector representation $D_R^{(1)}$. These vectors transform under the action of a twofold rotation 2_x as

$$2_x\mathbf{e}_x = \mathbf{e}_x \quad 2_x\mathbf{e}_y = -\mathbf{e}_y \quad 2_x\mathbf{e}_z = -\mathbf{e}_z,$$

which is expressed by the matrix:

$$D_R^{(1)}(2_x) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}.$$

We introduce standard typical vectors ($\mathbf{e}_{nx}$, $\mathbf{e}_{ny}$) in the $x_n y_n$ plane which transform by definition under the action of $g(\varphi)$ and 2_x according to equations:

$$g(\varphi)\mathbf{e}_{nx} = \mathbf{e}_{nx}.\cos n\varphi + \mathbf{e}_{ny}.\sin n\varphi,$$

$$g(\varphi)\mathbf{e}_{ny} = -\mathbf{e}_{nx}.\sin n\varphi + \mathbf{e}_{ny}.\cos n\varphi,$$

$$2_x\mathbf{e}_{nx} = \mathbf{e}_{nx}, \quad 2_x\mathbf{e}_{ny} = -\mathbf{e}_{ny}.$$

To these transformations there correspond the matrices

$$D_R^{(n)}[g(\varphi)] = \begin{pmatrix} \cos n\varphi & -\sin n\varphi \\ \sin n\varphi & \cos n\varphi \end{pmatrix} \quad \text{and} \quad D_R^{(n)}(2_x) = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

of a real vector representation $D_R^{(n)}$.

We introduce a standard transformation to complex vectors and variables:

$$\mathbf{e}_{n\xi} = \frac{1}{\sqrt{2}}(\mathbf{e}_{nx} - i\mathbf{e}_{ny}), \quad \mathbf{e}_{n\eta} = \frac{1}{\sqrt{2}}(\mathbf{e}_{nx} + i\mathbf{e}_{ny}),$$

$$\xi_n = \frac{1}{\sqrt{2}}(x_n + iy_n), \quad \eta_n = \frac{1}{\sqrt{2}}(x_n - iy_n).$$

The reciprocal transformation then reads:

$$\mathbf{e}_{nx} = \frac{1}{\sqrt{2}}(\mathbf{e}_{n\xi} + \mathbf{e}_{n\eta}), \quad \mathbf{e}_{ny} = \frac{i}{\sqrt{2}}(\mathbf{e}_{n\xi} - i\mathbf{e}_{n\eta}),$$

$$x_n = \frac{1}{\sqrt{2}}(\xi_n + \eta_n), \quad y_n = \frac{i}{\sqrt{2}}(\eta_n - \xi_n).$$

Vectors are then expressed in the two bases as

$$\mathbf{x}_n = x_n \mathbf{e}_{nx} + y_n \mathbf{e}_{ny} = \xi_n \mathbf{e}_{n\xi} + \eta_n \mathbf{e}_{n\eta},$$

and the transformation properties of complex vectors and bases are expressed by

$$g(\varphi)\mathbf{e}_{n\xi} = \mathrm{e}^{in\varphi}\mathbf{e}_{n\xi}, \quad g(\varphi)\mathbf{e}_{n\eta} = \mathrm{e}^{-i\varphi}\mathbf{e}_{n\eta}$$

$$2_x\mathbf{e}_{n\xi} = \mathbf{e}_{n\eta}, \quad 2_x\mathbf{e}_{n\eta} = \mathbf{e}_{n\xi},$$

so that the rotations are expressed by matrices:

$$D_C^{(n)}[g(\varphi)] = \begin{pmatrix} \mathrm{e}^{in\varphi} & 0 \\ 0 & \mathrm{e}^{-in\varphi} \end{pmatrix} \quad \text{and} \quad D_C^{(n)}(2_x) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

The real pair of variables (x_n, y_n) is transformed to a complex pair (ξ_n, η_n) and the real matrix irep $D_R^{(n)}$ to an equivalent complex matrix irep $D_C^{(n)}$. Both ireps are irreducible for groups D_n, $n \geq 3$ because the twofold rotation 2_x swaps the vectors $\mathbf{e}_{n\xi}$, $\mathbf{e}_{n\eta}$ as well as the variables ξ_n, η_n.

Matrices $D_C^{(n)}[g(\varphi)]$ are, however, quasidiagonal (in fact they are diagonal) and correspond to a pair of one-dimensional complex conjugate ireps. Two-dimensional representations of uniaxial groups and of groups T (23) and T_h ($m\overline{3}$) are therefore irreducible over the real field, but they split into a pair of one-dimensional complex conjugate ireps in the complex field. As a consequence, the pair of variables (x_n, y_n) transforms in the same way as the pair $(y_n, -x_n)$.

Kronecker products: If the basis vectors $(\mathbf{e}_{\alpha,1}, \mathbf{e}_{\alpha,2}, \ldots, \mathbf{e}_{\alpha,d_\alpha})$ of the carrier space V_α for an irep $D^{(\alpha)}(G)$ are combined with the basis vectors $(\mathbf{e}_{\beta,1}, \mathbf{e}_{\beta,2}, \ldots, \mathbf{e}_{\beta,d_\beta})$ of the carrier space V_β for an irep $D^{(\beta)}(G)$, we obtain a set of $d_\alpha d_\beta$ basis vectors $(\mathbf{e}_{\alpha,i}\mathbf{e}_{\beta,j})$ of the carrier space $V_\alpha \otimes V_\beta$ which is called the direct or tensor product of spaces V_α and V_β. The action of the group G on this space is defined by the relation:

$$g(\mathbf{e}_{\alpha,i_\alpha}\mathbf{e}_{\beta,i_\beta}) = \sum_{j_\alpha=1}^{d_\alpha} \sum_{j_\beta=1}^{d_\beta} D^{(\alpha)}_{j_\alpha i_\alpha}(g) D^{(\beta)}_{j_\beta i_\beta}(g)(\mathbf{e}_{\alpha,j_\alpha}\mathbf{e}_{\beta,j_\beta}).$$

The matrix representation $D^{(\alpha,\beta)}(G)$ in terms of matrices of elements $g \in G$,

$$D^{(\alpha,\beta)}_{(j_\alpha j_\beta)(i_\alpha i_\beta)}(g) = D^{(\alpha)}_{j_\alpha i_\alpha}(g) D^{(\beta)}_{j_\beta i_\beta}(g),$$

is called the direct or Kronecker product of matrix representations $D^{(\alpha)}(G)$ and $D^{(\beta)}(G)$ and denoted by $D^{(\alpha,\beta)}(G) = D^{(\alpha)}(G) \otimes D^{(\beta)}(G)$.

The latter space is generally reducible and spaces of the type V_γ appear in the reduction with certain multiplicities $m_{(\alpha,\beta|\gamma)} = (1/|G|)\sum_{g\in G} \chi_\alpha(g)\chi_\beta(g)\chi^*_\gamma(g)$. If the two spaces in the product belong to the same irep $D^{(\alpha)}(G)$, then the product space $V_\alpha \otimes V_\alpha$ splits into the space of symmetric and antisymmetric combinations:

$$\frac{1}{\sqrt{2}}(\mathbf{e}_{\alpha,i_\alpha}\mathbf{e}_{\alpha,j_\alpha} + \mathbf{e}_{\alpha,j_\alpha}\mathbf{e}_{\alpha,i_\alpha}) \quad \text{and} \quad \frac{1}{\sqrt{2}}(\mathbf{e}_{\alpha,i_\alpha}\mathbf{e}_{\alpha,j_\alpha} - \mathbf{e}_{\alpha,j_\alpha}\mathbf{e}_{\alpha,i_\alpha}).$$

The spaces are usually denoted as $[V_\alpha]^2$ for the symmetric case and $\{V_\alpha\}^2$ for the antisymmetric case and both spaces are invariant under the action of G and are generally reducible. The multiplicities then split into the sum of multiplicities for the symmetric and antisymmetric part: $m_{(\alpha,\alpha|\gamma)} = m_{[\alpha,\alpha|\gamma]} + m_{\{\alpha,\alpha|\gamma\}}$. This theory boils down in practice to tables of Kronecker products which are again given in the Spectroscopic and Standard notation. Rows and columns correspond to ireps in either of the notations and at the intersections are found direct sums of ireps into which the product of two ireps splits; if the resulting irep corresponds to a space of antisymmetric combinations, the respective symbol is given in braces.

These tables facilitate the calculation of selection rules and they are widely used in spectroscopy. They can be used to calculate the numbers of independent tensor components and hence to find how many new independent parameters appear in a tensor at a phase transition or the numbers of components in which two domain states differ. The tables of Clebsch–Gordan products, described in the next section, represent an explicit counterpart of the Kronecker product tables.

Clebsch–Gordan products: The calculations underlying this program were performed by the method of Clebsch–Gordan products in typical variables. The method stems originally from the theory of quantum momentum. Irreducible representations of the orthogonal group $\mathcal{O}(3)$ are labelled by the quantum number j of the total momentum and the wave functions ψ_{jm} form irreducible spaces of dimension $2j+1$ with $m = -j, \ldots, j-1, j$ where m defines the projection of the momentum on a chosen axis, usually the z axis. In a system of two particles in spherical field, the total wave function Ψ_{JM} is expressed as:

$$\Psi_{JM} = \sum_{m_1+m_2=M} (j_1 m_1 j_2 m_2 | JM) \psi_{j_1 m_1} \psi_{j_2 m_2}, \qquad \text{(iii)}$$

where $(j_1 m_1 j_2 m_2|JM)$ are the so-called Clebsch–Gordan coefficients, also called the coefficients of vector addition.

Quite analogously we can introduce Clebsch–Gordan coefficients for the multiplication of irreducible representations of any group G. The direct product $V_\alpha \otimes V_\beta$ of two typical irreducible spaces splits according to the fundamental theorem of representations into irreducible subspaces $V_{\gamma m}$, where $m = 1, 2, \ldots, m_{(\alpha,\beta|\gamma)} = \frac{1}{|G|} \sum_{g\in G} \chi_\alpha \chi_\beta \chi_\gamma^*$. The generalized Clebsch–Gordan formula reads:

$$\mathbf{E}_{\gamma k}^{(m)} = \sum_{i=1}^{d_\alpha} \sum_{j=1}^{d_\beta} (\alpha i \beta j | \gamma k)^{(m)} \mathbf{e}_{\alpha,i} \mathbf{e}_{\beta,j}. \qquad \text{(iv)}$$

The label m does not appear in the classical formula (iii) because multiplicities are in this case always $m(j_1, j_2|J) = 1$. We can also rewrite the latter formula in terms of the standard variables:

$$X_{\gamma k}^{(m)} = \sum_{i=1}^{d_\alpha} \sum_{j=1}^{d_\beta} (\alpha i \beta j | \gamma k)^{(m)*} x_{\alpha i} x_{\beta j}, \qquad \text{(v)}$$

and in the case $\alpha = \beta$ we also have to distinguish the symmetrized and antisymmetrized cases. Clebsch–Gordan coefficients $(\alpha i \beta j|\gamma k)^{(m)}$ for the crystal point groups were calculated by Koster, Dimmock, Wheeler & Statz (1963). They are important in quantum-mechanical calculations when orthonormality of wave functions is required.

Our aim is to find transformation properties of tensors and polynomials and we can disregard the normalization conditions. For calculations of this type, tables of Clebsch–Gordan products are more convenient. Without writing formulas, we define Clebsch–Gordan products as those $D^{(\gamma)}$-covariants whose components are bilinear combinations of components of a $D^{(\alpha)}$-covariant $(x_{\alpha 1}, \ldots, x_{\alpha d_\alpha})$ and a $D^{(\beta)}$-covariant $(x_{\beta 1}, \ldots, x_{\beta d_\beta})$. The number of such independent covariants is given by Kronecker products but their calculation for the crystal point groups is relatively easy. They are collected in tables where the heading of each table lists the typical $D^{(\gamma)}$-covariants and in the column headed by such a covariant are given bilinear combinations of typical variables which transform in the same way as the variables $(x_{\gamma 1}, \ldots, x_{\gamma d_\gamma})$. This is actually just another way of recording the full set of relations (v); to get the Clebsch–Gordan coefficients from tables of Clebsch–Gordan products it is sufficient to perform the normalization.

It is necessary to realize that variables in tables are just the representatives of actual variables. In the calculation of the tensor product of any two spaces V_1 and V_2, we first find the linear combinations of vector components in the two spaces which transform like the typical variables. In this procedure, several actual covariants may appear corresponding to some ireps. The tables give a prescription for how to form bilinear combinations of them with the desired transformation properties. Such tables were published and their use described a quarter of century ago (Kopský, 1976*a*; 1977).

Trivial Clebsch–Gordan products $\mathsf{x}_1(x_{\alpha 1}, \ldots, x_{\alpha d_\alpha})$ and $(x_{\alpha 1}, \ldots, x_{\alpha d_\alpha})\mathsf{x}_1$ are not explicitly written down in the tables; it is clear that they transform like $(x_{\alpha 1}, \ldots, x_{\alpha d_\alpha})$. The antisymmetric expressions like $x_1 y_1 - y_1 x_1$ express formally all possible bilinear combinations $x_1^{(a)} y_1^{(b)} - y_1^{(a)} x_1^{(b)}$, where a, b label various spaces and such combination vanishes when $a = b$. To a product such as $\mathsf{x}_3\mathsf{x}_4$ there naturally corresponds the product $\mathsf{x}_4\mathsf{x}_3$ which is not given in the tables. If replaced by actual variables, we have to distinguish the symmetric $(\mathsf{x}_3^{(a)}\mathsf{x}_4^{(b)} + \mathsf{x}_4^{(a)}\mathsf{x}_3^{(b)})$ and antisymmetric $(\mathsf{x}_3^{(a)}\mathsf{x}_4^{(b)} - \mathsf{x}_4^{(a)}\mathsf{x}_3^{(b)})$ combinations which both transform like the product $\mathsf{x}_3\mathsf{x}_4$. Analogous considerations hold in the case of products of the type $\mathsf{x}_\alpha(x_1, y_1, z_1)$ to which there correspond products $(x_1, y_1, z_1)\mathsf{x}_\alpha$. Quite generally, for a certain Clebsch–Gordan product which combines variables of two ireps of different classes in a certain order, there exists a Clebsch–Gordan product in which the order is reversed. If the typical variables are then replaced by actual ones, we should create the symmetric and antisymmetric combinations.

The tables are given in terms of variables which corresponds to relation (v). Analogous tables can be written for basis vectors. The presentation in terms of variables (components of vectors) is more convenient for us to proceed further.

Tensorial covariants: Let us now consider a tensor space $V^{(A)}$ under the action of the group $G \subseteq \mathcal{O}(3)$. According to the fundamental theorem of irreducible representations, the space splits into a direct sum $V^{(A)} = \oplus_{\alpha=1}^{|K|} \oplus_{a=1}^{n_\alpha} V_{\alpha a}^{(A)}$ of linearly independent subspaces $V_{\alpha a}^{(A)}$ which are irreducible under the action of G and in which we can find bases $\{\mathbf{e}_{\alpha a,1}^{(A)}, \mathbf{e}_{\alpha a,2}^{(A)}, \ldots, \mathbf{e}_{\alpha a,d_\alpha}^{(A)}\}$ which transform according to:

$$g\mathbf{e}_{\alpha a,i}^{(A)} = \sum_{j=1}^{d_\alpha} D_{ji}^{(\alpha)}(g)\mathbf{e}_{\alpha a,j}^{(A)}.$$

If we know the character $\mathcal{X}^{(A)}(g) = \mathrm{Tr}\ D^{(A)}(g)$ of the tensor representation of G on $V^{(A)}$, the number n_α of linearly independent subspaces which transform by an irep of the class $\chi_\alpha(G)$ can be found from character theory using $n_\alpha = (1/|G|)\sum_{g\in G} \mathcal{X}^{(A)}(g)\chi_\alpha^*(g)$.

Finally, if $n_\alpha > 1$, the decomposition $V_\alpha^{(A)} = \oplus_{a=1}^{n_\alpha} V_{\alpha a}^{(A)}$ of the G-invariant subspace $V_\alpha^{(A)}$ enveloping all subspaces $V_{\alpha a}^{(A)}$ which transform by ireps of the class χ_α is not unique. Each basis of the set of n_α bases $\{\mathbf{e}_{\alpha b,1}^{(A)}, \mathbf{e}_{\alpha b,2}^{(A)}, \ldots, \mathbf{e}_{\alpha b,d_\alpha}^{(A)}\}$ created by formula (i) transforms in the same way under G as the bases $\{\mathbf{e}_{\alpha a,1}^{(A)}, \mathbf{e}_{\alpha a,2}^{(A)}, \ldots, \mathbf{e}_{\alpha a,d_\alpha}^{(A)}\}$ and spans a subspace $V_{\alpha b}$, the direct sum of which is again the space $V_\alpha^{(A)} = \oplus_{b=1}^{n_\alpha} V_{\alpha b}^{(A)}$.

The tensor $\mathbf{A} \in V^{(A)}$ is expressed as

$$\mathbf{A} = \sum_{i \in I(\mathbf{A})} A_i \mathbf{e}_i^{(A)} = \sum_{\alpha=1}^{|K|} \sum_{a=1}^{n_\alpha} \sum_{i=1}^{d_\alpha} A_{\alpha a,i} \mathbf{e}_{\alpha a,i}^{(A)} = \sum_{\alpha=1}^{|K|} \sum_{b=1}^{n_\alpha} \sum_{i=1}^{d_\alpha} A_{\alpha b,i} \mathbf{e}_{\alpha b,i}^{(A)},$$

where A_i are its components in the Cartesian basis $\{\mathbf{e}_i\}_{i \in I(\mathbf{A})}$ while the sets $A_{\alpha a,i}$ and $A_{\alpha b,i}$ are its components in $D^{(\alpha)}(G)$-bases $\{\mathbf{e}_{\alpha a,1}, \mathbf{e}_{\alpha a,2}, \ldots, \mathbf{e}_{\alpha a,d_\alpha}\}$ or $\{\mathbf{e}_{\alpha b,1}, \mathbf{e}_{\alpha b,2}, \ldots, \mathbf{e}_{\alpha b,d_\alpha}\}$. The sets $\mathbf{A}_a^{(\alpha)} = (A_{\alpha a,1}, A_{\alpha a,2}, \ldots, A_{\alpha a,d_\alpha})$ and $\mathbf{A}_b^{(\alpha)} = (A_{\alpha b,1}, A_{\alpha b,2}, \ldots, A_{\alpha b,d_\alpha})$ are, by their transformation properties, $D^{(\alpha)}(G)$-covariants. We can now justify again the use of the term *"covariant"*. The linear combination of $D^{(\alpha)}(G)$-covariants is again a $D^{(\alpha)}(G)$-covariant and covariants themselves constitute linear spaces, so the concept of linear independence applies to them.

Calculation of tensorial covariants: As we concluded at the end of the section Tensorial representations, we want to avoid calculation of the matrices $D_{ij}^{(A)}(g)$. If, instead of that, we find the $D^{(\alpha)}(G)$-bases, we can handle the transformations of tensors in these bases in the simplest possible manner. It is even more suitable for our purposes to find the sets of linearly independent tensorial covariants to each point group.

The tables of tensorial covariants in this software describe the transformation properties of tensors whose symbols, intrinsic symmetries and numbers of independent components are given in Table 1.

Table 1. Symbols of tensors up to fourth rank

	Rank	Jahn symbol	Physical meaning of the tensor	Number of independent components
Tensors of material properties				
ε	0	ε	chirality, enantiomorphism	± 1
P_i	1	V	vector, polarization	3
u_i	2	$[V]^2$	stress or deformation tensor, permittivity	6
g_i	2	εV^2	gyrotropic tensor	6
d_{ij}	3	$V[V]^2$	piezoelectricity	18
A_{ij}	3	$\varepsilon V[V]^2$	electro-optic tensor	18
s_{ij}	4	$[[V]^2]^2$	tensor of the elastic stiffness	21
Q_{ij}	4	$([V]^2)^2$	elasto-optic tensor	36

The intrinsic symmetry of physical tensors is denoted by Jahn symbols (Jahn, 1949). A scalar does not need a symbol or it may be denoted by 1 and it always transforms as an invariant because it is the invariant of the group $\mathcal{O}(3)$. A pseudoscalar is denoted by ε. A vector is denoted by V. The last column of Table 1 indicates the number of independent components of each tensor considered. This number must be equal to $\sum_{\alpha=1}^{|K|} n_\alpha^{(A)} d_\alpha$, where $n_\alpha^{(A)}$ is the multiplicity with which an irep of the class $\chi_\alpha(G)$ appears in the tensor representation $\mathcal{X}^{(A)}(G)$ and d_α is its dimension. Therefore $n_\alpha^{(A)}$ is also the number of independent $D_\alpha(G)$-covariants.

Tables of tensorial covariants have been calculated by the consecutive use of Clebsch–Gordan products. In the first step, we determine the transformation properties of a vector, which is represented by the polarization $\mathbf{P} = (P_1, P_2, P_3)$, and of a pseudoscalar ε. The heading row of each table lists the typical variables in the form of $D^{(\alpha)}(G)$-covariants. We know that the components of the deformation tensor $\mathbf{u}$ (or alternatively of the permittivity ϵ) transform like symmetrized bilinear combinations of a vector, *i.e.* $u_1 \approx P_1^2$, $u_2 \approx P_2^2$, $u_3 \approx P_3^2$, $u_4 \approx (P_2P_3 + P_3P_2)$, $u_5 \approx (P_3P_1 + P_1P_3)$, $u_6 \approx (P_1P_2 + P_2P_1)$. Hence, if we know how P_1, P_2, P_3 map onto typical variables, we can read at once from tables of Clebsch–Gordan products how linear combinations of u_1, u_2, u_3, u_4, u_5, u_6 are mapped onto the typical variables. Next we know that the components d_{ij} of the piezoelectric tensor transform like the products $d_{ij} \approx P_i u_j$, the components of the elastic stiffness tensor transform like $s_{ij} \approx (u_i u_j + u_j u_i)$, the components of the gyrotropic tensor like $g_i \approx \varepsilon u_i$, the components of the electro-optic tensor like $A_{ij} \approx \varepsilon d_{ij}$ and the components of the elasto-optic tensor like $Q_{ij} \approx u_i u_j$. The symbol $\approx$ means here and from now on: transforms like.

Example: For the group D_6 $(6_z 2_x 2_y)$ we get the transformation properties as follows: $\varepsilon \approx \mathsf{x}_1$, $P_3 \approx \mathsf{x}_2$, $(P_1, P_2) \approx (x_1, y_1)$. From Clebsch–Gordan tables we further find: $u_1+u_2 \approx P_1^2+P_2^2 \approx x_1^2+y_1^2 \approx \mathsf{x}_1$, $u_3 \approx P_3^2 \approx (\mathsf{x}_2)^2 \approx \mathsf{x}_1$, $u_1-u_2 \approx P_1^2-P_2^2 \approx x_1^2-y_1^2 \approx x_2$. In the case of the component u_6 we have $u_6 \approx P_1P_2 \approx P_2P_1$ but the $D^{(2)}(D_6)$-covariant is $(P_1^2 - P_2^2, P_1P_2 + P_2P_1)$; hence the corresponding $D^{(2)}(D_6)$-covariant in components of tensor $\mathbf{u}$ is $(u_1 - u_2, 2u_6)$. Finally, from the $D^{(1)}(D_6)$-covariant $\mathsf{x}_2(y_1, -x_1)$ we get the $D^{(1)}(D_6)$-covariant $P_3(P_1, -P_2) \approx (u_4, -u_5)$. Thus we have a complete set of covariants for the tensor $\mathbf{u}$.

Let us now see the $D^{(1)}(D_6)$-covariant $(x_1x_2 + y_1y_2, x_1y_2 - y_1x_2)$ as a product of a $D^{(1)}(D_6)$-covariant (P_1, P_2) and of a $D^{(2)}(D_6)$-covariant $(u_1 - u_2, 2u_6)$. We get the $D^{(1)}(D_6)$-covariant $(d_{11} - d_{12} + 2d_{26}, 2d_{16} - d_{21} + d_{22})$. On the other hand, we have the $D^{(1)}(D_6)$-covariant $\mathsf{x}_1(x_1, y_1) \approx (u_1+u_2)(P_1, P_2) \approx (d_{11}+d_{21}, d_{22}+d_{21})$. The sum of these two covariants divided by 2 gives another $D^{(1)}(D_6)$-covariant $(d_{11} + d_{26}, d_{22} + d_{16})$ which is listed in the table together with the $D^{(1)}(D_6)$-covariant $(d_{11} + d_{21}, d_{22} + d_{21})$.

The tables of tensorial covariants presented in this software were calculated and published more than two decades ago (Kopský, 1979*a*,*b*). Together with tables of domain structures (here we mean the algebraic structure of tensor characteristics assigned to different domains) (Kopský, 1982, 1983) they constitute a background for various calculations connected with tensor changes at ferroic phase transitions including the distinction of domain pairs and the change of tensor properties on a path across domain walls. The tables in the software differ from the originals by the systematic choice of symbols and numerical labels of standard variables. While there exist several textbooks in which the invariant form of tensors for representative group orientations are given (Voigt, 1910;

Nye, 1957; Birss, 1964; Sirotin & Shaskolskaya, 1975), there exist, as far as we know, only attempts to calculate tensorial bases of ireps by Callen (1968) and later by Callen, Callen & Kalva (1970) for very low tensor rank. Janovec, Dvořák & Petzelt (1975) found some tensorial bases for ireps, but not always the lowest possible. The central tables of the software, which provide information about changes of tensors up to fourth rank and for both parities, are derived with the use of tables of tensorial covariants. In these tables appear generally linear combinations of tensor components as parameters of the transition. It is actually suitable to consider these components as the parameters of tensors and of their changes in ferroic transitions as shown below in the description of a procedure (Kopský, 2001*b*,*c*,*d*) consisting of the Labelling of covariants and calculation of Conversion equations.

Opechowski's magic relations: It is also worthwhile to mention that there exist systematic relations between tensorial covariants of different parities and groups of the same oriented Laue class. Investigation of such relations was inspired by Opechowski's question about the so-called "magic numbers" (Opechowski, 1975), which was rather promptly answered by Kopský (1976*b*). As an example we suggest that the reader looks up and compares tensorial covariants for the tensors $\mathbf{u}$ and $\mathbf{g}$. They have the same transformation properties for groups of proper rotations. In general, $\mathbf{g}$ transforms as $\varepsilon\mathbf{u}$ and $\varepsilon \approx \mathsf{x}_1$ for proper rotation groups. For other groups of the oriented Laue class, ε transforms like one of the variables x_2, x_3, x_4, and for centrosymmetric groups like x_1^+. We have the same relationship between tensors $\mathbf{A} \approx \varepsilon\mathbf{d}$.

If you go through the tables of tensorial covariants, you can observe that tensorial covariants of tensors of *even parity* with respect to space inversion i, which here are the tensors $\mathbf{u}$, $\mathbf{A}$, $\mathbf{s}$ and $\mathbf{Q}$, are identical for all groups of the oriented Laue class, and for a centrosymmetric group they acquire the superscript $^+$. On the other hand, tensors of *odd parity* with respect to space inversion i transform in the same manner as the respective tensors of even parity under the group of proper rotations, while for the remaining groups of the oriented Laue class the blocks of relative tensorial invariants exchange places and tensorial covariants are transformed according to rules that can be found from the Clebsch–Gordan tables. The basic rules were explained in the second paper on tensorial covariants (Kopský, 1979*b*) and later rediscovered by Grimmer (1991) in a less general form.

The relations which exist between tensorial covariants of tensors of the same intrinsic symmetries but different parities with respect to the space inversion i, time inversion e' and combined space–time inversion $i' = ie' = e'i$ under the action of magnetic groups of the same oriented Laue class deserve special attention in view of their prominence in a systematic approach. They are strongly connected with our choice of standard typical variables and it is our belief that they should be proliferated as a textbook material in tensor calculus. A complete scheme of their use under the name "Opechowski's magic relations" has been prepared for publication.

Labelling of covariants and Conversion equations: Any tensor $\mathbf{A} \in V^{(A)}$ can be expressed as

$$\mathbf{A} = \sum_{i \in I(\mathbf{A})} A_i \mathbf{e}_i^{(A)} = \sum_{\alpha=1}^{|K|} \sum_{a=1}^{n_\alpha^{(A)}} \sum_{j=1}^{d_\alpha} A_{\alpha a,j}(G) \mathbf{e}_{\alpha a,j}^{(A)}(G),$$

where the first expression depends only on the choice of the index set $I(\mathbf{A})$, while the second expression depends on the group G, on the choice of its ireps and even on the

possible choice of bases $\{\mathbf{e}^{(A)}_{\alpha a,1}(G), \mathbf{e}^{(A)}_{\alpha a,2}(G), \ldots, \mathbf{e}^{(A)}_{\alpha a,d_\alpha}(G)\}$.

The latter bases are linear combinations of Cartesian bases

$$\mathbf{e}^{(A)}_{\alpha a,j}(G) = \sum_{i\in I(\mathbf{A})} C^{(A)}_{i;\alpha a,j}(G)\mathbf{e}^{(A)}_i$$

and there exist relations which convert these bases back to Cartesian ones,

$$\mathbf{e}^{(A)}_i = \sum_{\alpha=1}^{|K|}\sum_{a=1}^{n_\alpha(A)}\sum_{j=1}^{d_\alpha} B^{(A)}_{\alpha a,j;i}(G)\mathbf{e}^{(A)}_{\alpha a,j}(G),$$

where $C^{(A)}_{i;\alpha a,j}(G)$ and $B^{(A)}_{\alpha a,j;i}(G)$ are elements of $n^{(A)} \times n^{(A)}$ mutually reciprocal matrices ($n^{(A)} = \dim V^{(A)}$), so that $CB = BC = I_{n^{(A)}}$ or explicitly:

$$\sum_{\alpha=1}^{|K|}\sum_{a=1}^{n^{(A)}_\alpha}\sum_{j=1}^{d_\alpha} C^{(A)}_{i;\alpha a,j}(G)B^{(A)}_{\alpha a,j;k}(G) = \delta_{ik} \quad \text{and} \quad \sum_{j\in I(\mathbf{A})} B^{(A)}_{\alpha a,i;j}(G)C^{(A)}_{j;\beta b,k}(G) = \delta_{\alpha\beta}\delta_{ab}\delta_{ik}.$$

Applying transformations to tensor components instead of to tensorial bases, we obtain the relations

$$A_{\alpha a,j}(G) = \sum_{i\in I(\mathbf{A})} B^{(A)}_{\alpha a,j;i}(G)A_i \quad \text{and} \quad A_i = \sum_{\alpha=1}^{|K|}\sum_{a=1}^{n_\alpha}\sum_{j=1}^{d_\alpha} C^{(A)}_{i;\alpha a,j}(G)A_{\alpha a,j}(G).$$

The pairs of these relations are given in Appendix E, where the first relations are listed as the Labelling of covariants, the second as the Conversion equations. The relations are given for groups of proper rotations and for tensors that are invariant under the space inversion i starting from the tetragonal groups. They are not necessary for groups up to orthorhombic because ireps of these groups are one-dimensional and covariants (relative invariants) to these ireps for groups in standard orientations are identical with Cartesian components.

The first set of these relations simply assigns certain symbols to covariant tensor components as they are given in tables of tensorial covariants. The rules for the labelling of covariants are very simple. For each tensor we use the same letter as for the Cartesian components. Relative invariants are denoted by sans serif fonts with the same index as the respective typical variable. If there is more than one relative invariant to a given irep, a second index is used to distinguish these invariants. Covariants are denoted by a boldface letter with a superscript in parentheses indicating the label of the irep, and a subscript labelling individual covariants. Their components contain the irep label followed by a letter x, y or z indicating the component.

Example 1: We consider the group $6_z2_x2_y$ (D_6) and the electro-optic tensor $\mathbf{A}$. There is only one invariant denoted by A_1, three χ_2-covariants $\mathsf{A}_{2,1}$, $\mathsf{A}_{2,2}$, $\mathsf{A}_{2,3}$, one χ_3-covariant A_3, and one χ_4-covariant A_4. Then there are four $D^{(1)}_R$-covariants $\mathsf{A}^{(1)}_1 = (A_{1x,1}, A_{1y,1})$, $\mathsf{A}^{(1)}_2 = (A_{1x,2}, A_{1y,2})$, $\mathsf{A}^{(1)}_3 = (A_{1x,3}, A_{1y,3})$, $\mathsf{A}^{(1)}_4 = (A_{1x,4}, A_{1y,4})$, and two $D^{(2)}_R$-covariants $\mathsf{A}^{(2)}_1 = (A_{2x,1}, A_{2y,1})$, $\mathsf{A}^{(2)}_2 = (A_{2x,2}, A_{2y,2})$.

It is important to realize that the number of independent covariant components is the same as the number of independent Cartesian tensor components. The invariant components are suitable tensor parameters for describing a tensor allowed by the symmetry $6_z2_x2_y$, while covariant components are suitable tensor parameters for considering the change of tensor properties at a transition with parent group $6_z2_x2_y$, as we show below.

Example 2: We shall now illustrate briefly how the labelling of covariants and hence also the conversion equations can be extended to other tensors of the same intrinsic symmetry and to other groups of the same oriented Laue class. The piezoelectric tensor $\mathbf{d}$ has the same transformation properties under the group $6_z2_x2_y$ as the electro-optic tensor $\mathbf{A}$. The labelling of covariants and the conversion equations for this tensor are therefore obtained if we replace all letters A by letter d, using the same font types and the same indices and superscripts.

Let us now consider the group $6_zm_xm_y$ (C_{6v}). Comparing tensorial covariants we see that they contain the same linear combinations as in the previous case; the only thing which changes is the labelling of these combinations. Thus we have now three invariants $\mathsf{d}_{1,1} = d_{31} + d_{32}$, $\mathsf{d}_{1,2} = d_{15} + d_{24}$, $\mathsf{d}_{1,3} = d_{33}$, one χ_2-covariant $\mathsf{d}_2 = d_{14} - d_{25}$, one χ_3-covariant $\mathsf{d}_3 = d_{22} - d_{21} - 2d_{16}$, and one χ_4-covariant $\mathsf{d}_4 = d_{11} - d_{12} - 2d_{26}$. In the case of $D_R^{(\alpha)}$-covariants we have to replace $d_{\alpha x,i}$ by $d_{\alpha y,i}$ and $d_{\alpha y,i}$ by $-d_{\alpha x,i}$.

Example 3: We shall illustrate the calculation of tensor forms with use of the conversion equations. The linear combination $\mathsf{d}_1 = d_{14} - d_{25}$ of the components of the piezoelectric tensor is invariant under the action of the group $6_z2_x2_y$. We find that a first component of one of the two $D^{(2)}(D_6)$-covariants is $d_{2x,2} = d_{14} + d_{25}$. We have at once the conversion equations which involve the components d_{14} and d_{25}:

$$d_{14} = \frac{1}{2}(\mathsf{d}_1 + d_{2x,2}) \quad \text{and} \quad d_{25} = \frac{1}{2}(-\mathsf{d}_1 + d_{2x,2}).$$

All other Cartesian components are expressed as linear combinations of covariant components which belong to non-identity ireps. In the equilibrium state of symmetry $6_z2_x2_y$, all these covariant components as well as the $d_{2x,2}$ vanish. The invariant d_1 is the sole nonvanishing independent component and there are two Cartesian components which are expressed through it as

$$d_{14} = -d_{25} = \frac{1}{2}\mathsf{d}_1.$$

Hence an invariant d_1 can be interpreted as an independent parameter which defines the form of the piezoelectric tensor for the symmetry $6_z2_x2_y$.

We consider now the same tensor under the symmetry group $6_zm_xm_y$. There are three independent invariants: $\mathsf{d}_{1,1} = d_{31}+d_{32}$, $\mathsf{d}_{1,2} = d_{15}+d_{24}$, and $\mathsf{d}_{1,3} = d_{33}$; the third coincides with a Cartesian component. The Cartesian components which occur in the first two also occur in covariant components: $d_{2x,1} = d_{32} - d_{31}$ and $d_{2x,2} = d_{24} - d_{15}$. From this we obtain the conversion equations:

$$d_{31} = \frac{1}{2}(\mathsf{d}_{1,1} - d_{2x,1}) \quad \text{and} \quad d_{32} = \frac{1}{2}(\mathsf{d}_{1,1} + d_{2x,1}),$$

$$d_{15} = \frac{1}{2}(\mathsf{d}_{1,2} - d_{2x,2}) \quad \text{and} \quad d_{24} = \frac{1}{2}(\mathsf{d}_{1,2} + d_{2x,2}).$$

Setting the covariant components to zero, we have the nonvanishing Cartesian components: $d_{31} = d_{32} = \frac{1}{2}\mathsf{d}_{1,1}$, and $d_{15} = d_{24} = \frac{1}{2}\mathsf{d}_{1,2}$ and, of course, $d_{33} = \mathsf{d}_{1,3}$, which may be called a trivial conversion equation.

Invariant tensor components are therefore suitable parameters for the specification of a tensor under certain symmetry. It will be shown in Part B that covariant components are suitable parameters for describing the changes of tensors at symmetry descents.

Extended integrity bases: The extended integrity bases are a powerful tool for the determination of the form of thermodynamic potentials, and for finding the "faint interactions" and "switching interactions". All these tasks require the knowledge of transformation properties of polynomials in certain variables. We start with a space $V(n)$ and consider the space $\mathcal{P}(\mathbf{x})$ of polynomials $p(x_1, x_2, \ldots, x_n)$ in components of a vector $\mathbf{x} = \sum_{i=1}^{n} x_i \mathbf{e}_i \in V(n)$. Such space splits into subspaces $\mathcal{P}^{(k)}(\mathbf{x})$ of polynomials of the same order k. Let us assume that an action of the group G is given on $V(n)$; this action induces the action of G on the polynomial space and the subspaces $\mathcal{P}^{(k)}(\mathbf{x})$ remain invariant under this action. Just like any space invariant under the action of G, these subspaces split further into subspaces $\mathcal{P}_a^{(\alpha,k)}(\mathbf{x})$ which transform by ireps $D^{(\alpha)}(G)$ and whose direct sum is the whole space $\mathcal{P}^{(k)}(\mathbf{x})$. To each of the subspaces $\mathcal{P}_a^{(\alpha,k)}(\mathbf{x})$ there corresponds a polynomial $D^{(\alpha)}(G)$-covariant $\mathbf{p}_a^{(\alpha,k)}(\mathbf{x}) = [p_{a,1}^{(\alpha,k)}(\mathbf{x}), \ldots, p_{a,d_\alpha}^{(\alpha,k)}(\mathbf{x})]$, the components of which span the subspace. Components of all these $D^{(\alpha)}(G)$-covariants are linearly independent and span the whole subspace $\mathcal{P}^{(k)}(\mathbf{x})$ of homogeneous polynomials of the same order k. The transformation properties of these polynomials are the same as those of completely symmetrized tensors; in other words, if $n = 3$, then the space of the polynomials behaves like the space $[V(3)]^k$.

We denote in the following by $I(\mathbf{x})$ the polynomial invariants for which

$$GI(\mathbf{x}) = I(\mathbf{x})$$

for every $g \in G$, by $p^{(\alpha)}(\mathbf{x})$ the polynomial $\chi_\alpha(G)$-covariants (relative invariants) which transform by one-dimensional irep $\chi_\alpha(G)$, so that

$$gp^{(\alpha)}(\mathbf{x}) = \chi_\alpha(g) p^{(\alpha)}(\mathbf{x}),$$

and by $\mathbf{p}^{(\alpha)}(\mathbf{x}) = [p_1^{(\alpha)}(\mathbf{x}), \ldots, p_{d_\alpha}^{(\alpha)}(\mathbf{x})]$ the polynomial $D^{(\alpha)}(G)$-covariants, the components of which transform according to

$$gp_i^{(\alpha)}(\mathbf{x}) = \sum_{j=1}^{d_\alpha} D_{ij}^{(\alpha)}(g) p_j^{(\alpha)}(\mathbf{x}).$$

Hence the transformation properties of polynomial covariants and their components are, by definition, again identical with the transformation properties of typical covariants and typical variables. The whole space $\mathcal{P}(\mathbf{x})$ of polynomials splits under the action of G into a direct sum of irreducible subspaces

$$\mathcal{P}(\mathbf{x}) = \oplus_{k=0}^{\infty} \oplus_\alpha \oplus_a \mathcal{P}_a^{(\alpha,k)}$$

and there is a one-to-one correspondence between each such decomposition and the complete sets of linearly independent $D^{(\alpha)}(G)$-covariants $\mathbf{p}_a^{(\alpha,k)}(\mathbf{x}) = [p_{a,1}^{(\alpha,k)}(\mathbf{x}), \ldots, p_{a,d_\alpha}^{(\alpha,k)}(\mathbf{x})]$.

Calculation of polynomial invariants and covariants can again be performed consecutively, with the use of Clebsch–Gordan multiplication, as in the case of tensorial covariants. While the tensor spaces of each rank and intrinsic symmetry are of finite dimensions, the space of all polynomials is of an infinite dimension. In practical calculations of the thermodynamic potential or of faint and switching interactions we use, as a rule, the expansion in a power series in the respective variables so that we actually also need to know the polynomial covariants only to a certain finite order.

There exists an important difference between the calculation and recording of tensorial and polynomial covariants. Tensors form linear spaces while polynomials form an algebra.

Let us recall the difference: In a linear space, each linear combination of its elements also belongs to the space. In an algebra, the product of elements and hence a polynomial in the elements also belongs to the algebra. As a result, tensorial $D^{(\alpha)}(G)$-covariants form linear spaces and we have to find bases of linearly independent covariants of each tensor. A linear combination of polynomial $D^{(\alpha)}(G)$-covariants is again a polynomial $D^{(\alpha)}(G)$-covariant, as in case of tensorial covariants. In addition, if we replace in any polynomial $P_o(z_1, \ldots, z_n)$ its variables z_j by invariant polynomials $I_j(\mathbf{x})$, then the resulting polynomial $\mathcal{I}(\mathbf{x}) = P_o[I_1(\mathbf{x}), \ldots, I_n(\mathbf{x})]$ is again an invariant polynomial. Finally, a multiplication of a polynomial $D^{(\alpha)}(G)$-covariant by a polynomial invariant results again in a polynomial $D^{(\alpha)}(G)$-covariant. Using these relations we have developed a special algorithm (Kopský, 1975, 1979*c*,*d*,*e*) to calculate so-called extended integrity bases of polynomial algebras. This elegant and powerful mathematical result, which enables us to describe the whole polynomial algebra through a finite set of polynomials, has deep historical roots. It was proved a long time ago that a finite set of polynomial invariants exists such that any other polynomial invariant can be expressed as a polynomial in these invariants (Hilbert, 1890, 1893; Noether, 1916; Weyl, 1946). This statement is referred to as Noether's theorem and such sets received the name integrity bases of polynomial invariants. Such bases were actually calculated for the point groups by Döring (1958) in the study of magnetic anisotropy. It appears, however, that finite bases also exist for polynomial covariants; these have the property that any polynomial $D^{(\alpha)}$-covariant can be expressed as a linear combination of basic $D^{(\alpha)}$-covariants with polynomial covariants as coefficients. A series of papers was published in the 1970s (Killingbeck, 1972; McLellan, 1974; Patera & Winternitz, 1975; Patera, Sharp & Winternitz, 1978; Kopský, 1975, 1979*c*,*d*,*e*) in which methods for the calculation of polynomial covariants were developed and extended integrity bases actually calculated for ireps of crystallographic point groups and double crystallographic point groups. The Montreal group of Patera, Sharp and Winternitz used the theory of Molien series to calculate the numbers of polynomial covariants in such bases and then calculated them by brute force. Kopský used a special algorithm to achieve analogous results. The main theoretical result reads:

Fundamental theorem on extended integrity bases:

Let $\mathbf{x} = (x_1, x_2, \ldots, x_n)$ be a vector of an n-dimensional space $V(n)$ on which the action of a finite group G is defined. Let further $D^{(\alpha)}(G)$ be a complete set of irreducible matrix representations of the group G. We consider the space of polynomials on $V(n)$. The following statements hold:

1. There exists a finite set of polynomial invariants $I_j(\mathbf{x})$, $j = 1, 2, \ldots, n$, called free (another term is numerator) invariants and a finite set of so-called transient (another term is denominator) invariants $J_k(\mathbf{x})$, $k = 1, 2, \ldots$, such that any polynomial invariant $\mathcal{I}(\mathbf{x})$ can be expressed as:

$$\mathcal{I}(\mathbf{x}) = P_o[I_1(\mathbf{x}), \ldots, I_n(\mathbf{x})] + \sum_k P_k[I_1(\mathbf{x}), \ldots, I_n(\mathbf{x})] J_k(\mathbf{x}). \qquad \text{(J)}$$

2. For each irep $D^{(\alpha)}(G)$ there exists a finite set of polynomial $D^{(\alpha)}(G)$-covariants $\mathbf{p}^{(\alpha)}_a(\mathbf{x}) = [p^{(\alpha)}_{a,1}(\mathbf{x}), \ldots, p^{(\alpha)}_{a,d_\alpha}(\mathbf{x})]$ such that any other $D^{(\alpha)}(G)$-covariant can be expressed as:

$$\mathbf{p}^{(\alpha)}(\mathbf{x}) = \sum_a P_{\alpha a}[I_1(\mathbf{x}), \ldots, I_n(\mathbf{x})] \mathbf{p}^{(\alpha)}_a(\mathbf{x}). \qquad \text{(K)}$$

The set of basic invariants is called the integrity basis of polynomial invariants on the space $V(n)$ under the action of the group G. The integrity basis together with sets of basic covariants $\mathbf{p}_a^{(\alpha)}(\mathbf{x})$ is called the extended integrity basis of polynomial algebra $\mathcal{P}(\mathbf{x})$ under the action of the group G.

Notice that the number of free invariants is the same as the number of variables $(x_1, x_2, \ldots, x_n)$; the number of transient invariants is connected in a rather refined manner with the characters. Other names of these invariants – denominator and numerator – are connected with the appearance of their numbers either in the numerator or denominator of Molien series.

From the relations (J) and (K) we get relations for transformation properties of *"well behaving functions"* by which we mean the functions which can be approximated by polynomials.

1. A well behaving function $\mathcal{F}(\mathbf{x})$ on the space $V(n)$, invariant under the action of the group G can be expressed as:

$$\mathcal{F}(\mathbf{x}) = F_o[I_1(\mathbf{x}), \ldots, I_n(\mathbf{x})] + \sum_k F_k[I_1(\mathbf{x}), \ldots, I_n(\mathbf{x})] J_k(\mathbf{x}).$$

2. A functional $D^{(\alpha)}$-covariant $\mathcal{F}^{(\alpha)}(\mathbf{x}) = (F_1^{(\alpha)}(\mathbf{x}), \ldots, F_{d_\alpha}^{(\alpha)})$ whose components are well behaving functions can be expressed as:

$$\mathcal{F}^{(\alpha)}(\mathbf{x}) = \sum_a F_{\alpha a}[I_1(\mathbf{x}), \ldots, I_n(\mathbf{x})] \mathbf{p}_a^{(\alpha)}(\mathbf{x}).$$

Here $F_o[I_1(\mathbf{x}), \ldots, I_n(\mathbf{x})]$, $F_k[I_1(\mathbf{x}), \ldots, I_n(\mathbf{x})]$, $F_{\alpha a}[I_1(\mathbf{x}), \ldots, I_n(\mathbf{x})]$ are well behaving functions whose arguments are the free invariants.

On the face of it, this is very general result which might prove useful in other instances. However, in the usual models we use the power expansion in terms of $\mathbf{x}$, so that the use of the extended integrity bases is rather in the realm of basic polynomials from which such an expansion to any degree can easily be derived. In addition, we cannot present all spaces on which a group G may act and it is also not necessary. For practical purposes, it is sufficient to have the extended integrity bases only for the typical spaces V_α.

Extended integrity bases of irreducible matrix groups: Our final practical aim is to give the extended integrity bases from which all interactions occurring in the theory of phase transitions can be derived. It appears that we actually only need the extended integrity bases of irreducible matrix groups. Let us consider the simplest example, when the irep $\chi_\alpha(G)$ is real one-dimensional, so that the variable which belongs to it is x_α. Whatever the group G and whatever the label α, we always face the same situation: (i) The integrity basis of invariants contains only the invariant x_α^2. (ii) The basis of $\chi_\alpha(G)$-covariants (relative invariants) contains only the $\chi_\alpha(G)$-covariant x_α. (iii) No functions of x_α exist which will be the components of covariants belonging to any other irep of G.

Points (i) and (ii) are just another expression of the fact that all invariants are, in this case, even functions of x_α, all $\chi_\alpha(G)$-covariants are odd functions of x_α. Other covariants are not generated by functions of x_α.

We shall now consider the general case of an irep $D^{(\alpha)}(G)$, so that our variables are now the components of a typical $D^{(\alpha)}(G)$-covariant $\mathbf{x}^{(\alpha)} = (x_{\alpha 1}, \ldots, x_{\alpha d_\alpha})$. We denote by $H_\alpha \subseteq G$ that subgroup of G of elements $h \in H_\alpha$ for which $D^{(\alpha)}(h) = I_{d_\alpha}$ – the d_α-dimensional unit matrix. This group is the kernel of the irep $D^{(\alpha)}(G)$ and each coset in the resolution

$$G = H_\alpha \cup g_2 H_\alpha \cup \ldots \cup g_p H_\alpha,$$

where $p = [G : H_\alpha]$ is the index of H_α in G, contains elements $g_i h$ ($h \in H_\alpha$) to which the irep assigns the same matrix $D^{(\alpha)}(g_i) = D^{(\alpha)}(g_i h)$.

The action of the group G on the space V_α can therefore be viewed as an action of a group $\mathcal{H}_\alpha \approx G/H_\alpha$, isomorphic with the factor group of G over H_α. Each operator $\gamma_i \in \mathcal{H}_\alpha$ represents the identical action of the elements of the whole coset $g_i H_\alpha$ on the space V_α. The group $\mathcal{H}_\alpha$ has its own set of classes of ireps $\chi_\beta(\mathcal{H}_\alpha)$ to which there correspond the typical spaces V_β. In each of these classes we choose a certain matrix form $D^{(\beta)}(\mathcal{H}_\alpha)$ which defines the typical covariants $\mathbf{x}^{(\beta)} = (x_{\beta 1}, \ldots, x_{\beta d_\beta})$. Each of these classes defines uniquely a class $\chi_\beta(G)$ and a specific matrix form $D^{(\beta)}(G)$ of an irep of the group G by assigning to each element $g \in G$ the character $\chi_\beta(g) = \chi_\beta(\gamma_i)$ and matrix $D^{(\beta)}(g) = D^{(\beta)}(\gamma_i)$ of that element $\gamma_i \in \mathcal{H}_\alpha$ which corresponds to the coset $g_i H_\alpha$ to which g belongs. Such classes of ireps and such specific matrix ireps of the group G are called engendered by respective classes and by specific matrix ireps of the group $\mathcal{H}_\alpha$.

Now we consider the algebra of polynomials in the variables $(x_{\alpha 1}, \ldots, x_{\alpha d_\alpha})$. From the consideration above we see that the *extended integrity basis* of this algebra depends only on the matrix group $D^{(\alpha)}(\mathcal{H}_\alpha)$. Indeed, we consider the space V_α under the action of the group $\mathcal{H}_\alpha$ to get the integrity basis of invariants $I_j(\mathbf{x}^{(\alpha)})$, $J_k(\mathbf{x}^{(\alpha)})$ and the bases of covariants $\mathbf{p}_a^{(\beta)}(\mathbf{x}^{(\alpha)})$, where $D^{(\beta)}(\mathcal{H}_\alpha)$ are matrix ireps of the group $\mathcal{H}_\alpha$. Each invariant of this group is at the same time an invariant of the group G and each $D^{(\beta)}(\mathcal{H}_\alpha)$-covariant is at the same time a $D^{(\beta)}(G)$- covariant where $D^{(\beta)}(G)$ is an irep of G engendered by the irep $D^{(\beta)}(\mathcal{H}_\alpha)$ of $\mathcal{H}_\alpha$. This relationship between ireps of a group and those of its factor group has another important consequence formulated as the representation generating theorem (Burnside, 1955).

Representation generating theorem: The ireps of the class $\chi_\alpha(\mathcal{H}_\alpha)$ are faithful and the representation generating theorem asserts that a faithful representation (not necessarily irreducible) generates all other representations *via* polynomials. In other words, to each irep $D^{(\beta)}(\mathcal{H}_\alpha)$ there exists a polynomial $D^{(\beta)}(\mathcal{H}_\alpha)$-covariant $\mathbf{p}_{(\beta)}(\mathbf{x}^{(\alpha)})$ in variables of the $D^{(\alpha)}(\mathcal{H}_\alpha)$-covariant $\mathbf{x}^{(\alpha)} = (x_{\alpha,1}, \ldots, x_{\alpha,d_\alpha})$.

For the group G this implies that to each irep $D^{(\beta)}(G)$ engendered by an irep $D^{(\beta)}(\mathcal{H}_\alpha)$ there exists a polynomial $D^{(\beta)}(G)$-covariant $\mathbf{p}_{(\beta)}(\mathbf{x}^{(\alpha)})$ in variables of the $D^{(\alpha)}(G)$-covariant $\mathbf{x}^{(\alpha)} = (x_{\alpha,1}, \ldots, x_{\alpha,d_\alpha})$. The physical significance of representation generating theorem (Kopský, 1979*f*) will be discussed below in connection with "faint interactions" and "switching of domain states" by external fields in the theory of structural phase transitions.

Here we shall give two examples of its consequences. In the history of magnetic materials the concept of a *"cubic ferromagnet"* appears. However, a cubic ferromagnet cannot exist because the existence of magnetization in a sample contradicts cubic symmetry. According to the representation generating theorem there must exist an interaction (magnetostriction) which distorts the cubic symmetry. Since the magnitude of this interaction is usually small, such a distortion was found later by more precise measurements.

In the early stages of the investigation of ferroic phase transitions, the question arose whether to each irep of a point group a tensorial basis (covariant) exists. Again, the answer is yes, because vector representation of each point group is faithful. This can be easily extended to magnetic point groups as well.

Part B: Ferroic and equitranslational phase transitions

We consider structural phase transitions in a Landau sense, *i.e.* those which are accompanied by a symmetry descent. Such a structural phase transition is called "ferroic" if it is accompanied by a change of the point symmetry of the material. The results of tensor analysis also apply to the cases of order–disorder transitions accompanied by symmetry descent. Every equitranslational phase transition is ferroic; non-ferroic transitions are always associated with a symmetry descent in which the unit cell of the low-symmetry phase contains several original unit cells.

It is well known that the point symmetry restricts the form of tensors which express material properties. These restrictions can be expressed in two ways:

(i) Nonvanishing Cartesian tensor components can be specified. If they are not independent, then relations between them must be also given.

(ii) The tensor components can be expressed in terms of independent parameters. Such parameters are the invariants of the tensor and they are generally expressed as linear combinations of Cartesian components. *Vice versa*, the Cartesian components are then expressed as linear combinations of these parameters.

Each ferroic phase transition is characterized by an onset of new tensor parameters which are forbidden by the symmetry of the parent phase but allowed in the ferroic phase. These parameters are again generally linear combinations of Cartesian tensor components which transform under the parent group in a certain well defined manner. In other words, they can be interpreted as covariant tensor components related to certain suitable choices of ireps. Such are those choices when a covariant tensor component with reference to the parent symmetry turns into an invariant with reference to the ferroic symmetry. These components are considered here as tensor parameters of the ferroic transition and of the domain states arising in such a transition. The tables of symmetry descents within the classical point groups provide information about tensor parameters for tensors up to fourth rank and this information can be transferred to the Cartesian form of tensors in different domain states with the use of *"Conversion equations"*.

The physical background of the origin of structural phase transitions lies in instabilities of certain modes of motion and analysis in terms of the Landau model requires mode analysis with a subsequent consideration of the Landau potential. In the case of non-equitranslational transitions, the *"soft mode"* transforms by a certain irep of the parent space group which is associated with a nontrivial wavevector $\mathbf{k}$. Equitranslational transitions are associated with *"homogeneous"* instabilities, associated with wavevector $\mathbf{k} = \mathbf{0}$. All ireps of the parent space group which correspond to homogenous modes engender ireps of the respective point group.

Strictly speaking, an equitranslational structural phase transition, considered as a transition without any change of the translational symmetry, is actually a theoretical fiction. In fact, the structures of a crystal above and below the phase transition line are not rigid structures; at least the lattice parameters and parameters of Wyckoff positions (when positions with free parameters are occupied) change continuously with variations of temperature and of hydrostatic pressure above as well as below the transition line in the phase diagram. Accordingly, the space symmetries change continuously within the regions of the same phase. What remains invariant within this region is the structure type and the respective space-group type.

At the transition point we encounter a change of the structure type as well as of the type of the space-group symmetry. If the transition is continuous, small deviations from

the high-symmetry structure type develop with small deviations of the external conditions from the transition line into the region of the low-symmetry phase.

The central point of this software contains information about changes of tensor properties of crystals at ferroic phase transitions and about the form of relevant interactions. This information is contained in tables with headings Symmetry descent $G \Downarrow H$ or Symmetry descent $G \Downarrow F_1, \ldots, F_p$, where G is the parent point symmetry, H the ferroic symmetry if it is a normal subgroup, and $F_1, \ldots F_p$ is the set of conjugate ferroic symmetries. Access to these tables is through the choice of the item Subgroups. On choosing this item, a lattice of subgroups of the point group G under consideration appears on the screen.

Lattices of subgroups

Lattices: In this context, the term lattice means a special type of a partially ordered set, the general properties of which are described in detail by Birkhoff (1948). Lattices of subgroups are considered in the textbook by Hall (1959); their importance in the theory of structural phase transitions was realized by Ascher (1968), who prepared the first lattices of equitranslational subgroups of space groups. Lattices of subgroups of the point groups are considered in this context by Kopský (1982). One should realize that between subgroups of a given group there exist inclusion relations, so that we can say that a certain group F is larger than another group K in the sense that F contains K; written as $K \subset F$. However, such a relation does not generally exist between any pair of subgroups of a given group. The set of subgroups is therefore suitably presented in the form of a special graph, in which the original group is on the top, connected by lines with its maximal subgroups which, in their turn, are connected by lines with their maximal subgroups and so on until we come to the trivial subgroup C_1 at the bottom. Subgroups of the same index in the original group and hence of the same order are presented on the same level and each subgroup is connected by lines downwards to all its maximal subgroups and by lines upwards to all its minimal supergroups. From such a presentation we see all the chains of consecutive subgroups. More than that, from the lattice we can also find unions $F \vee K$ and intersections $F \wedge K$ of any pair F and K of subgroups. Thus the lattice is certainly more informative than a simple list of subgroups.

Note: Let us recall that the union of groups $F \vee K$ does not mean the set-theoretical union of their elements, which is usually not a group at all. The union of groups F and K contains all products of the elements of both groups and it is also the minimal group which contains both groups F and K. On the other hand, the intersection $F \wedge K$ of groups F and K is the maximal group contained in both F and K and it coincides with the set-theoretical intersection $F \cap K$. The symbols $\vee$ (vee) and $\wedge$ (wedge) are used quite generally in lattice theory for the *least upper bound* and *greatest lower bound*, which coincide with our definitions of group-theoretical *union* and *intersection*. Although lattices are formally presented in the form of graphs in the sense defined by graph theory (Ore, 1972), only a few concepts of this theory are used.

The lattices are prepared in a certain default form but the user can rearrange each lattice into another form either for one-time use or to make it their own default. In the original arrangement, we collect the sets of conjugate subgroups into blocks. Each subgroup is framed and the blocks of conjugate subgroups look like a stack of sheets of paper.

The lattices serve as a menu for calling up informative tables about phase transitions from the original group to any of its subgroups. Before we describe these tables, we

would like to introduce a few group-theoretical concepts which will prove useful later. In this treatment we follow the concepts developed a long time ago in the booklet on fine structure of domain states (Kopský, 1982) and in three subsequent papers (Kopský, 1983).

Dual lattices: If we take a certain lattice and invert it so that the bottom goes to the top and *vice versa*, we obtain a lattice that is called dual to the original one. In the dual lattice, all inclusion relations are reversed and unions interchange with intersections. In other words, if we invert the lattice and denote all elements by tilde, then from $F \subset K$, $M = F \wedge K$, $N = F \vee K$ follows $\widetilde{K} \subset \widetilde{F}$, $\widetilde{M} = \widetilde{F} \vee \widetilde{K}$, $\widetilde{N} = \widetilde{F} \wedge \widetilde{K}$. This, rather abstract, algebraic relation has a certain interesting and useful bearing on the theory of phase transitions as shown below.

Stability spaces: Anticipating the use of group-theoretical concepts for the description of the structural phase transitions, we first explain the relationship between lattices of subgroups and carrier spaces of ireps of the original group. Let us consider a tensor space $V^{(A)}$. It contains subspaces $V^{(A)}(G)$ and $V^{(A)}(F)$ of tensors which are invariant under the groups G and F, respectively. Such spaces are called the stability spaces of groups G and F. The subspace $V^{(A)}(G)$ is described by tensorial invariants of the group G, while the complementary subspace is defined by components of tensorial $D^{(\alpha)}_R(G)$-covariants. In considering the symmetry descent $G \Downarrow F$, we have to find those covariant components which became invariant under the group F. Though in general there may exist no such components for a given tensor $\mathbf{A}$, there always exist tensors for which such covariant components exist and hence the stability space $V^{(A)}(F)$ always contains the stability space $V^{(A)}(G)$ and, for some tensors, this subspace is a proper subspace. The approach *via* typical variables and typical carrier space enables the use of the systematic approach.

The typical carrier space $V_o = \oplus_\alpha V_\alpha$ of the original group G (referred to in the tables as the Parent group) is a direct sum of the carrier spaces V_α of R-irreducible spaces with bases $\{\mathbf{e}_{\alpha,1}, \mathbf{e}_{\alpha,2}, \ldots, \mathbf{e}_{\alpha,d_\alpha}\}$. All invariants of the group G are represented by a single vector $\mathbf{e}_1$ or by a single variable x_1.

Let us now consider a subgroup F of the group G which is potentially the symmetry of a certain ferroic state. To this subgroup there corresponds a subspace $V_o(F) = \oplus_\alpha V_\alpha(F)$ of the typical space V_o which contains all those vectors of V_o which are invariant under the action of the subgroup F. This space is called the typical stability space of the subgroup F, while individual $V_\alpha(F)$ are the typical stability spaces of F in the carrier spaces V_α of individual ireps. Expressing the stability spaces in terms of standard variables, we obtain the set of invariants of the group F expressed as linear combinations of these variables. Comparing them with tensorial covariants we obtain immediately those linear combinations of tensor components which onset at the phase transition from the parent group G to the ferroic subgroup F. More than that, we can also identify the ireps of the parent group G to which the onsetting parameters belong. Here we simply use the fact that subspaces $V^{(A)}_{\alpha a}(G)$ behave under the action of the group G like copies of the typical spaces $V_\alpha(G)$.

Duality theorem: It is worth mentioning that the typical stability spaces $V_o(F)$ form a lattice which is dual to the lattice of subgroups. This is the content of the duality theorem, which we give without proof. In other words, if $F \subset K$, then $V_o(K) \subset V_o(F)$, so the typical stability space grows as we go down the lattice of subgroups. Let us point out that the typical stability spaces $V_o(F)$ are the stability spaces of subgroups F in the

typical carrier space V_o of the parent group G and that this is the least space for which the stability spaces $V_o(F)$ form a lattice dual to the lattice of the parent group G. The stability space $V_o(G)$ of the group G itself in its typical carrier space is the one-dimensional space V_1 which contains only the products $\mathsf{x}_1\mathbf{e}_1$ of an invariant typical vector $\mathbf{e}_1$ with an invariant typical variable x_1, while the stability space of the trivial subgroup C_1 is the whole typical carrier space V_o of the group G.

The physical content of this statement is clear – a subgroup always allows some tensor properties which its supergroup does not allow, because every typical variable is represented by components of some tensors (in fact, tensors up to fourth rank cover all cases). Thus, the typical stability spaces provide information about newly onsetting tensorial properties.

The dimensions of stability spaces have an interesting property. It is well known that

$$\sum_\alpha d_\alpha^2 = |G|,$$

or, in words, that the sum of squares of dimensions of ireps is equal to the order of the group. This statement is sometimes referred to as the Burnside theorem. Let us now denote by $s_\alpha(F)$ the dimension of the stability space $V_\alpha(F)$. This number is one of the subduction coefficients – it says how many times an irep of the class $\chi_\alpha(G)$ subduces the identity irep of the subgroup F. Then the following relation holds

$$\sum_\alpha s_\alpha(F) d_\alpha = [G:F],$$

which we call the *generalized Burnside theorem*. In particular, if $F = H$ is a normal subgroup, then $s_\alpha(H) = d_\alpha$ for those ireps of G which are engendered by ireps of the factor group $\mathcal{H} = G/H$ and $s_\alpha = 0$ otherwise. The latter relation results in $[G:H]$, which is identical with the order of the factor group $|\mathcal{H}|$.

Stabilizers and orbits: Let us consider now the action of a group G on a set $\mathcal{S}$. The elements of $\mathcal{S}$ are called points and denoted by S. The action of G assigns to each element $g \in G$ and to each point $\mathsf{S} \in \mathcal{S}$ a point $g\mathsf{S}$. Let us pick up a certain point S. Some elements $f \in G$ may leave the point S invariant, so that $f\mathsf{S} = \mathsf{S}$. It is easy to show that all elements of G which leave the point invariant must constitute a group, which is called the stabilizer of the point S under the action of G.

We denote this group by F_1 and the point by S_1. Performing coset resolution

$$G = F_1 \cup g_2 F_1 \cup \ldots \cup g_p F_1,$$

we can see that all elements of the coset $g_i F_1$ send the point S_1 to the same point $\mathsf{S}_i = g_i F_1 \mathsf{S}_1 = g_i \mathsf{S}_1$. The set of points S_i is called the orbit. If we pick any point S_i of the orbit and apply an element of the group G to it, we obtain another point of the orbit. Indeed, $g\mathsf{S}_i = g g_i \mathsf{S}_1 = g_j \mathsf{S}_1 = \mathsf{S}_j$.

The stabilizer of a point S_i is a group $F_i = g_i F_1 g_i^{-1}$ conjugate to the group F_1. We consider now the first normalizer $N_G^{(1)}(F_1)$ of the subgroup F_1 in G. From coset resolutions

$$G = N_G^{(1)}(F_1) \cup t_2 N_G^{(1)}(F_1) \cup \ldots \cup t_q N_G^{(1)}(F_1)$$

and

$$N_G^{(1)}(F_1) = F_1 \cup s_2 F_1 \cup \ldots \cup s_r F_1$$

we obtain

$$
\begin{aligned}
G = \quad & F_1 \cup s_2 F_1 \cup \ldots s_r F_1 \cup \\
& t_2 F_1 \cup t_2 s_2 F_1 \cup \ldots t_2 s_r F_1 \cup \\
& \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \\
& t_q F_1 \cup t_q s_2 F_1 \cup \ldots t_q s_r F_1 .
\end{aligned}
$$

Changing the indexing of points, starting with $\mathsf{S}_1 \to \mathsf{S}_{11}$ through to $\mathsf{S}_{ij} = t_i s_j \mathsf{S}_1$, we find that the orbit splits into q subsets labelled by indices from the set $i = 1, 2, \ldots, q$ and each of these subsets contains r points S_{ij} with fixed index i and $j = 1, 2, \ldots, r$. The points with the same i have the same stabilizer $F_i = g_i F_1 g_i^{-1}$. The numbers q and r are indices of subgroups: $q = [G : N_G^{(1)}(F_1)]$, $r = [N_G^{(1)}(F_1) : F_1]$ and $p = qr = [G : F_1]$.

Permutation representation: The set $\mathcal{S}$ therefore splits under the action of the group G into *disjoint* sets, called *orbits*. The action of the elements $g \in G$ is transitive on each orbit; transitivity means that every element of the orbit is obtained when elements of the group G act on any chosen element of the orbit. Elements of the group G are therefore permuting points of the orbit thus defining a permutation representation of the group G. The kernel of this representation is the group $H = \text{core}\, F_i = \bigcap_{i=1}^{q} F_i$, which is a normal subgroup of G.

Linear orbits and strata: If the set $\mathcal{S}$ on which the group G acts is a linear space $V(n)$, then the elements are vectors $\mathbf{x} \in V(n)$. If F_1 is a stabilizer of a vector $\mathbf{x}_{11} \in V(n)$ then, using the same coset resolution as in the case of the set $\mathcal{S}$, we obtain an orbit of vectors $\mathbf{x}_{ij} = t_i s_j \mathbf{x}_{11}$ for which we use the name linear orbit. Since linear spaces are sets of some special properties, we can expect that linear orbits also have some properties characteristic for the linear action of the group G. Indeed, if vector $\mathbf{x}_{11}$ generates an orbit of vectors $\mathbf{x}_{ij}$, then every vector $a\mathbf{x}_{11}$, $a \neq 0$, generates an orbit of vectors $a\mathbf{x}_{ij}$. From this we can get the wrong impression that vectors with the same stabilizer F_1 form linear spaces. This, however, is not true, as we can see already by considering the trivial vector $\mathbf{x} = \mathbf{0}$ which belongs to every linear space and generates an orbit with one vector – itself. Also, if linearly independent vectors $\mathbf{x}$ and $\mathbf{y}$ have the same stabilizer F_1, then the stabilizer of their linear combination $a\mathbf{x} + b\mathbf{y}$ certainly contains F_1 but is not necessarily identical with it.

This means that while all vectors of the stability space $V(F_1)$ are by definition invariant under the group F_1, the group F_1 is not necessarily the stabilizer of an arbitrary vector from $V(F_1)$. The set of all vectors of $V(n)$ which have F_1 as a stabilizer will be called here the stratum of F_1 in $V(n)$. The stratum of F_1 in a certain space $V(n)$ can be empty. If it is not, then we find it as follows: We consider the stability space $V(F_1)$. This is never empty, it contains at least the trivial vector $\mathbf{x} = \mathbf{0}$. If the stability space is nontrivial, it is at least of dimension 1. The stratum is then the set of all vectors of $V(F_1)$ with the exception of the trivial vector. If the stability space is of higher dimension, it may contain subspaces, which are stability spaces of supergroups of F_1. To get the stratum, we have to take all these stability spaces out of the space $V(F_1)$. Since these subspaces are of lower dimensions than $V(F_1)$, the stratum of F_1 in $V(F_1)$ is always a dense subset of $V(F_1)$. We shall use the more customary expression that vector $\mathbf{x}$ is a general vector of the stability space $V(F_1)$, as is more usual in the literature. Indeed, the vectors that do not belong to the stratum can be considered as vectors of special symmetry.

Remark: The original definition of stratum as used, *e.g.* in the book by Tolédano & Dmitriev (1996), is the union of all strata as defined here for the set of conjugate subgroups and it coincides with our concept of strata for a normal subgroup. If it is necessary

to use both concepts, we suggest using a capital S in the symbol for the original stratum.

Kernels and epikernels: Let us now replace the set $\mathcal{S}$ by a typical carrier space V_α. If the corresponding R-irep $\chi_\alpha(G)$ is one-dimensional, Ker $\chi_\alpha(G) = H_\alpha$, then the space V_α contains only two types of orbits:

(i) The trivial vector $\mathbf{x}^{(\alpha)} = \mathbf{0}$, whose stabilizer under the action of G is the group G itself.

(ii) If $\mathbf{x}^{(\alpha)} = \mathsf{x}_\alpha \mathbf{e}^{(\alpha)}$, then the stabilizer of this vector is the halving subgroup H_α. From coset resolution $G = H_\alpha \cup g_2 H_\alpha$ we obtain the second vector of the orbit, which is $g_2\mathbf{x}^{(\alpha)} = -\mathbf{x}^{(\alpha)}$.

Notice that the set of all vectors with stabilizer H_α is the whole space V_α with the exception of the trivial vector. This set is the stratum of H_α.

If the dimension of the R-irep is at least two, we have to analyse the structure of the space V_α as follows:

(i) The stabilizer of the trivial vector $\mathbf{x}^{(\alpha)} = \mathbf{0}$ is again the group G itself.

(ii) The stabilizer of any other vector $\mathbf{x}^{(\alpha)}$ is at least the group $H_\alpha = \text{Ker } D_R^{(\alpha)}(G)$. The index of H_α is now higher than two and we find the orbit in the usual manner. If every vector of the space has this group for its stabilizer, then we take the trivial vector out and get the stratum of H_α. The stratum of the group G always consists of the trivial vector with the exception of the space V_1 of invariants. This and the trivial space are the only spaces which are at the same time strata.

(iii) There may, however, exist vectors of the space V_α, the stabilizers of which are greater than H_α. Let us assume that such a vector $\mathbf{x}_1^{(\alpha)}$ exists. The stabilizer of this vector is called an "epikernel" of the R-irep $D_R^{(\alpha)}(G)$ and we denote it by $F_{\alpha 1}$. This group cannot be normal in G because normal subgroups leave invariant either all vectors or only the trivial vector in each of the spaces V_α. Epikernels therefore appear as sets of conjugate subgroups.

The stability space $V_\alpha(F_{\alpha 1})$ is of the dimension $s_\alpha(F_{\alpha 1}) < d_\alpha$. If $s_\alpha(F_{\alpha 1}) > 1$, which may happen only if $d_\alpha > 2$, there may exist vectors of $V_\alpha(F_{\alpha 1})$, the stabilizer of which is greater than $F_{\alpha 1}$. The dimension of the stability space of this stabilizer is smaller than $s_\alpha(F_{\alpha 1})$.

The structure of the space V_α can therefore be described as follows: A general vector of this space has the stabilizer $H_\alpha = \text{Ker } \chi_\alpha(G)$. All vectors with exactly this stabilizer form the stratum of the group H_α. This will be obtained if the trivial vector and vectors of stability spaces of epikernels are excluded from the space V_α.

Epikernels appear as sets of conjugate subgroups $F_{\alpha i}^{(u)}$, where the superscript u labels different sets of conjugate subgroups and the index i labels subgroups of the set. Intersections core $F_\alpha^{(u)} = \bigcap_i F_{\alpha i}^{(u)} = H_\alpha$ of all conjugate epikernels always result in the kernel. If one epikernel $F_{\alpha 1}^{(v)}$ is a subgroup of another epikernel $F_{\alpha 1}^{(u)}$, then the stability space $V_\alpha(F_{\alpha 1}^{(u)})$ is a subspace of the stability space $V_\alpha(F_{\alpha 1}^{(v)})$. The stratum of each epikernel is therefore obtained by excluding from its stability space the trivial vector and stability spaces of all epikernels which are subgroups of this epikernel.

The lattice of normal subgroups: The intersection and union of normal subgroups are again normal subgroups. From this it follows that normal subgroups form a sublattice $\mathcal{L}_N(G)$ of the whole lattice $\mathcal{L}(G)$. Among normal subgroups we distinguish those which are kernels of ireps. Hence we have a set of normal subgroups H_α which can be labelled

by the same labels as the ireps. One normal subgroup can be simultaneously the kernel of more than one irep. These kernels have the property that they generate the whole lattice $\mathcal{L}_N(G)$ by intersections. In other words, each normal subgroup is either a kernel of one or of more ireps, or it is some intersection of such kernels. In the second case, the kernel may be generally obtained in several ways as the intersection of kernels of ireps.

The whole lattice: Epikernels play the same role with reference to the whole lattice as kernels do with reference to the lattice of normal subgroups. Namely, every subgroup is either an epikernel of some irep or an intersection of epikernels. In this statement, the word epikernel also includes kernel, which is a special case of an epikernel. Let us also mention without proof that an intersection of epikernels of the same irep $\chi_\alpha(G)$ is again an epikernel of this irep. Hence, if a subgroup is not an epikernel, it must be an intersection of epikernels belonging to different ireps.

If the subgroup is an intersection of kernels or epikernels of ireps, it is suitable when considering phase transitions to consider all such possible intersections which have the property that all kernels or epikernels in this intersection are necessary to get the desired subgroup. In other words, if some group can be excluded from the intersection without changing it, then this group should be excluded. We shall say that the intersection $F_1 = \bigcap_\alpha F_{\alpha 1}$ is a true intersection if omission of any of $F_{\alpha 1}$ results in a supergroup of F_1.

Remark: We consider it appropriate to make the following remark of historical and terminological character. The term epikernel was introduced by Ascher (1977) [see also Kobayashi & Ascher (1977)] in connection with his study of the direct and inverse Landau problem. Unfortunately, the terms little group or isotropy group crept into the literature instead of it. In our opinion, this is taking jargon too far. A little linguistic analysis seems not out of place here. The older terms little group or isotropy group are now frequently replaced by the term stabilizer. The term was introduced in connection with the group action on any set. The stabilizer of a point of the set is then that subgroup which contains all those elements of the group which leave the point invariant. In this sense, an epikernel of an irep $D_R^{(\alpha)}(G)$ is a stabilizer (little group or isotropy group) of a certain *vector* of the carrier space V_α under the action of the group G (it is in no way the stabilizer of its irep). In addition, the term little group (isotropy group) of an irep has its own meaning in the theory of representations of space groups, which is a quite different story.

The fine structure of a typical linear orbit: We shall consider now again the typical stability space $V_o(F_1)$ of a subgroup F_1 of the group G. This space is a direct sum of the stability spaces $V_\alpha(F_1)$ of the group F_1 in individual typical carrier spaces V_α. We denote by $F_{\alpha 1}$ the stabilizer of a general vector $\mathbf{x}_{11}^{(\alpha)} \in V_\alpha(F_1)$. The stability space $V_\alpha(F_1)$ is identical with the stability space $V_\alpha(F_{\alpha 1})$ and all stabilizers $F_{\alpha 1}$ contain the group F_1. We perform the coset resolution

$$G = F_{\alpha 1} \cup g_2^{(\alpha)} F_{\alpha 1} \cup \ldots \cup g_{p_\alpha}^{(\alpha)} F_{\alpha 1}$$

and the more detailed

$$G = N_G^{(1)}(F_{\alpha 1}) \cup t_2^{(\alpha)} N_G^{(1)}(F_{\alpha 1}) \cup \ldots \cup t_{q_\alpha}^{(\alpha)} N_G^{(1)}(F_{\alpha 1})$$

and

$$N_G^{(1)}(F_{\alpha 1}) = F_{\alpha 1} \cup s_2^{(\alpha)} F_{\alpha 1} \cup \ldots \cup s_{r_\alpha}^{(\alpha)} F_{\alpha 1},$$

which combine into

$$
\begin{aligned}
G = \quad & F_{\alpha 1} \cup s_2^{(\alpha)} F_{\alpha 1} \cup \ldots s_{r_\alpha}^{(\alpha)} F_{\alpha 1} \cup \\
& t_2^{(\alpha)} F_{\alpha 1} \cup t_2^{(\alpha)} s_2^{(\alpha)} F_{\alpha 1} \cup \ldots t_2^{(\alpha)} s_{r_\alpha}^{(\alpha)} F_{\alpha 1} \cup \\
& \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \\
& t_{q_\alpha}^{(\alpha)} F_{\alpha 1} \cup t_{q_\alpha}^{(\alpha)} s_2^{(\alpha)} F_{\alpha 1} \cup \ldots t_{q_\alpha}^{(\alpha)} s_{r_\alpha}^{(\alpha)} F_{\alpha 1}
\end{aligned}
$$

to obtain the orbit of vector $\mathbf{x}_{11}^{(\alpha)} \in V_\alpha(F_{\alpha 1}) = V_\alpha(F_1)$. This orbit contains $p_\alpha = q_\alpha r_\alpha$ vectors $\mathbf{x}_{ij}^{(\alpha)} = t_i^{(\alpha)} s_j^{(\alpha)} \mathbf{x}_{11}^{(\alpha)} \in V_\alpha(F_{\alpha i})$ and splits into q_α subsets labelled by indices from the set $i = 1, 2, \ldots, q_\alpha$, and each of these subsets contains r_α vectors $\mathbf{x}_{ij}^{(\alpha)}$ with fixed index i and index $j = 1, 2, \ldots, r_\alpha$. The vectors with the same i have the same stabilizer $F_{\alpha i} = g_i^{(\alpha)} F_{\alpha 1} g_i^{(\alpha)-1}$. The numbers q_α and r_α are indices of subgroups: $q_\alpha = [G : N_G^{(1)}(F_{\alpha 1})]$, $r_\alpha = [N_G^{(1)}(F_{\alpha 1}) : F_{\alpha 1}]$ and $p_\alpha = q_\alpha r_\alpha = [G : F_{\alpha 1}]$.

A vector $\mathbf{x}_{11}$ of the typical stability space $V_o(F_1)$ of the subgroup F_1 generates an orbit of $p = qr$ vectors $\mathbf{x}_{ij} = t_i s_j \mathbf{x}_{11}$ with stabilizers F_i, where $p = [G : F_1] = qr$, where $q = [G : N_G^{(1)}(F_1)]$ and $r = [N_G^{(1)}(F_1) : F_1]$. This vector splits into components $\mathbf{x}_{11}^{(\alpha)}$ in the typical irreducible subspaces V_α. Each of these components has its own stabilizer $F_{\alpha 1} \supseteq F_1$. Vectors $\mathbf{x}_{ij} = t_i s_j \mathbf{x}_{11}$ of the orbit also split into components $\mathbf{x}_{ij}^{(\alpha)}$. While all vectors $\mathbf{x}_{ij}$ of the typical orbit are distinct, the components $\mathbf{x}_{ij}^{(\alpha)}$ are also distinct only if $F_{\alpha 1} = F_1$. Notice that this means that these components are distinct only if F_1 is an epikernel of the irep $D_R^{(\alpha)}(G)$. On the other hand, if $F_{\alpha 1} \supset F_1$, the number p_α of distinct components is a divisor of the total number p of vectors of the orbit; it is $p : p_\alpha = [F_{\alpha 1} : F_1]$.

If we label the components $\mathbf{x}_{ij}^{(\alpha)}$ by the original labels ij, then certain groups of these labels denote the same component. To label them uniquely, we use the coset resolutions associated with the stabilizer $F_{\alpha 1}$ which results in a certain unique labelling $\mathbf{x}_{i_\alpha j_\alpha}^{(\alpha)}$. Each label $i_\alpha j_\alpha$ then corresponds to $k_\alpha = p : p_\alpha$ labels ij. The set of vectors

$$
\mathbf{x}_{ij} = (\ldots, \mathbf{x}_{i_\alpha j_\alpha}^{(\alpha)}, \ldots, \mathbf{x}_{i_\beta j_\beta}^{(\beta)}, \ldots)
$$

will be called the typical linear orbit and its representation in terms of components in irreducible typical subspaces will be referred to as the fine structure of the typical linear orbit. Tables of these structures (under the less precise name *fine domain structures*) were published a long time ago (Kopský, 1982).

Examples: We shall illustrate these theoretical results using, as an example of a parent group, the point group $4_z/m_z m_x m_{xy}$ (D_{4hz}). In Table B1 are listed all subgroups of this group and for each of the subgroups its typical stability space in terms of nonvanishing typical variables is given. If such a vector is framed, then the corresponding subgroup is an epikernel (or kernel) of that irep to which the covariant belongs.

In Table B2 are shown the fine structures of typical orbits for a few symmetry descents from the same parent group and some cases of descents from other parent groups. The descent $D_6 \Downarrow C_3$ is exomorphic (*cf.* the section following these examples) with the descent $D_{4hz} \Downarrow C_{4z}$ and the descent $D_{4z} \Downarrow (C_{2x}, C_{2y})$ with the descent $D_{4hz} \Downarrow (C_{2hx}, C_{2hy})$. The advantage of typical variables is clear if we recall that tables of tensorial covariants assign to each of these variables all covariant tensor components up to fourth order (and if extension to higher orders is necessary, we know how to do this).

Table B1: Epikernels and stability spaces for the group $D_{4hz} - 4_z/m_z m_x m_{xy}$

C_{4hz}	$4_z/m_z$	$\boxed{\mathsf{x}_2^+}$
D_{2h}	$m_x m_y m_z$	$\boxed{\mathsf{x}_3^+}$
$\widehat{D}_{2hz}$	$m_{x\overline{y}} m_{xy} m_z$	$\boxed{\mathsf{x}_4^+}$
D_{4z}	$4_z 2_x 2_{xy}$	$\boxed{\mathsf{x}_1^-}$
C_{4vz}	$4_z m_x m_{xy}$	$\boxed{\mathsf{x}_2^-}$
D_{2dz}	$\overline{4}_z 2_x m_{xy}$	$\boxed{\mathsf{x}_3^-}$
$\widehat{D}_{2dz}$	$\overline{4}_z m_x 2_{xy}$	$\boxed{\mathsf{x}_4^-}$
C_{2hz}	$2_z/m_z$	$\mathsf{x}_2^+, \mathsf{x}_3^+, \mathsf{x}_4^+$
C_{4z}	4_z	$\mathsf{x}_2^+, \mathsf{x}_1^-, \mathsf{x}_2^-$
D_2	$2_x 2_y 2_z$	$\mathsf{x}_3^+, \mathsf{x}_1^-, \mathsf{x}_3^-$
$\widehat{D}_{2z}$	$2_{x\overline{y}} 2_{xy} 2_z$	$\mathsf{x}_4^+, \mathsf{x}_1^-, \mathsf{x}_4^-$
S_{4z}	$\overline{4}_z$	$\mathsf{x}_2^+, \mathsf{x}_3^-, \mathsf{x}_4^-$
C_{2vz}	$m_x m_y 2_z$	$\mathsf{x}_2^-, \mathsf{x}_3^+, \mathsf{x}_4^-$
$\widehat{C}_{2vz}$	$m_{x\overline{y}} m_{xy} 2_z$	$\mathsf{x}_2^-, \mathsf{x}_3^-, \mathsf{x}_4^+$
C_{2z}	2_z	$\mathsf{x}_2^+, \mathsf{x}_3^+, \mathsf{x}_4^+, \mathsf{x}_1^-, \mathsf{x}_2^-, \mathsf{x}_3^-, \mathsf{x}_4^-$
C_{2hx}	$2_x/m_x$	x_3^+ $\boxed{(x_1^+, 0)}$
C_{2hy}	$2_y/m_y$	x_3^+ $\boxed{(0, x_1^+)}$
C_{2hxy}	$2_{xy}/m_{xy}$	x_4^+ $\boxed{(x_1^+, x_1^+)}$
$C_{2hx\overline{y}}$	$2_{x\overline{y}}/m_{x\overline{y}}$	x_4^+ $\boxed{(x_1^+, -x_1^+)}$
C_i	$\overline{1}$	$\mathsf{x}_2^+, \mathsf{x}_3^+, \mathsf{x}_4^+$ $\boxed{(x_1^+, y_1^+)}$

C_{2vx}	$2_x m_y m_z$	x_3^+	$\boxed{(x_1^-, 0)}$
C_{2vy}	$m_x 2_y m_z$	x_3^+	$\boxed{(0, x_1^-)}$
C_{2vxy}	$m_{x\overline{y}} 2_{xy} m_z$	x_4^+	$\boxed{(x_1^-, x_1^-)}$
$C_{2vx\overline{y}}$	$2_{x\overline{y}} m_{xy} m_z$	x_4^+	$\boxed{(x_1^-, -x_1^-)}$
C_{sz}	m_z	$\mathsf{x}_2^+, \mathsf{x}_3^+, \mathsf{x}_4^+$	$\boxed{(x_1^-, y_1^-)}$
C_{2x}	2_x	$\mathsf{x}_3^+, \mathsf{x}_1^-, \mathsf{x}_3^-$	$(x_1^+, 0)$ $(x_1^-, 0)$
C_{2y}	2_y	$\mathsf{x}_3^+, \mathsf{x}_1^-, \mathsf{x}_3^-$	$(0, x_1^+)$ $(0, x_1^-)$
C_{2xy}	2_{xy}	$\mathsf{x}_4^+, \mathsf{x}_1^-, \mathsf{x}_4^-$	(x_1^+, x_1^+) (x_1^-, x_1^-)
$C_{2x\overline{y}}$	$2_{x\overline{y}}$	$\mathsf{x}_4^+, \mathsf{x}_1^-, \mathsf{x}_4^-$	$(x_1^+, -x_1^+)$ $(x_1^-, -x_1^-)$
C_{sx}	m_x	$\mathsf{x}_3^+, \mathsf{x}_2^-, \mathsf{x}_4^-$	$(x_1^+, 0)$ $(0, x_1^-)$
C_{sy}	m_y	$\mathsf{x}_3^+, \mathsf{x}_2^-, \mathsf{x}_4^-$	$(0, x_1^+)$ $(x_1^-, 0)$
C_{sxy}	m_{xy}	$\mathsf{x}_4^+, \mathsf{x}_2^-, \mathsf{x}_3^-$	(x_1^+, x_1^+) $(x_1^-, -x_1^-)$
$C_{sx\overline{y}}$	$m_{x\overline{y}}$	$\mathsf{x}_4^+, \mathsf{x}_2^-, \mathsf{x}_3^-$	$(x_1^+, -x_1^+)$ (x_1^-, x_1^-)
C_1	1	$\mathsf{x}_2^+, \mathsf{x}_3^+, \mathsf{x}_4^+, \mathsf{x}_1^-, \mathsf{x}_2^-, \mathsf{x}_3^-, \mathsf{x}_4^-$	(x_1^+, y_1^+) (x_1^-, y_1^-)

Table B2: Examples of the fine structure of typical orbits

Symmetry descent: $D_{4hz} \Downarrow D_{2h}$

D_{4hz}	D_{2h}	$4_z D_{2h}$
D_{2h}	x_3^+	$-\mathsf{x}_3^+$

Symmetry descent: $D_{4hz} \Downarrow C_{4z}$

D_{4hz}	C_{4z}	iC_{4z}	$2_x C_{4z}$	$m_x C_{4z}$
C_{4hz}	x_2^+	x_2^+	$-\mathsf{x}_2^+$	$-\mathsf{x}_2^+$
D_{4z}	x_1^-	$-\mathsf{x}_1^-$	x_1^-	$-\mathsf{x}_1^-$
C_{4vz}	x_2^-	$-\mathsf{x}_2^-$	$-\mathsf{x}_2^-$	x_2^-

Symmetry descent: $D_{4hz} \Downarrow (C_{2hx}, C_{2hy})$

First normalizer $N_{D_{4hz}}(C_{2hx}) = N_{D_{4hz}}(C_{2hy}) = D_{2h}$ = normal subgroup

D_{4hz}	D_{2h}		4_zD_{2h}	
	C_{2hx}	2_zC_{2hx}	4_zC_{2hx}	$4_z^{-1}C_{2hx}$

	C_{2hx}		C_{2hy}	
D_{2h}	x_3^+	x_3^+	$-\mathsf{x}_3^+$	$-\mathsf{x}_3^+$
C_{2hi}	$(x_1^+, 0)$	$(-x_1^+, 0)$	$(0, x_1^+)$	$(0, -x_1^+)$

Symmetry descent: $D_{4hz} \Downarrow C_{sz}$

D_{4hz}	C_{sz}	4_zC_{sz}	2_zC_{sz}	$4_z^{-1}C_{sz}$
C_{4hz}	x_2^+	x_2^+	x_2^+	x_2^+
D_{2h}	x_3^+	$-\mathsf{x}_3^+$	x_3^+	$-\mathsf{x}_3^+$
$\widehat{D}_{2hz}$	x_4^+	$-\mathsf{x}_4^+$	x_4^+	$-\mathsf{x}_4^+$
C_{sz}	(x_1^-, y_1^-)	$(-y_1^-, x_1^-)$	$(-x_1^-, -y_1^-)$	$(y_1^-, -x_1^-)$

	2_xC_{sz}	$2_{xy}C_{sz}$	2_yC_{sz}	$2_{x\overline{y}}C_{sz}$
C_{4hz}	$-\mathsf{x}_2^+$	$-\mathsf{x}_2^+$	$-\mathsf{x}_2^+$	$-\mathsf{x}_2^+$
D_{2h}	x_3^+	$-\mathsf{x}_3^+$	x_3^+	$-\mathsf{x}_3^+$
$\widehat{D}_{2hz}$	$-\mathsf{x}_4^+$	x_4^+	$-\mathsf{x}_4^+$	x_4^+
C_{sz}	$(x_1^-, -y_1^-)$	(y_1^-, x_1^-)	$(-x_1^-, y_1^-)$	$(-y_1^-, -x_1^-)$

Symmetry descent: $D_{4hz} \Downarrow (C_{2x}, C_{2y})$

First normalizer $N_{D_{4hz}}(C_{2x}) = N_{D_{4hz}}(C_{2y}) = D_{2h}$ = normal subgroup

D_{4hz}	D_{2h}				4_zD_{2h}			
	C_{2x}	iC_{2x}	2_zC_{2x}	m_zC_{2x}	4_zC_{2x}	$\overline{4}_zC_{2x}$	$4_z^{-1}C_{2x}$	$\overline{4}_z^{-1}C_{2x}$
	C_{2x}				C_{2y}			
D_{2h}	x_3^+	x_3^+	x_3^+	x_3^+	$-\mathsf{x}_3^+$	$-\mathsf{x}_3^+$	$-\mathsf{x}_3^+$	$-\mathsf{x}_3^+$
D_4	x_1^-	$-\mathsf{x}_1^-$	x_1^-	$-\mathsf{x}_1^-$	x_1^-	$-\mathsf{x}_1^-$	x_1^-	$-\mathsf{x}_1^-$
D_{2dz}	x_3^-	$-\mathsf{x}_3^-$	x_3^-	$-\mathsf{x}_3^-$	$-\mathsf{x}_3^-$	x_3^-	$-\mathsf{x}_3^-$	x_3^-
C_{2hi}	$(x_1^+, 0)$	$(x_1^+, 0)$	$(-x_1^+, 0)$	$(-x_1^+, 0)$	$(0, x_1^+)$	$(0, x_1^+)$	$(0, -x_1^+)$	$(0, -x_1^+)$
C_{2vi}	$(x_1^-, 0)$	$(-x_1^-, 0)$	$(-x_1^-, 0)$	$(x_1^-, 0)$	$(0, x_1^-)$	$(0, -x_1^-)$	$(0, -x_1^-)$	$(0, x_1^-)$

Symmetry descent: $D_4 \Downarrow (C_{2x}, C_{2y})$

First normalizer $N_{D_{4z}}(C_{2x}) = N_{D_{4z}}(C_{2y}) = D_2 =$ normal subgroup

D_{4z}	D_2		$4_z D_2$	
	C_{2x}	$2_z C_{2x}$	$4_z C_{2x}$	$4_z^{-1} C_{2x}$

	C_{2x}		C_{2y}	
D_2	x_3	x_3	$-\mathsf{x}_3$	$-\mathsf{x}_3$
C_{2i}	$(x_1, 0)$	$(-x_1, 0)$	$(0, x_1)$	$(0, -x_1)$

Symmetry descent $D_6 \Downarrow C_3$

D_{6z}	C_{3z}	$2_z C_{3z}$	$2_x C_{3z}$	$2_y C_{3z}$
C_6	x_2	x_2	$-\mathsf{x}_2$	$-\mathsf{x}_2$
D_{3x}	x_3	$-\mathsf{x}_3$	x_3	$-\mathsf{x}_3$
D_{3y}	x_4	$-\mathsf{x}_4$	$-\mathsf{x}_4$	x_4

Symmetry descent: $O \Downarrow (D_{3p}, D_{3q}, D_{3r}, D_{3s})$

First normalizers: $N_O(D_{3p}) = D_{3p}$, $N_O(D_{3q}) = D_{3q}$, $N_O(D_{3r}) = D_{3r}$, $N_O(D_{3s}) = D_{3s} =$ self-normalizers

O	D_{3p}	$2_z D_{3p}$	$2_x D_{3p}$	$2_y D_{3p}$
	D_{3p}	D_{3q}	D_{3r}	D_{3s}
D_{3j}	(x_1, x_1, x_1)	$(-x_1, -x_1, x_1)$	$(x_1, -x_1, -x_1)$	$(-x_1, x_1, -x_1)$

Symmetry descent: $O_h \Downarrow (D_{4z}, D_{4x}, D_{4y})$

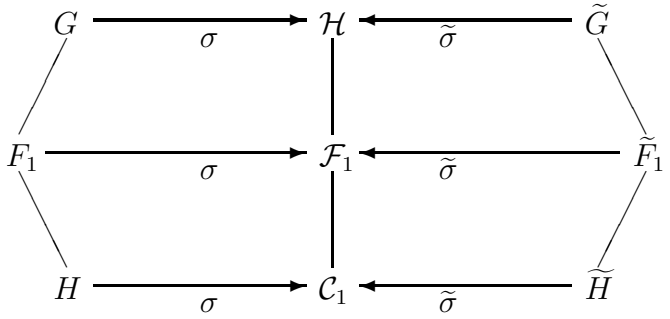
First normalizers: $N_{O_h}(D_{4hz}) = D_{4hz}$, $N_{O_h}(D_{4hx}) = D_{4hx}$, $N_{O_h}(D_{4hy}) = D_{4hy} =$ self-normalizers

	O_h	D_{4hz}		$3_p D_{4hz}$		$3_p^2 D_{4z}$	
		D_{4hz}		D_{4hx}		D_{4hy}	
		D_{4z}	iD_{4z}	$3_p D_{4z}$	$\overline{3}_p D_{4z}$	$3_p^2 D_{4z}$	$\overline{3}_p^5 D_{4z}$
		D_{4z}		D_{4x}		D_{4y}	
	O	x_1^-	$-\mathsf{x}_1^-$	x_1^-	$-\mathsf{x}_1^-$	x_1^-	$-\mathsf{x}_1^-$
D_{4j}	D_{4hj}	$(x_3^+, 0)$	$(x_3^+, 0)$	$(-ax_3^+, bx_3^+)$	$(-ax_3^+, bx_3^+)$	$(-ax_3^+, -bx_3^+)$	$(-ax_3^+, -bx_3^+)$
	D_{4j}	$(x_3^-, 0)$	$(-x_3^-, 0)$	$(-ax_3^-, bx_3^-)$	$(ax_3^-, -bx_3^-)$	$(-ax_3^-, -bx_3^-)$	(ax_3^-, bx_3^-)

Exomorphic symmetry descents: Let us consider two symmetry descents: $G \Downarrow F_1$ and $\widetilde{G} \Downarrow \widetilde{F}_1$. First we construct the intersections $H = \text{core } F_i = \bigcap_i F_i$ and $\widetilde{H} = \text{core } \widetilde{F}_i = \bigcap_i \widetilde{F}_i$, which are normal subgroups of G and $\widetilde{G}$, respectively.

If the factor groups G/H and $\widetilde{G}/\widetilde{H}$ are isomorphic, then there exist homomorphisms σ and $\tilde{\sigma}$, with kernels $\text{Ker } \sigma = H$, $\text{Ker } \tilde{\sigma} = \widetilde{H}$ which map the groups G and $\widetilde{G}$ onto the same group $\mathcal{H} = \sigma(G) = \tilde{\sigma}(\widetilde{G})$. If these homomorphisms also map the groups F_1 and $\widetilde{F}_1$ onto the same subgroup $\mathcal{F}_1 = \sigma(F_1) = \tilde{\sigma}(\widetilde{F}_1)$, then we say that the symmetry descents (group–subgroup relations) $G \Downarrow F_1$ and $\widetilde{G} \Downarrow \widetilde{F}_1$ are exomorphic or of the same exomorphic type.

Diagram of exomorphic relations



The exomorphism of symmetry descents has powerful consequences:

(i) There exists a one-to-one mapping of ireps $\alpha \longleftrightarrow \tilde{\alpha}$ of G and $\widetilde{G}$ engendered by ireps of the factor group $\mathcal{H}$. There also exists a one-to-one mapping of cosets $g_i F_1 \longleftrightarrow \tilde{g}_i \widetilde{F}_i$ such that elements of these cosets act in the same way on spaces of engendered ireps. Indeed, both cosets act in the same way as the element γ_i of the factor group $\mathcal{H}$.

(ii) From this it follows that the stability spaces, strata and typical orbits have identical structures.

(iii) In addition, all polynomials in variables which belong to engendered ireps have the same transformation properties under the action of elements of corresponding cosets.

The concept was introduced by Kopský (1978) for equitranslational phase transitions. In this context, we can say that the consideration of two exomorphic transitions is based on the same algebraic relations. In view of this, the classification of symmetry descents into exomorphic types facilitates systematic investigation. Thus in terms of crystallographic point groups we find 44 exomorphic types. Among them we find 28 cases where the subgroup is an epikernel of some irep, and in five cases out of these the subgroup is simultaneously an epikernel of two ireps. Extending the investigation to magnetic crystallographic point groups, we find another 25 exomorphic types, none of which corresponds to an epikernel.

The number of distinct descents within classical crystallographic point groups is 212, within magnetic crystallographic point groups it goes up to 1599. In terms of equitranslational symmetry descents between ordinary or magnetic space groups this number will go up into the thousands.

Domain states in structural phase transitions

The abstract picture outlined above is applicable to structural phase transitions with symmetry descent, the phenomenological theory of which stems from the work of Landau (1937). The role of parameters which transform by R-ireps was already recognized in this work; Landau calls them *"races of functions"*. The basic idea of the Landau theory is well known. A physical system of symmetry G, called the parent symmetry, allows only such states the parameters of which are invariants of G. These are represented in the abstract picture for point groups by x_1 or x_1^+. Deviations from such states are described by parameters which transform by non-identity R-ireps of the group G. In the abstract picture these are described by typical variables, to which, in models of real situations, correspond some real physical parameters. The typical linear orbits describe, in an abstract manner, the set of domain states; these are those states of the low symmetry which are equivalent with reference to the parent symmetry (Janovec, 1972). The models of structural phase transitions can be developed on different levels of approximation; to describe them we need a few concepts which are not yet commonly used.

Space and subperiodic groups: It is well known that symmetries of crystals are described by space groups. There exist 230 types of such groups, which are described in Vol. A of *International Tables for Crystallography* (2002). It is useful to extend the concept of space groups as well as the concept of crystallographic groups in a manner which will be described below. All groups we shall consider are groups of "isometries" (*"Euclidean motions"* is another term in which we should, however, consider mirror reflections as motions as well). We denote isometries by Seitz symbols $\{g|\mathbf{t}\}_P$, where P is an origin of Euclidean space $E(3)$, $\mathbf{t} \in V(3)$ is the translation of this space, $g \in \mathcal{O}(3)$ is an orthogonal operator on $V(3)$ and $\mathcal{O}(3)$ is the orthogonal group. Any point of $X \in E(3)$ can be expressed as $X = P + \mathbf{x}$, where $\mathbf{x} \in V(3)$ and the action of isometry on points is expressed by:

$$\{g|\mathbf{t}\}_P X = \{g|\mathbf{t}\}_P(P + \mathbf{x}) = P + g\mathbf{x} + \mathbf{t}.$$

We shall now introduce a symbol

$$\mathcal{G} = \{G, T_G, P, \mathbf{u}_G\},$$

for the group of isometries $\{g|\mathbf{t}\}_P$. This set is a group of isometries if the following conditions are satisfied: elements g constitute a point group G, T_G is a G-invariant group of translations $\mathbf{t}$, and $\mathbf{u}_G(g) : G \longrightarrow V(3)$ is a function which assigns to each element g a vector $\mathbf{u}_G(g)$ and which satisfies the following conditions:

$$\mathbf{w}(g, h) = \mathbf{u}_G(g) + g\mathbf{u}_G(h) - \mathbf{u}_G(gh) \in T_G.$$

The function satisfying such conditions is called the system of nonprimitive translations and the function $\mathbf{w}(g, h)$ is called the factor system.

A rigorous mathematical approach to the theory of Euclidean groups has been developed in two exacting papers by Ascher & Janner (1965, 1968/69) in terms of *"cohomology groups"*. The authors thank Professor Procházka from the Mathematical Faculty of Charles University in Prague who deciphered this algebraic theory for us. It applies not only to space groups in their usual meaning but to all Euclidean groups. Combining algebraic background with geometrical interpretation and with the use of groups in problems which go beyond classical crystallography, we found that a slight amendment of the concepts of *"crystallographic"* and of *"space groups"* is desirable. These amendments

were discussed at Commissions of IUCr and publicly proposed at the ECM 9 in Prague (1998). We suggested the following use of terms (for details see Kopský, 2001*a*):

(i) A point group G is crystallographic if it leaves a certain discrete three-dimensional translation subgroup (crystallographic lattice) T_G invariant.

(ii) A Euclidean group $\mathcal{G}$ is crystallographic if G is crystallographic.

(iii) A group $\mathcal{G}$ is a space group if the translation subgroup T_G spans the whole space $V(3)$.

(iv) A group $\mathcal{G}$ is a layer or rod group, if the translation subgroup T_G spans a two-dimensional or one-dimensional subspace of $V(3)$ and it is a site point group if $T_G = \{\mathbf{0}\}$.

This terminology enables us to develop a rigorous approach to the theory of Landau-type phase transitions and of the respective domain walls in the continuous approximation. Indeed, what is the symmetry of a crystal in the continuous approximation? This is a group $\mathcal{G}$ with point group G and translation subgroup $T_G = V(3)$. In view of this, the system of nonprimitive translations can be chosen as trivial, so that the group is denoted by $\mathcal{G} = \{G, V(3), P, \mathbf{u}_G = \mathbf{0}\}$. This group has the property that the symmetry at each point X of the space is G_X. We suggest using the name point-like space groups for such groups. Analogously, we define point-like layer and rod groups, for which $T_G = V(2)$ or $V(1)$, respectively.

Although this terminology sounds unusual, it is more natural than that generally adopted. The main property of crystals is not their *"discreteness"*. All materials are discrete in the same sense. The main property of crystals is their three-dimensional periodicity and its invariance under the point groups. On the other hand, what is the most natural term for groups the translation subgroup of which is the whole space $V(3)$? We believe that *"space groups"* is the most appropriate. In such terminology, the usual space groups are now the crystallographic space groups and, on the other hand, the groups with continuous translation subgroup are crystallographic once their point group is crystallographic. Using this terminology, we can develop the models of structural phase transitions and of domains on different levels of approximation:

1. Microscopic (full-scale) level: In this case we consider the structure described either by atomic positions or by density functions and the symmetries and their descents $\mathcal{G} \Downarrow \mathcal{F}_1$ in terms of space groups. This consideration is always the most rigorous; it is quite necessary in the case of non-ferroic transitions, where the point class of the symmetry group does not change. Indeed, at the level of the continuous approximation (*cf.* the next paragraph) no symmetry change will have a meaning for a non-ferroic transition. The approach certainly also applies in the case of ferroic transitions. The "Scanning Tables" of *International Tables for Crystallography* Vol. E, *Subperiodic Groups* (Kopský & Litvin, 2002) are designed for use when considering domain walls at this level.

2. Continuous approximation: The material is treated as an infinite homogeneous and anisotropic medium and its symmetry is the point-like space group. The microscopic structure is neglected and considerations are confined only to morphic effects, *i.e.* to the change of tensor properties, to the tensor distinction of domain states and to the character of tensors across the domain wall.

This approximation can be used for considering ferroic phase transitions. We should distinguish here two cases:

2.1. Non-equitranslational transitions: In this case we neglect all parameters associated with those ireps of the actual space group which correspond to non-homogeneous modes (wavevectors $\mathbf{k} \neq \mathbf{0}$).

2.2. Equitranslational phase transitions: All ireps associated with the transition are

taken into account but microscopic parameters (displacements of atoms) are ignored.

The concept of transition parameter(s) (generally plural) is of basic importance in phase-transition theory. We should, however, distinguish between transition parameters which appear in the Landau model and transition parameters which are described by morphic effects, *i.e.* by the change of tensor properties. The latter are used in the continuous model.

General case of space structures: Structural phase transitions are characterized by symmetry descents: $\mathcal{G} \Downarrow \mathcal{H}$ or $\mathcal{G} \Downarrow \mathcal{F}_i$, where $\mathcal{G}$ is the parent space group and the low-symmetry space group is either normal, denoted here as $\mathcal{H}$, or there exists a set of equivalent low symmetries $\mathcal{F}_i$ which are conjugate subgroups of $\mathcal{G}$. In the analysis of domain states we first use coset resolution

$$\mathcal{G} = \mathcal{F}_1 \cup \{g_2|\mathbf{u}_G(g_2)\}_P\mathcal{F}_1 \cup \ldots \{g_p|\mathbf{u}_G(g_p)\}_P\mathcal{F}_1 \cup$$

$$\{e|\mathbf{t}_2 + \mathbf{u}_G(g_2)\}_P\mathcal{F}_1 \cup \{g_2|\mathbf{t}_2 + \mathbf{u}_G(g_2)\}_P\mathcal{F}_1 \cup \ldots \{g_p|\mathbf{t}_2 + \mathbf{u}_G(g_p)\}_P\mathcal{F}_1 \cup$$

$$\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots$$

$$\{e|\mathbf{t}_q + \mathbf{u}_G(g_2)\}_P\mathcal{F}_1 \cup \{g_2|\mathbf{t}_q + \mathbf{u}_G(g_2)\}_P\mathcal{F}_1 \cup \ldots \{g_p|\mathbf{t}_q + \mathbf{u}_G(g_p)\}_P\mathcal{F}_1$$

of the space (parent) symmetry $\mathcal{G} = \{G, T_G, P, \mathbf{u}_G(g)\}_P$ of the original (parent) state S into left cosets of the subgroup $\mathcal{F}_1$, which is the symmetry of one of the domain states S_1.

Applying the left coset representatives $\{g_i|\mathbf{t}_j + \mathbf{u}_G(g_i)\}_P$ to the first domain state S_1 we obtain the set of equivalent low-symmetry states:

$$\begin{array}{cccc} \mathsf{S}_1 & \mathsf{S}_2 & \ldots & \mathsf{S}_p \\ \mathsf{S}_1(\mathbf{t}_2) & \mathsf{S}_2(\mathbf{t}_2) & \ldots & \mathsf{S}_p(\mathbf{t}_2) \\ \ldots\ldots & \ldots\ldots & \ldots\ldots & \ldots\ldots \\ \mathsf{S}_1(\mathbf{t}_q) & \mathsf{S}_2(\mathbf{t}_q) & \ldots & \mathsf{S}_p(\mathbf{t}_q) \end{array}$$

where $\mathsf{S}_i(\mathbf{t}_j) = \{g_i|\mathbf{t}_j + \mathbf{u}_G(g_i)\}_P\mathsf{S}_1$. The total number of domain states $pq = [\mathcal{G} : \mathcal{H}] = [G : H][T_G : T_H]$ splits into $p = [G : H]$ sets of orientation states, as representatives of which we may use the states

$$\mathsf{S}_1, \mathsf{S}_2, \ldots, \mathsf{S}_p.$$

To each set there belong $q = [T_G : T_{F_1}]$ translational states

$$\mathsf{S}_i, \mathsf{S}_i(\mathbf{t}_2), \ldots, \mathsf{S}_i(\mathbf{t}_q).$$

Domain states $\mathsf{S}_i(\mathbf{t}_j)$, $i = 1, 2, \ldots, p$, $j = 1, 2, \ldots, q$ in this consideration represent the *"same"* structure in p different orientations and q different locations. Mode analysis is the tool needed to determine domain states with reference to the parent state S. Domains are regions in space occupied by different domain states, and to analyse a *"multidomain"* sample one has to take into account the geometry of the domain structure and the structure of the domain walls (interfaces). Such an analysis begins with the determination of pairs of domain states; representatives of such pairs are in a one-to-one correspondence with double cosets (Janovec, 1972).

Enantiomorphism: If the parent group $\mathcal{G}$ does not contain improper rotations (rotations or screw rotations combined with space inversion), then there exists a mirror image $\widehat{\mathsf{S}}$ of the original structure; the structures S and $\widehat{\mathsf{S}}$ are known as mutually enantiomorphic

structures. The symmetry of the structure $\widehat{\mathsf{S}}$ is the group $\widehat{\mathcal{G}}$, an enantiomorphic partner of $\mathcal{G}$ if $\mathcal{G}$ belongs to one of the 11 pairs of enantiomorphic space-group types; otherwise $\widehat{\mathcal{G}} = \mathcal{G}$. The low-symmetry groups $\mathcal{F}_{\alpha,i}$ then also do not contain improper rotations and there exists a phase transition from the structure $\widehat{\mathsf{S}}$ of symmetry $\widehat{\mathcal{G}}$ to the set of structures $\widehat{\mathsf{S}}_{ij}$ with symmetries $\widehat{\mathcal{F}}_{\alpha,i}$.

If the parent group $\mathcal{G}$ contains improper rotations, then the structure S is mirror-symmetric (some rotations combined with a mirror are its symmetry operations). If the low-symmetry groups $\mathcal{F}_{\alpha,i}$ also contain improper rotations (if one of them does, then all of them do), then the domain states S_{ij} are also mirror-symmetric.

If the parent group $\mathcal{G}$ contains improper rotations while the low-symmetry groups $\mathcal{F}_{\alpha,i}$ do not (again, if one of them does not, then none does), then the set of domain states S_{ij} splits into two subsets; the domain states within each of these subsets differ only by orientation and location, while all domain states of one of the sets are mirror images (subject to rotation and translation) of domain states of the other set.

Geometric description of domain states. In the theory of displacive phase transitions we can describe domain states as follows. We assume that we know the original parent structure S. Various modes of motion of this structure are classified by ireps $\chi_\alpha(\mathcal{G})$ of the parent group $\mathcal{G}$. Quite generally, the mode analysis consists of the determination of carrier spaces $V_{\alpha a}$, belonging to these ireps, in terms of atomic displacements. As long as the temperature and hydrostatic pressure remain in the region of the parent phase, the displacements over the time average vanish. Only those invariants are allowed which account for possible changes of lattice parameters and motion of atoms without leaving their Wyckoff positions. The space-group type and the structure type do not change.

At the transition point on a (T, p) line of a phase diagram, some of the modes are frozen so that the atoms are displaced from their original positions, which leads to the change of the structure type and of the space-group type. If the low symmetry is the subgroup $\mathcal{F}_1$ of $\mathcal{G}$, the frozen displacements are those which belong to stability spaces $V_{\alpha a}(\mathcal{F}_1)$. These stability spaces are copies of the typical stability spaces $V_\alpha(\mathcal{F}_1)$ and the number of spaces $V_{\alpha a}(\mathcal{F}_1)$ is equal to the number of modes which transform by the irep $D_R^{(\alpha)}(\mathcal{G})$. We can use the same coset resolution as for the typical orbit to obtain the orbit of vectors

$$\mathbf{x}_{ij} = (\ldots, \mathbf{x}^{(\alpha)}_{a,i_\alpha j_\alpha}, \ldots, \mathbf{x}^{(\beta)}_{b,i_\beta j_\beta}, \ldots),$$

each of which describes one of the equivalent domain states S_{ij} of the low symmetry. Here, equivalence means that whatever pair of domain states we choose, there exists an element of the parent group $\mathcal{G}$ which sends one of them to the other (in fact, it is always the whole coset of elements). Here, indices i, j are related to those used in labelling the vectors of the typical orbit.

Primary and secondary parameters: In the Landau theory we assume that one of the modes becomes unstable at the transition line and is therefore frozen. Parameters of this mode are usually described by letters η. In our consideration this will be the components of a certain vector $\mathbf{x}^{(\alpha)}_{o,11} \in V_{\alpha o}$. This parameter is usually called the primary order parameter (or primary transition parameter). Since the low symmetry $\mathcal{F}_1$ is the stabilizer of this vector, all domain states differ in this parameter. In this case, the set of domain states is called full in this parameter. The onset of this parameter is to be considered as the cause of the symmetry descent. Since the parameter belongs to a certain irep $D_R^{(\alpha)}(\mathcal{G})$, the low-symmetry group has to be an epikernel of this irep.

The descent of symmetry leads generally to an onset of other parameters. For the time being we simply assume that such parameters appear because they are allowed. These parameters are called the secondary parameters and three different types of them may exist:

(i) If there exist other modes $\mathbf{x}_{a,11}^{(\alpha)}$ which belong to the same irep as the primary parameter, they should also freeze in the low-symmetry states.

As we have seen in the consideration of the typical orbit, in general parameters $\mathbf{x}_{b,11}^{(\beta)}$ belonging to other ireps should also onset. There are two possibilities:

(ii) The low-symmetry group is simultaneously an epikernel of another irep $D_R^{(\beta)}(\mathcal{G})$ and hence it is the stabilizer of some vectors $\mathbf{x}_{b,11}^{(\beta)}$.

(iii) The stability space of the low symmetry is nontrivial in the typical space $V_\beta(\mathcal{F}_1)$ and hence in all spaces $V_{\beta b}(\mathcal{F}_1)$, but the stabilizer of a general vector of such a subspace is a group $\mathcal{F}_{\beta 1}$ which contains $\mathcal{F}_1$.

The set of domain states is full in secondary parameters in cases (i) and (ii). In case (iii), several domain states correspond to one value of the parameter. We say that the set of domain states is partial in this parameter. The names *"full"* and *"partial"* for the set of domain states as well as the term *"faint"* for coupling of secondary parameters with the transition parameter are borrowed from the work of Aizu (1969, 1970, 1972, 1979).

Interactions: Primary parameter. In the consideration of the Landau potential we should generally write down invariant polynomials in terms of all transition parameters. Since the ireps which are used are orthogonal and irreducible over the field of real numbers, the form of an invariant in every parameter $\mathbf{x}^{(\alpha)}$ has the form $\sum_{i=1}^{d_\alpha} x_{\alpha i}^2$. In the Landau potential we assume that the constant at this term for the primary transition parameter $\mathbf{x}_o^{(\alpha)}$ is proportional to the difference $(T - T_c)$, where T_c is the transition temperature. The remaining terms have the form of polynomials which can be found in the integrity basis of invariants.

Faint interactions: The secondary parameters $\mathbf{x}^{(\beta b)}$ transform like $\mathbf{x}^{(\beta)}$, which forms an invariant $\sum_{j=1}^{d_\beta} x_{\beta j}^2$. This means that invariants of the form

$$\sum_{j=1}^{d_\beta} x_{\beta b,j} p_{\beta j}(\mathbf{x}_o^\alpha)$$

also exist, where $p_{\beta,j}(\mathbf{x}_o^\alpha)$ transform like $x_{\beta j}$, so that they are components of a polynomial $D_R^{(\beta)}(\mathcal{G})$-covariant in components of a $D_R^{(\alpha)}(\mathcal{G})$-covariant $\mathbf{x}_o^\alpha$. The components of these covariants are proportional to the forces which are exerted by primary parameter on the secondary parameters. In continuous phase transitions, the value of primary parameter slowly grows from zero. The forces acting on secondary parameters behave like powers of the primary parameter and are therefore smaller the higher the degree of the lowest polynomial $p_{\beta,j}(\mathbf{x}_o^\alpha)$. Aizu uses the name "faintness index" for this power and we shall accordingly call the interactions of the primary parameter with secondary parameters the "faint interactions". The lowest-degree polynomials are contained in the extended integrity bases in terms of the primary parameter. According to the representation generating theorem, faint interactions always exist and determine the forces exerted by the primary parameter which bring the secondary parameters to life (Kopský 1979*f*).

A secondary parameter $\mathbf{x}_a^\alpha$ may also belong to the same irep as the primary parameter $\mathbf{x}_o^\alpha$. In this case, there exists an invariant of the form $\sum_i x_{\alpha o,i} x_{\alpha a,i}$. It is always possible

to eliminate such invariants by a diagonalization procedure and it is also advisable to do so. Indeed, the existence of such interactions indicates that $\mathbf{x}_o^\alpha$ is not an *"eigenmode"*. In other words, the index of faintness should never be 1. Polynomials $p_{\alpha,i}(\mathbf{x}_a^\alpha)$ always exist and the ones of lowest order couple with the primary parameter $\mathbf{x}^\alpha$ into faint interactions $\sum_i x_{\alpha o,i} p_{\alpha,i}(\mathbf{x}_a^\alpha)$ (*cf.* the example of two approaches to the ferrielectric behaviour of ammonium sulfate below).

Remark: In application to ferroelectrics and ferroelastics, the terms proper, improper (Dvořák, 1971, 1972; Levanyuk & Sannikov, 1970, 1974) and pseudoproper (Petzelt, Grigas & Mayerová, 1974) are widely used. The first means that polarization or deformation is the primary parameter, in the second case it is the secondary parameter, the third case applies if polarization or deformation is a secondary parameter transforming in the same way as the primary parameter. With reference to microscopic theory, this terminology seems to have rather historical value. Thus in the example of ammonium sulfate, polarization is neither primary nor secondary parameter. In this case, the primary parameter is a certain linear combination of modes which carries part of the polarization, the secondary parameter is another combination which carries the other part. At the same time, both components transform by the same irep. Let us recall the historical experiment on gadolinium molybdate (Cross, Fousková & Cummins, 1968) where a ferroelectric phase transition was not accompanied by a pronounced peak in permittivity, which would be predicted by phenomenological theory with polarization as a transition parameter. Cochran (1971) introduced the concept of the "soft mode", which is identical with primary order parameter. This mode is not necessarily homogeneous, so it cannot be in general identified with any macroscopic parameter.

Switching interactions: Parameters which transform by ireps of space groups which correspond to a wavevector $\mathbf{k} = \mathbf{0}$ also interact with external fields. These interactions with an electric field can be expressed as invariants of the form

$$\sum_{i=1}^{d_\alpha} x_{\alpha i} p_{\alpha i}(\mathbf{E}),$$

while the interactions with an external mechanical stress are expressed as

$$\sum_{i=1}^{d_\alpha} x_{\alpha i} p_{\alpha i}(\sigma).$$

Remark 1: It nearly became traditional to denote the components of the primary transition parameter by η_i; this corresponds to the subscript "o" in our treatment.

Remark 2: You can find switching interactions with electric field in tables for every parameter. The fact that an electric field can, in principle, always switch the domain states while mechanical forces can always switch domain states associated with tensors of even parity is again a consequence of the representation generating theorem (Kopský, 2001*c*). On the basis of this theorem combined with parity reasoning we can find analogous laws for the switching of domain states in cases when magnetic properties are involved.

Many-parametric structural phase transitions: The consideration above assumes that the transition parameter belongs to a certain irep of the parent group and hence that the low-symmetry group is a kernel or epikernel of this irep. We shall say that such transitions are single parametric, which means that they are associated with a single irep. There exist, however, symmetry descents to subgroups which are neither kernels nor epikernels

of ireps. On the other hand, every normal subgroup is either a kernel or an intersection of kernels and every other subgroup is either an epikernel or an intersection of epikernels. The low symmetry can therefore always be attained by simultaneous onset of two or more parameters. The model of such transitions was proposed by Holakovský (1973) under the name triggered phase transitions. Other models are considered in Section 2.5 of the book by Kociński (1990) and in Section 4.4 of the book by Tolédano & Dmitriev (1996).

The direct and inverse Landau problem. There are two possible approaches to a group-theoretical part of an analysis of feasible structural phase transitions with a certain parent symmetry $\mathcal{G}$, which were formulated by Kobayashi & Ascher (1977):

(i) The direct problem: Assuming that we know the class $\chi_\alpha(\mathcal{G})$ of ireps to which the primary transition parameter belongs (*i.e.* according to which it transforms), find possible low-symmetry groups $\mathcal{F}_\alpha$. The term epikernel was actually introduced in connection with this formulation.

(ii) The inverse problem: Assuming that we know the low-symmetry group $\mathcal{F}$, find the ireps that are candidates for being the ireps of the primary transition parameter. In other words, find ireps of which the group is an epikernel.

The subduction and chain subduction criteria: Under these names criteria were introduced (Birman, 1966; Goldrich & Birman, 1968; Jarič, 1981, 1982, 1983) which actually represent auxiliary procedures for determination of epikernels of ireps and hence for the solution of the direct problem. Hatch & Stokes (1986) and Stokes & Hatch (1988), with the use of a mainframe computer, determined epikernels (using the name *"isotropy subgroups"*) of all those ireps of the space groups which correspond to points of special symmetry in the Brillouin zone. Thus they solved the direct Landau problem for a large class of feasible transitions.

The Ker-core criterion: To solve the inverse Landau problem in a certain particular case, one can use the Ker-core criterion by Ascher (1977). The use of this criterion facilitates the solution of the inverse problem, *i.e.* the search for ireps to which the transition parameter may belong including the cases when the transition is many-parametric. In application of this criterion we find first the intersection of the set of conjugate low-symmetry groups: core $\mathcal{F}_i = \bigcup_i \mathcal{F}_i = \mathcal{H}$, which is the normal subgroup of the parent group $\mathcal{G}$, and then we find the factor group $\mathcal{G}/\mathcal{H}$. If this group contains faithful R-ireps, then $\mathcal{F}_i$ are epikernels of engendered R-ireps of the original group $\mathcal{G}$. If the only faithful representations of the factor group are reducible, then groups $\mathcal{F}_i$ are intersections of epikernels of those R-ireps which are contained in the reducible representation of $\mathcal{G}$ engendered by faithful representation of the factor group.

It is our opinion that these approaches will soon be replaced by electronic databases and software, which will readily answer both the direct and inverse Landau problem for structural phase transitions associated with special points of the Brillouin zone, like the present software does for ferroic transitions. The current situation in the topic of phase transitions is similar to early studies of crystal structures. At the time when the first tables of space groups appeared [references to *International Tables* which are based on group theory, starting with the pioneering book by Niggli (1919), are listed at the end of bibliography], only a few space symmetries were represented by known structures. The number of known structural phase transitions grows [see the last report by Tomaszewski (1992)] which justifies systematic research, especially in the case of ferroic transitions in connection with the development of so-called *"domain engineering"*. The aim of such research is not only to save the tedious work in interpretation of experimental results; its importance also lies in setting standards by which such results may be expressed.

Tensor calculus of domain states in ferroic phase transitions

In our consideration of ferroic phase transitions we adopt the following philosophy: *"The full investigation of a structural phase transition requires mode analysis, which may differ from one material to another even if the symmetry groups of parent and low-symmetry phase are identical. Changes of material properties in ferroic transitions and the relationship between these properties in different domains can, however, be investigated on the grounds of group–subgroup relations in complete independence of specific materials."* In other words, our analysis in this section and the results in the accompanying software do not depend on particular microscopic models. The development of tensor calculus for domain states is a prerequisite in a strategy for a general investigation of multidomain materials which may play an important role in the development of *"domain engineering"*. As usual, such investigations supply only qualitative results and cannot predict the magnitude of effects.

The consideration of changes of material properties in ferroic phase transitions is based on the same scheme as the analysis of structural changes with mode coordinates replaced by tensor components. This approach is useful because it provides important information, but it cannot replace the mode analysis even in the case of equitranslational phase transitions. Two important points of this analysis will now be briefly scrutinized.

Principal and secondary tensor parameters. The first point concerns the fact that material properties cannot be considered as the order parameters in the Landau sense, *i.e.* as parameters which appear in the Landau potential. Changes of these properties at ferroic transitions are described as morphic effects. Spontaneous polarization and strain should also be considered as morphic effects, although they were and still are considered as order parameters in proper ferroelectric and ferroelastic phase transitions. This is, however, possible only if they are so strongly connected with modes that their use does not lead to any confusion. In this connection we recall the case of the ferrielectric behaviour of ammonium sulfate (Unruh, 1970). Two models were proposed to explain this behaviour (Kopský, 1976*c*; Dvořák & Ishibashi, 1976). Two components of polarization, each connected with its own mode, were introduced in both cases. This example is very illustrative. On symmetry grounds there is no reason to split polarization into two components. The ferrielectric behaviour can, however, be explained in analogy with well known ferrimagnetic models if we assume the existence of two modes, each of which carries part of the polarization. In the model by Dvořák & Ishibashi (1976) one mode is considered as the primary parameter. The other mode has the same transformation properties and therefore there exist bilinear interactions between the two modes which lead to a shift of the originally assumed transition temperature. The existence of bilinear interactions, however, implies that the first mode is not an *"eigenmode"*. In the model by Kopský (1976*c*), linear combination of the two modes such that the bilinear interaction is eliminated is assumed to be the primary order parameter. Both models predict the same temperature dependence of polarization but the second does not need introduction of the shift of transition temperature. This example shows clearly that on the level of morphic effects we cannot use the concept of the *"primary order parameter"* unless specific conditions are met. For example, if there is only one mode which carries polarization and this mode is the primary parameter, then polarization can also be safely considered as the primary parameter.

It is, however, possible to apply to morphic effects the same principle of *"cause ⟶ consequence"* as to the modes. The relationship between symmetry and allowed parameters is twofold. If we observe an onset of a new material property, not allowed by the parent group, with the change of temperature T and hydrostatic pressure p, we can certainly conclude that a ferroic transition took place, leading to symmetry descent and consequently to the appearance of other new properties allowed by the ferroic group. We should, of course, remember that behind this change there lies a deeper *"cause"* in the structural changes which are beyond the macroscopic observation.

If an experimentalist observes an onset of some tensor parameters which are not allowed by the parent symmetry G, he can certainly conclude that a transition with symmetry descent to some subgroup F_1 took place. On the other hand, such symmetry descent is accompanied by an onset of all those parameters which are covariant components allowed by symmetry F_1 while forbidden by G. Some of these parameters themselves may, however, result in higher symmetry then F_1 though lower than G.

In tables analogous to Table B1 which, in different form, were also published a long time ago (Kopský, 1982, 1983), we clearly distinguish, in terms of typical variables, parameters which lead to a subgroup F_1 from those which are consequently allowed. Those variables which are framed represent the cause of the transition to an epikernel. In some cases there may exist two types of framed variables belonging to different R-ireps in the case of point groups. If a subgroup is not an epikernel to any R-irep, then it can be expressed as a *"true intersection of epikernels"*, perhaps in several ways. In this case, we should consider simultaneously the parameters of these epikernels as the cause of the descent. The remaining parameters are then the consequence of the descent. Tables of tensorial covariants enable us to interpret these variables in terms of tensor parameters. Although we use here the term tensor parameter in the singular, we should realize that they may contain several components.

We shall say that a tensor parameter is a principal tensor parameter of a symmetry descent $G \Downarrow F_1$ if it is the cause of the descent; in this case F_1 is the stabilizer of a tensor corresponding to these parameters. Other parameters will be called the secondary tensor parameters. There are infinitely many principal tensor parameters, but we are limited by experimental facilities. Even with tensors, considered in this work, there are usually several principal tensor parameters of different tensor character. In cases where the low-symmetry group is not an epikernel but an intersection of epikernels, some of the parameters may have different tensor character to the others. The principal tensor parameters are in a certain sense analogous to the primary order parameter and secondary tensor parameters are analogous to faint variables. One of the manifestations of the difference between the consideration of structural changes and of morphic effects is the fact that we can consider several tensor parameters as the principal ones, while there is always one primary order parameter.

Tensor parameters of a symmetry descent are certain covariant components of a tensor. To see the change of the tensor in its Cartesian form in the transition, we should use the conversion relations. Detailed analysis of particular cases can be performed with use of our tables and of conversion relations. There exist cases which might seem strange at first sight. Thus it may happen that part of a certain Cartesian tensor component appears as the principal parameter while another contribution to the same component is a secondary parameter, so that the structure of domain states is full in one of these contributions and partial in the other part. Let us finally observe that the invariant linear combinations of Cartesian components also represent the independent parameters of tensors of a given type for a given symmetry.

Continuous model of ferroic transitions. In the case of ferroic phase transitions we consider the crystal as a homogeneous anisotropic continuum. The appropriate symmetry is, in this case, a certain point-like space group VG whose isometries are all $\{g|\mathbf{t}\}_P$ with $g \in G$ and $\mathbf{t} \in V(3)$. In other words, this is the space group which contains all translations of the space and its elements which leave a certain but arbitrary point P of the space invariant form just the site point group G_P. Rigorously speaking, we should consider the point-like space groups as the symmetry groups of crystals in the continuous description and homogeneous tensor fields as their material properties.

This also concerns the case of equitranslational phase transitions, which it is virtually traditional to treat in terms of point groups. The reason why there is no seeming contradiction is of a group-theoretical nature. The translation subgroup is not changed in such transitions and hence all quantities which became invariant in the low-symmetry group transform by those ireps of the parent space group which are engendered by ireps of its point group. Since the tensor fields are constant throughout the space, we express the results in terms of point groups and tensor components. This approach should be considered merely as a suitable way of presenting the information and we should realize that it will fail the moment we try to consider domain walls. In this case, we cannot speak about the point symmetry of the wall; its symmetry in a continuous description is a point-like layer group and it is a sectional layer group of the point-like space group.

In the case of equitranslational transitions, there exist tensor parameters which transform like the primary order parameters (or a set of parameters in many-parametric transitions). In the case of non-equitranslational transitions, no tensor parameter transforms like the primary order parameter. All tensor parameters are then secondary parameters from the viewpoint of the Landau model. However, even in these cases we shall distinguish the principal and secondary tensor parameters of the ferroic transition.

Comment: The point-like space, layer and rod groups were introduced by Kopský (1993*a*,*b*) and used in the description of domain walls by Přívratská & Janovec (1999).

Ferroic domain states: Ferroic phase transitions are defined as transitions in which the point symmetry G of the crystal decreases, either to a normal subgroup H of G or to one of the set of conjugate subgroups F_i. As long as we are interested only in morphic effects, we can consider these transitions in the continuous approximation. As shown in the preceding paragraph, the point-like space groups VG should be used as the symmetry of crystal, VH or VF_i as symmetries of the domain bulk, point-like layer groups as symmetries of sections (interfaces) and tensor fields should be used instead of tensor components. However, as long as the analysis of domain walls is not included, we can use point groups and tensor components to describe the morphic effects in all domain states. This simplification is suitable for both theoretical consideration and tabular presentation, and the results can be easily amended.

Let us therefore consider a ferroic phase transition $G \Downarrow F_i$. The first domain state S_1 corresponds to the low symmetry F_1. The coset resolution

$$G = F_1 \cup g_2F_1 \cup \ldots g_pF_1$$

of G into left cosets of F_1 is again used to derive the set of $p = [G : F]$ orientation domain states

$$\mathsf{S}_1,\ \mathsf{S}_2 = g_2\mathsf{S}_1,\ \ldots,\ \mathsf{S}_p = g_p\mathsf{S}_1$$

from a chosen first domain state S_1.

We can also consider the fine structure $\mathsf{S}_{ij} \approx (\mathbf{x}_{ij}^{(\alpha)}, \ldots, \mathbf{x}_{i_\beta j_\beta}^{(\beta)}, \ldots)$ of domain states in terms of morphic effects. Such structures were found for all ferroic phase transitions by Kopský (1982) in terms of typical variables. The main tables of the present work describe the fine structure of the first domain state in terms of onsetting tensors, and they were obtained by the joint use of these tables and of tables of tensorial covariants (Kopský, 1979*a*,*b*). The tables of this work describe the fine structure of the first domain state in all nonmagnetic ferroic transitions in terms of point groups and tensor components.

An overview of the general analysis.

1. As a first step of the general analysis we consider representatives of all symmetry descents $G \Downarrow H$ or $G \Downarrow F_i$ in terms of crystallographic point groups. For each such symmetry descent we want to find the answers to the following questions:

(i) What are the changes of tensor properties at $G \Downarrow F_i$ or, more precisely, what new tensor parameters distinguish the first domain state S_1 (and the other domain states S_i) from the parent state S?

(ii) How do the tensors distinguish domain states of a pair S_i and S_j?

(iii) What combinations of stress and electric field force the switching of domain states?

2. Consideration of domain walls (interfaces) of different orientations is the next step. It is important to realize at this point that domains are regions occupied by the same phase; domain states refer to various orientations of this phase in space. At this stage, it is desirable to analyse orientation scanning, *i.e.* to find the dependence of point-like layer symmetries on interface orientations.

3. *Domain engineering.* To analyse the behaviour of multidomain samples we need all the information from the previous points and, in addition, we have to know (or assume) the geometry of the domains.

Pairs of domain states and twinning group: Although the tables of fine structure of typical orbits represent the relationship between any pair of domain states, it is sufficient to consider, in particular situations, only certain representative pairs of domain states. It has been shown by Janovec (1972) that the sets of equivalent domain pairs correspond to double cosets of the low-symmetry group in the parent group. There may appear situations when the original structure is not known or does not exist at all. If we know the pair of domain states S_1 and $\mathsf{S}_2 = g\mathsf{S}_1$, it is possible to find the tensor distinction of such a pair with the use of the so-called "twinning group" $K = \{F_1, g\}$ (Fuksa & Janovec, 1995), generated by the symmetry F_1 of the state S_1 and by the "twinning operation" g. The two domain states may then be considered as a result of presumed transition $K \Downarrow F_1$. Analogously, a set of domain states S_1, $\mathsf{S}_2 = g_2\mathsf{S}_1$, ..., $\mathsf{S}_k = g_k\mathsf{S}_1$ can be considered as a result of a transition $K \Downarrow F_1$, where $K = \{F_1, g_2, \ldots, g_k\}$ is the group generated by F_1 and elements g_2, ..., g_k.

Completely transposable domain pairs: The case of symmetry descent $G \Downarrow H$ where the low-symmetry group H is a halving subgroup of the parent group G represents the simplest case of symmetry descent, associated with a single one-dimensional irep $\chi_\alpha(G)$ to which there corresponds one typical variable x_α. The subgroup H is the kernel of the irep $\chi_\alpha(G)$ and it has only one coset $gH = Hg$, the elements of which change the sign of the variable x_α, so that $gh\mathsf{x}_\alpha = -\mathsf{x}_\alpha$ for every $gh \in gH$. Hence only two domain states

exist, the parameters of which differ only in the sign.

In general, there also exist pairs of domain states $(\mathsf{S}_1, \mathsf{S}_2)$ in symmetry descents which have otherwise a rather complicated structure of domain states but which have the property that they are completely transposable. The complete theory and information about general types of domain pairs and about their tensor distinction is still being developed, but in this particular case we know the answer. The pair is called completely transposable if both states have the same symmetry H and if there exists an element $g \in G$ which swaps the domain states, so that $g\mathsf{S}_1 = \mathsf{S}_2$, $g\mathsf{S}_2 = \mathsf{S}_1$. The twinning group of such a pair of states is then the group $K = H \cup gH$. There exists an irep $\chi_\alpha(G)$ of the twinning group K of which H is a kernel and we can consider the relationship between the two domain states as a result of symmetry descent $K \Downarrow H$. From this we conclude immediately which of the tensor components are identical in both states and which differ in sign. Every point group which has a halving subgroup appears as a twinning group K for some pairs of completely transposable domain pairs. To emphasize that the group is interpreted as a twinning group, we distinguish the elements of the coset by a star (originally an asterisk was used, but this clashes with notation in reciprocal space). For the twinning groups we use Schönflies symbols of the form $G^\star(H)$, while in their Hermann–Mauguin symbols a star is used as a superscript at those generators which belong to the coset gH. These symbols are analogous to symbols of magnetic groups and sometimes the twinning groups are also considered as *black-and-white* groups as if the domain states are distinguished as black and white. This, however, is not a correct interpretation. Twinning groups are ordinary point groups and the star is only a suitable label for distinguishing elements that change the domain states from those that do not.

Tables of ferroic transitions

Below we give an account of the information which can be explicitly found in the main tables of the software. Each table is accessible when lattice of the parent group G is displayed on the screen by choosing the low-symmetry group and the menu item Domains. The following tensors are involved in these tables: enantiomorphism (chirality) ε, polarization $\boldsymbol{P}$, deformation tensor $\boldsymbol{u}$, tensor of optical activity $\boldsymbol{g}$, piezoelectricity $\boldsymbol{d}$, electro-optics $\boldsymbol{A}$, elastic stiffness $\boldsymbol{s}$, elasto-optics $\boldsymbol{Q}$. In terms of these tensors the main tables describe:

1. Tensor components common to all domains – invariant under the parent group G.
2. New tensor components which appear in the first domain state of the symmetry F_1.

These tensor components are distinguished according to the ireps to which they belong. This enables us to specify principal tensor parameters with "full" structure of domain states and secondary parameters with "partial" structure of domain states in the sense defined by Aizu.

3. The number of conjugate subgroups, total number of domain states, number of ferroelectric states and of ferroelastic states is given for each partial set of domain states.
4. In the case of transitions that are not associated with one particular irep (irreducible representation), the ferroic subgroup is expressed in terms of true intersections of epikernels (groups associated with one irep).
5. Algebraic expressions for the construction of the Landau potential.

Remark: To abbreviate expressions of certain polynomials, we use in this part of the tables special symbols of standard polynomials, the form of which and some relations are

expressed in Appendix D.

Representative ferroic symmetry descents: As already pointed out, the use of point groups and tensor components in the description of ferroic transitions is conventional. It simplifies the tabulation and the user can always replace point groups by point-like space groups and tensor components by homogeneous tensor fields as necessary when considering domain walls or twin boundaries. A ferroic phase transition is therefore characterized below by its parent point group G and by the set F_i of its conjugate subgroups. In tables we refer to that relation as the symmetry descent $G \Downarrow F_i$ and each table gives the tensor parameters of the first domain state S_1 corresponding to the symmetry F_1. Both parent group G and ferroic subgroup F_1 must be completely specified with reference to the Cartesian coordinate system to which the tensor components are related. From the viewpoint of the macroscopic (continuous) description, it would be sufficient to consider one parent group of a specific orientation for each geometric crystallographic class so that altogether we should describe symmetry descents from the 32 parent point groups. We use a slightly broader viewpoint by considering pairs of parent groups of different orientations in the following cases:

Geometric class	First parent group	Second parent group
$D_{2d} - \overline{4}2m$	$D_{2dz} - \overline{4}_z 2_x m_{xy}$	$\widehat{D}_{2dz} - \overline{4}_z m_x 2_{xy}$
$D_3 - 32$	$D_{3x} - 3_z 2_x$	$D_{3y} - 3_z 2_y$
$C_{3v} - 3m$	$C_{3vx} - 3_z m_x$	$C_{3vy} - 3_z m_y$
$D_{3d} - \overline{3}m$	$D_{3dx} - \overline{3}_z m_x$	$D_{3dy} - \overline{3}_z m_y$
$D_{3h} - \overline{6}2m$	$D_{3h} - \overline{6}_z 2_x m_y$	$\widehat{D}_{3h} - \overline{6}_z m_x 2_y$

The reason will become clear on inspection of the space groups of these geometric classes in Vol. A of *International Tables for Crystallography* (2002). If the crystallographic basis (**a**,**b**,**c**) of the respective space groups is chosen in the same way with reference to the Cartesian basis, then in each of these geometric classes we shall obtain point groups of two standard orientations as listed above.

From the macroscopic viewpoint it is also not necessary to distinguish between such symmetry descents as, for example, $D_2 - 2_x 2_y 2_z \Downarrow C_{2x} - 2_x$, $D_2 - 2_x 2_y 2_z \Downarrow C_{2y} - 2_y$, $D_2 - 2_x 2_y 2_z \Downarrow C_{2z} - 2_z$, or $D_{4z} - 4_z 2_x 2_{xy} \Downarrow (C_{2x} - 2_x, C_{2y} - 2_y)$ and $D_{4z} - 4_z 2_x 2_{xy} \Downarrow (C_{2xy} - 2_{xy}, C_{2x\overline{y}} - 2_{x\overline{y}})$ and others, which are nevertheless given in the tables as distinct symmetry descents.

As a result, the total number of symmetry descents considered in the main tables is 278, although the number of macroscopically different types is only 212.

An overview and characterization of symmetry descents: There is no natural order of subgroups of a given group because the subgroups form lattices which are only partially ordered sets. This makes the search of particular symmetry descents rather unpleasant in the printed form (Kopský, 2001*b*), while in the software we can pick up the desired table directly. Auxiliary information about representative symmetry descents is given in Appendix F of this file, where each symmetry descent is characterized according to the following criteria:

A: Symmetry descent $G \Downarrow H$ where H is a normal subgroup of G:

A0. H is a halving subgroup of G.

A1a. H is a kernel of an irep $D^{(\alpha)}(G)$, which does not generate ireps other than the trivial. No faint variables.
A1b. H is a kernel of one specific irep $D^{(\alpha)}(G)$, which generates other ireps $D^{(\beta)}(G)$.
A1c. H is simultaneously a kernel of two ireps $D^{(\alpha_1)}(G)$, $D^{(\alpha_2)}(G)$.
A2. H is an intersection of two or more kernels but is itself not a kernel of any irep.

B. Symmetry descents $G \Downarrow F_i$ where F_i is a set of conjugate subgroups:

B1a. F_i are epikernels of one specific irep $D^{(\alpha)}(G)$ and there are no faint variables for other ireps.
B1b. F_i are epikernels of one specific irep $D^{(\alpha)}(G)$, and there are faint variables for some other ireps $D^{(\beta)}(G)$.
B1c. F_i are simultaneously epikernels of two ireps $D^{(\alpha_1)}(G)$, $D^{(\alpha_2)}(G)$.
B2. F_i are intersections of epikernels of two or more ireps but they are not epikernels of any ireps.

The first column of the list contains the parent groups, the second their subgroups. In the next column, the characteristic of the descent by the criteria above is given, followed by its exomorphic type as defined by Kopský (1982).

The contents of the tables: The main tables have the following common features:

1. Each table begins with a title Symmetry descent $G \Downarrow H$ (cases A) or Symmetry descent $G \Downarrow F_i$ (cases B) in embellished Hermann–Mauguin symbols.

2.1. The heading block bears the specification Parent point group G followed by both embellished Hermann–Mauguin and Schönflies symbols. The form of tensors which are allowed by this group is given below.

2.2. In cases of symmetry descents $G \Downarrow H$, where H is a halving subgroup of the parent group G, an alternative specification or twinning point group K is given followed by a Hermann–Mauguin symbol in which elements which belong to the coset gH are distinguished by a star ($\star$) in the superscript and by a Schönflies symbol of the form $G^{\star}(H)$ ($cf.$ the description of the case A0).

3. The rest of the table is divided into rows, each of which corresponds to an irep $\chi_\beta(G)$ for which the stability space $V_\beta(H)$ or $V_\beta(F_1)$ [and hence of all $V_\beta(F_i)$] of the ferroic subgroup(s) is nontrivial. These rows cross the columns which give the following information about each irep $\chi_\beta(G)$:

3.1. The spectroscopic symbol and description of stability space $V_\beta(H)$ or $V_\beta(F_1)$ in terms of typical variables is given in the first column.

3.2. The symmetry $F_{\beta 1}$ of the first domain state with reference to the general vector (vector of stratum) of the space $V_\beta(F_1)$ in both embellished Schönflies and Hermann–Mauguin symbols is specified in the second column.

3.3. The third column contains tensorial $D^{(\beta)}(G)$-covariants of the tensors considered.

3.4. The last four columns give in order the numbers:
n_f = the total number of domain states in the space V_β;
n_F = the number of conjugate subgroups $F_{\beta,i}$;
n_a = the number of ferroel<u>a</u>stic domain states in the space V_β;
n_e = the number of ferroel<u>e</u>ctric domain states in the space V_β.

An asterisk at the domain number in a specific row means that this number of domains does not correspond to the irep of this row.

If the transition is single parametric so that the ferroic subgroup is an epikernel (kernel) of some irep or of two ireps, then the last row corresponds to the irep of the principal tensor parameters (plural) or, in cases A1c and B1c, the last two rows correspond to the two potential principal tensor parameters.

If the ferroic subgroup is neither a kernel nor an epikernel of one irep but an intersection of kernels or epikernels (cases A2 and B2), then the second part of the table begins again with rows which describe the stability spaces (strata) of the ferroic group in individual carrier spaces. These rows indicate the stabilizers to these strata (kernels and epikernels) and describe the tensors and domain states in the same manner as above. None of the stabilizers is the desired ferroic group in this case. The next part has a special subheading; the first column headed by Reducible representations contains in each row a direct sum of stability spaces corresponding to each of the subgroups which lie between epikernels and the ferroic group; in most cases there is only one such row and the subgroup is already the ferroic group. The second column headed Ferroic Point Group F; Intersections shows how such a subgroup can be expressed as a true intersection of epikernels and what transition parameters correspond to each such intersection. The last four columns contain again the numbers n_f, n_F, n_a and n_e.

In the bottom block of each table the interactions are given in the form:

Integrity basis: Basic invariant polynomials for the transition parameter.

Faint interactions: Linear coupling of faint variables with polynomials in the transition parameter.

Electric and elastic switching interactions: Linear coupling of the transition parameter as well as of faint variables with polynomials in components of electric field $\mathbf{E}$ or of elastic field σ.

Specific features corresponding to the characteristics of symmetry descents given above are:

A0. In this case, H is a kernel of a certain one-dimensional real irep χ_α and hence a halving subgroup of the parent group G. All onsetting properties transform like the respective variable x_α and there are two domain states in which all tensor parameters of this type differ in sign. With reference to the distinction of pairs of domain states, the parent group can be interpreted as a twinning group $K = G^\star(H)$.

A1. This indicates a type of symmetry descent $G \Downarrow H$ where the ferroic subgroup H is a kernel of an irep $D^{(\alpha)}(G)$ of dimension 2 or 3. The subgroup H is therefore the stabilizer of a general vector (vector of stratum) of the space $V_\alpha(H)$. All tensor components which transform like (x_α, y_α) or $(x_\alpha, y_\alpha, z_\alpha)$ are allowed in the ferroic state and the respective domain states form a full set in Aizu's terminology. If the transition is equitranslational, then these components also transform like the transition parameter. The row corresponding to the irep $D^{(\alpha)}(G)$ and subgroup H is located at the bottom of the central part of the table immediately above the block containing interactions.

B1. This indicates a type of symmetry descent $G \Downarrow F_i$ where the ferroic subgroups F_i are conjugate epikernels of an irep $D^{(\alpha)}(G)$ of dimension 2 or 3. The table is related to the conventionally chosen first subgroup F_1 which is the stabilizer of a general vector (vector of stratum) of the stability space $V_\alpha(F_1)$. This stability space is specified in terms

of variables (x_α, y_α) or $(x_\alpha, y_\alpha, z_\alpha)$ with conditions which define $V_\alpha(F_1)$ as a subspace of $V_\alpha(d_\alpha)$ [for example $(x_\alpha, 0)$, (x_α, x_α) or $(x_\alpha, x_\alpha, z_\alpha)$]. The corresponding tensor components onset in the ferroic state and the respective domain states again form a full set in Aizu's terminology. If the transition is equitranslational, then these components also transform like the transition parameter. The row corresponding to the irep $D^{(\alpha)}(G)$ and subgroup F_1 is located at the bottom of the central part of the table immediately above the block containing interactions.

A1a. and B1a. There is only one row in the central part of the table and the entry Faint interactions: *none* indicates the absence of faint variables.

A1b. and B1b. The sequence of rows corresponding to ireps $D^{(\beta)}(G)$ starts with ireps of lower dimensions and continues to the last row, which corresponds to the irep $D^{(\alpha)}(G)$ of the principal tensor parameters (primary transition parameter).

A1c. and B1c. In a few cases of this type, both rows corresponding to ireps $D^{(\alpha_1)}(G)$, $D^{(\alpha_2)}(G)$ are located at the bottom of the central table. The domain structure is full with respect to tensor components belonging to both ireps. Since only one irep defines the transition parameter in the case of equitranslational phase transitions, it is not *a priori* clear which of the ireps characterizes the transition parameter. Group theory cannot provide an answer.

Application to domain walls. *"Hic sunt leones."*

A method for the study of domain walls has been described by Janovec (1981) and applied by Janovec, Schranz, Warhanek & Zikmund (1989) and Janovec & Zikmund (1993). The Scanning Tables of *International Tables for Crystallography* Vol. E, *Subperiodic Groups* (Kopský & Litvin, 2002) are a prerequisite for such studies in microscopic models (Janovec & Kopský, 1997; Saint Grégoire, Janovec, & Kopský, 1997). In the case of the continuous model we need to begin with tensor distinction of domain states. Several papers have been devoted to its solution: Janovec, Richterová & Litvin (1992, 1993), Janovec, Litvin & Richterová (1994), Janovec, Litvin & Fuksa (1995), Litvin & Janovec (1997) in the last decade. All these papers given only information about the number of independent components by which the domain states differ. With the use of current software and of *conversion relations* it is possible to find explicit tensor components in which the domain states differ. Simple examples are given in the paper by Kopský (2001*b*). Notice that all results of this type are based on the technique of Clebsch–Gordan products, which enables the easy handling of tensorial and polynomial bases.

Final note: All results can be easily extended to magnetic point groups and magnetic properties with the use of Opechowski's magic relations. The skilful reader can use the current material themselves, but a subsequent version of the software is in preparation which will provide the results explicitly.

Lattices of equitranslational subgroups of the space groups

Lattice isomorphism: To facilitate the consideration of equitranslational phase transitions, the software includes an option for describing lattices of equitranslational subgroups of space groups. Here we use the well known relationship between the point groups and space groups: The translation subgroup (crystallographic lattice) of any space group is its normal subgroup and its point group is the respective factor group. As a consequence, the equitranslational subgroups of the space group can be arranged in a lattice which is identical with the lattice of subgroups of its point group. In other words, if you replace the parent point group G in any of the lattices of subgroups of the point groups by a space group $\mathcal{G}$ of which G is its point group, then any of the point groups H or F_i is uniquely replaced by the corresponding equitranslational subgroup $\mathcal{H}$ or $\mathcal{F}_i$ of the space group $\mathcal{G}$.

Lattices of equitranslational subgroups of the space groups were published some time ago by Ascher (1968) but his tables do not contain the full information. They are given in terms of Schönflies symbols of space-group types and the information you can obtain from them is the following:

"If you replace the parent point group in the lattice by a certain space-group type, then the symbols in the lattice show you the type of the space group by which each point group should be replaced".

The present software provides information about equitranslational subgroups of space groups in two modes which are activated by the choice of item Space under the pull-down menu Groups when the lattice of subgroups of a certain point group G is displayed on the screen. The conventions for the interpretation of Schönflies symbols of oriented space-group types and for the interpretation of Hermann–Mauguin symbols as symbols of quite specific groups will follow the preliminary guidelines.

After the choice of the option Space, a new panel appears on the screen. In its left-hand part is a window which contains all Hermann–Mauguin symbols of space groups of the geometric class G as they appear in Vol. A. These symbols are arranged as closely as possible to the order in which the space-group types are listed in Vol. A. Deviations from this order are due to deviations of the standard sequence of space-group types from the systematic sequence in which groups of the same arithmetic class are listed sequentially with the symmorphic group as the first. Hence, for example, in the case of cubic system, groups with lattice type cP are listed first, and then groups with lattice type cF and finally groups with lattice type cI.

Simplified mode: Each Hermann–Mauguin symbol is accessible by scrolling through this window. If you click on a chosen symbol, the sequential number of the respective space-group type, oriented Schönflies symbol of this type and corresponding setting or cell choice (where applicable) appear in the left-hand part of the panel. At the same time, the Schönflies symbols of oriented space-group types replace the symbols of the point groups in the lattice. While this information is more precise than that given in Ascher's lattices, it is still not complete.

Complete mode: The choice of the Hermann–Mauguin symbol specifies the parent group exactly. After clicking on the box of any of the Schönflies symbols of oriented space-group types, the full information about the respective subgroup appears in the lower bar of the panel. The reason for such a choice of presentation is rather prosaic; the

exact specification of the subgroup is usually too long to be accommodated within frames without disturbing the view of the lattice. It consists in general of three parts:

(i) Hermann–Mauguin symbol,

(ii) a shift of origin which specifies the location of the subgroup if it is not the standard one,

(iii) specification of the crystallographic basis in cases where it is different from the basis of the parent group.

When using the complete mode, we should realize that this is the first time that complete information about equitranslational subgroups is provided and that Hermann–Mauguin symbols in their traditional interpretation cannot describe the relationship between the parent group and its equitranslational subgroups properly. This is because the Hermann–Mauguin symbols do not include the specification of the origin, which is customarily given separately in the "origin statement". On the other hand, the Hermann–Mauguin symbols are perfectly adaptable to be interpreted as symbols of specific groups. In this software we embark from the notation of Vol. A because no better source is available. Our interpretation of Hermann–Mauguin symbols is subject to several conventions:

Convention 1: Interpretation of basic symbols: Each Hermann–Mauguin symbol together with the crystallographic coordinate system $(P; \mathbf{a}, \mathbf{b}, \mathbf{c})$, where $(\mathbf{a}, \mathbf{b}, \mathbf{c})$ is the conventional crystallographic basis, has the meaning of a quite specific space group. Normally we interpret the Hermann–Mauguin symbol as the symbol of that space group which is defined by isometries listed in Vol. A under the heading *Symmetry operations* or which can be deduced from the general Wyckoff positions. Groups listed in Vol. A with two origin choices are further distinguished by specification of the choice behind the symbol. These descriptions are identical with the description from the diagram of the space group in the *"standard setting"*.

For Hermann–Mauguin symbols of space groups of the orthorhombic system in *"non-standard settings"*, only the description *via* a diagram is available. In these cases, we interpret the symbol as the symbol of that space-group type which will be obtained from the diagram if we assume that, with reference to the location of the symbol, the origin P is located in the upper left corner of the diagram, vector $\mathbf{a}$ down from the origin and vector $\mathbf{b}$ to the right from this origin. In the case of monoclinic groups, there also appear symbols which correspond to different choices of the unique axis and in some cases to different choices of the conventional cell. The exact meaning of these symbols can again be deduced from their diagrams.

Convention 2: Lattice symbols: Below we give the ordinary lattice letters (symbols) in terms of vectors of the conventional basis $(\mathbf{a}, \mathbf{b}, \mathbf{c})$. The symbol $T(\mathbf{a}, \mathbf{b}, \mathbf{c})$ means the translation group generated by these basis vectors.

$$P(\mathbf{a}, \mathbf{b}, \mathbf{c}) = T(\mathbf{a}, \mathbf{b}, \mathbf{c})$$

$$C(\mathbf{a}, \mathbf{b}, \mathbf{c}) = T(\mathbf{a}, \mathbf{b}, \mathbf{c}) \left[\mathbf{0} \cup \frac{\mathbf{a} + \mathbf{b}}{2} \right]$$

$$A(\mathbf{a}, \mathbf{b}, \mathbf{c}) = T(\mathbf{a}, \mathbf{b}, \mathbf{c}) \left[\mathbf{0} \cup \frac{\mathbf{b} + \mathbf{c}}{2} \right]$$

$$B(\mathbf{a},\mathbf{b},\mathbf{c}) = T(\mathbf{a},\mathbf{b},\mathbf{c}) \left[\mathbf{0} \cup \frac{\mathbf{c}+\mathbf{a}}{2}\right]$$

$$I(\mathbf{a},\mathbf{b},\mathbf{c}) = T(\mathbf{a},\mathbf{b},\mathbf{c}) \left[\mathbf{0} \cup \frac{\mathbf{a}+\mathbf{b}+\mathbf{c}}{2}\right]$$

$$F(\mathbf{a},\mathbf{b},\mathbf{c}) = T(\mathbf{a},\mathbf{b},\mathbf{c}) \left[\mathbf{0} \cup \frac{\mathbf{a}+\mathbf{b}}{2} \cup \frac{\mathbf{b}+\mathbf{c}}{2} \cup \frac{\mathbf{c}+\mathbf{a}}{2}\right]$$

$$R_o(\mathbf{a},\mathbf{b},\mathbf{c}) = T(\mathbf{a},\mathbf{b},\mathbf{c}) \left[\mathbf{0} \cup \frac{2\mathbf{a}+\mathbf{b}+\mathbf{c}}{3} \cup \frac{\mathbf{a}+2\mathbf{b}+2\mathbf{c}}{3}\right]$$

$$R_r(\mathbf{a},\mathbf{b},\mathbf{c}) = T(\mathbf{a},\mathbf{b},\mathbf{c}) \left[\mathbf{0} \cup \frac{\mathbf{a}+2\mathbf{b}+\mathbf{c}}{3} \cup \frac{2\mathbf{a}+\mathbf{b}+2\mathbf{c}}{3}\right]$$

Vectors (**a**,**b**,**c**) constitute here the hexagonal basis, to which vectors of rhombohedral bases in obverse and reverse settings are related by

$$\begin{aligned} \mathbf{a}_o &= \tfrac{1}{3}(2\mathbf{a}+\mathbf{b}+\mathbf{c}) & \qquad \mathbf{a}_r &= \tfrac{1}{3}(-2\mathbf{a}-\mathbf{b}+\mathbf{c}) \\ \mathbf{b}_o &= \tfrac{1}{3}(-\mathbf{a}+\mathbf{b}+\mathbf{c}) & \qquad \mathbf{b}_r &= \tfrac{1}{3}(\mathbf{a}-\mathbf{b}+\mathbf{c}) \\ \mathbf{c}_o &= \tfrac{1}{3}(-\mathbf{a}-2\mathbf{b}+\mathbf{c}) & \qquad \mathbf{c}_r &= \tfrac{1}{3}(\mathbf{a}+2\mathbf{b}+\mathbf{c}). \end{aligned}$$

Vice versa, the hexagonal vectors are expressed through rhombohedral bases as follows:

$$\begin{aligned} \mathbf{a} &= \mathbf{a}_o - \mathbf{b}_o & &= \mathbf{b}_r - \mathbf{a}_r \\ \mathbf{b} &= \mathbf{b}_o - \mathbf{c}_o & &= \mathbf{c}_r - \mathbf{b}_r \\ -\mathbf{a}-\mathbf{b} &= \mathbf{c}_o - \mathbf{a}_o & &= \mathbf{a}_r - \mathbf{c}_r. \end{aligned}$$

As in Vol. A, we use only the obverse rhombohedral setting, using the letter R without a subscript.

Convention 3: Conventional versus Cartesian bases: Conventional crystallographic bases are natural and useful for the description of crystal structures as well as for the description of the space groups. Cartesian bases are, on the other hand, at least suitable if not mandatory when considering tensor properties. This is why we introduced embellished Schönflies and Hermann–Mauguin symbols for specifically oriented point groups. As an artefact of this notation we have the symbols of oriented space-group types in the simplified mode. In the complete mode we express the groups with reference to crystallographic bases. It is therefore desirable to correlate the choice of these bases with Cartesian ones. We use the following correspondences:

Triclinic	irrelevant
Monoclinic a	$\mathbf{b} = a\mathbf{e}_x$, $\mathbf{c} = b_1\mathbf{e}_x + b_2\mathbf{e}_y$, $\mathbf{a} = c\mathbf{e}_z$
Monoclinic b	$\mathbf{c} = a\mathbf{e}_x$, $\mathbf{a} = b_1\mathbf{e}_x + b_2\mathbf{e}_y$, $\mathbf{b} = c\mathbf{e}_z$
Monoclinic c	$\mathbf{a} = a\mathbf{e}_x$, $\mathbf{b} = b_1\mathbf{e}_x + b_2\mathbf{e}_y$, $\mathbf{c} = c\mathbf{e}_z$
Orthorhombic	$\mathbf{a} = a\mathbf{e}_x$, $\mathbf{b} = b\mathbf{e}_y$, $\mathbf{c} = c\mathbf{e}_z$
Tetragonal	$\mathbf{a} = a\mathbf{e}_x$, $\mathbf{b} = a\mathbf{e}_y$, $\mathbf{c} = c\mathbf{e}_z$
Hexagonal	$\mathbf{a} = a\mathbf{e}_x$, $\mathbf{b} = -\frac{1}{2}a\mathbf{e}_x + \frac{\sqrt{3}}{2}a\mathbf{e}_y$, $\mathbf{c} = c\mathbf{e}_z$
Cubic	$\mathbf{a} = a\mathbf{e}_x$, $\mathbf{b} = a\mathbf{e}_y$, $\mathbf{c} = a\mathbf{e}_z$

The point groups C_1 and C_i of the triclinic system are normal in the orthogonal group $\mathcal{O}(3)$. Orientation has no meaning for them and the relation between the crystallographic and Cartesian bases is irrelevant. For the groups of the monoclinic system we identify the unique axes a, b, c with Cartesian directions $\mathbf{e}_x$, $\mathbf{e}_y$, $\mathbf{e}_z$, respectively. For groups of the hexagonal family we identify the secondary crystallographic direction with the Cartesian direction $\mathbf{e}_x$.

Convention 4: Changes of the conventional basis: Hermann–Mauguin symbols specify the group with reference to the conventional basis and the admissible choices of this basis depend on the point group. When considering an equitranslational subgroup which belongs to the same family as the original group, the conventional bases of the group and of the subgroup are identical. The conventional basis of an equitranslational subgroup which belongs to a lower system is, however, frequently different from the conventional basis of the original group. Below we list all cases where this happens and specify the conventions and changes of the notation we use in such cases. In Table B3 are collected all embellished lattice symbols which are defined below.

Triclinic Family of Parent Groups:

There are only two types of triclinic space group: C_1^1 and C_i^1. The specific groups of these types are denoted by $P1$ and $P\overline{1}$ (**s**). In the first case, the group is completely specified by its lattice $P = T(\mathbf{a}, \mathbf{b}, \mathbf{c})$ and a shift in space does not change the group. In the second case, the complete specification of the group also requires the specification of the shift **s**.

The first group type appears as an equitranslational subgroup of every space group, the second as the equitranslational subgroup of any centrosymmetric group. The lattice type is always aP with the standard lattice symbol P. When a triclinic group appears in tables as a subgroup, we replace its standard lattice symbol by the lattice symbol of the original group.

Monoclinic Family of Parent Groups:

The lattice type of a group of the monoclinic family does not change for its monoclinic subgroups. All lattice types turn into the type aP for triclinic subgroups and we use the lattice symbol of the original group for the subgroup as well, as stated above.

Table B3. Bravais types of lattices, standard and non-conventional lattice symbols

Family/ system	Bravais type	Standard lattice symbols	Non-conventional lattice symbols
triclinic (anorthic)	aP	P	A, B, C, I, F
monoclinic	mP	P	$\widehat{P}_a$, $\widehat{P}_b$, $\widehat{P}_c$
UNIQUE AXIS c	mS	A, B, I	$\widehat{I}_a$, $\widehat{I}_b$, $\widehat{I}_c$; $\widehat{C}$; $\widehat{A}$, $\widehat{B}$
UNIQUE AXIS b	mS	C, A, I	C_1, C_2, C_3; I_1, I_2, I_3
UNIQUE AXIS a	mS	B, C, I	$\overline{I}_a$, $\overline{I}_b$, $\overline{I}_c$; $\widehat{C}_a$, $\widehat{C}_b$, $\widehat{C}_c$ $\widehat{A}_a$, $\widehat{A}_b$, $\widehat{A}_c$; $\widehat{B}_a$, $\widehat{B}_b$, $\widehat{B}_c$
orthorhombic	oP, oF, oI	P, F, I	$\widehat{C}$, $\widehat{F}$; C_1, C_2, C_3
	oS	C, A, B	$\widehat{C}_a$, $\widehat{C}_b$, $\widehat{C}_c$; $\widehat{F}_a$, $\widehat{F}_b$, $\widehat{F}_c$ $\overline{I}_a$, $\overline{I}_b$, $\overline{I}_c$
tetragonal	tP, tI	P, I	P_a, P_b, P_c I_a, I_b, I_c; $\overline{I}_a$, $\overline{I}_b$, $\overline{I}_c$
hexagonal/ trigonal	hP, hR	P, R	$R_{P,p}$, $R_{P,q}$, $R_{P,r}$, $R_{P,s}$ $R_{F,p}$, $R_{F,q}$, $R_{F,r}$, $R_{F,s}$ $R_{I,p}$, $R_{I,q}$, $R_{I,r}$, $R_{I,s}$
hexagonal	hP	P	none
cubic	cP, cI, cF	P, I, F	none

Orthorhombic Family of Parent Groups:

Orthorhombic to Monoclinic groups:

Case (a): Orthorhombic lattices of types oP and oI: With reference to monoclinic subgroups, the lattices of the types oP and oI correspond to types mP and mS, respectively. In addition, the conventional bases of orthorhombic groups can also be chosen as the conventional bases of their monoclinic subgroups. We therefore express the monoclinic subgroups by their Hermann–Mauguin symbols with reference to these bases using the same lattice symbols P and I.

Case (b): Orthorhombic lattices of the type oS: These orthorhombic lattices are denoted by letters A, B or C depending on the setting. Two cases should be distinguished:

Case (b1): The orthorhombic lattice of the type oS is of the type mS with reference to a monoclinic subgroup in the following cases:

(i) If the setting of the orthorhombic group is characterized by letter C and the unique axis of the monoclinic subgroup is either a or b.

(ii) If the setting of the orthorhombic group is characterized by letter A and the unique axis of the monoclinic subgroup is either b or c.

(iii) If the setting of the orthorhombic group is characterized by letter B and the unique axis of the monoclinic subgroup is either c or a.

In these cases we retain the original lattice letter and the conventional basis for the monoclinic subgroups.

Case (b2): The orthorhombic lattice of the type oS is of the type mP with reference to monoclinic subgroups in the following cases:

(i) Monoclinic subgroup with unique axis c of an orthorhombic group in a setting with lattice letter C.

(ii) Monoclinic subgroup with unique axis b of an orthorhombic group in a setting with lattice letter B.

(iii) Monoclinic subgroup with unique axis a of an orthorhombic group in a setting with lattice letter A.

In these cases we use embellished lattice symbols $\widehat{P}_c$, $\widehat{P}_a$, $\widehat{P}_b$, respectively, where relations

$$\widehat{P}_c = T[(\mathbf{a}-\mathbf{b})/2, (\mathbf{a}+\mathbf{b})/2, \mathbf{c}], \quad \widehat{P}_a = T[\mathbf{a}, (\mathbf{b}-\mathbf{c})/2, (\mathbf{b}+\mathbf{c})/2],$$

$$\widehat{P}_b = T[(\mathbf{c}+\mathbf{a})/2, \mathbf{b}, (\mathbf{c}-\mathbf{a})/2]$$

define simultaneously the embellished lattice symbol and the conventional basis of the monoclinic subgroup.

Case (c): Orthorhombic lattice of the type oF: The orthorhombic lattice of this type is always of the type mS with reference to all monoclinic subgroups. We choose the conventional bases of monoclinic subgroups so that they correspond to lattice symbols $\widehat{I}_c$, $\widehat{I}_a$, $\widehat{I}_b$ defined together with conventional monoclinic bases by:

$$\widehat{I}_c = I[(\mathbf{a}-\mathbf{b})/2, (\mathbf{a}+\mathbf{b})/2, \mathbf{c}], \quad \widehat{I}_a = I[\mathbf{a}, (\mathbf{b}-\mathbf{c})/2, (\mathbf{b}+\mathbf{c})/2],$$

$$\widehat{I}_b = I[(\mathbf{c}+\mathbf{a})/2, \mathbf{b}, (\mathbf{c}-\mathbf{a})/2].$$

Notice that in both choices of $\widehat{P}_c$, $\widehat{P}_a$, $\widehat{P}_b$ and $\widehat{I}_c$, $\widehat{I}_a$, $\widehat{I}_b$, the subscripts indicate the unique axis of the monoclinic subgroup and that the a, b and c unique axes correspond to the first, second and third positions in the Hermann–Mauguin symbol of the subgroup.

Tetragonal Family of Parent Groups:

Tetragonal to Orthorhombic groups:

Case (a): The conventional bases of tetragonal groups are compatible with the conventional bases of orthorhombic subgroups with point groups D_{2h}; C_{2vz}, C_{2vx}, C_{2vy}; and D_2 and the tetragonal lattice types tP and tI correspond in these cases to orthorhombic

lattice types oP and oI. Lattice symbols and conventional bases are retained.

Case (b): The tetragonal lattices of the types tP and tI turn into lattice types oS and oF with reference to orthorhombic subgroups with the point groups $\widehat{D}_{2hz}$; $\widehat{C}_{2vz}$, $\widehat{C}_{2vx}$, $\widehat{C}_{2vy}$; $\widehat{D}_2$. We choose the conventional orthorhombic bases and define lattice letters as follows:

$$\widehat{C} = C[(\mathbf{a}-\mathbf{b}),(\mathbf{a}+\mathbf{b}),\mathbf{c}], \quad \widehat{F} = F[(\mathbf{a}-\mathbf{b}),(\mathbf{a}+\mathbf{b}),\mathbf{c}].$$

Tetragonal to Monoclinic groups:

Case (a): The conventional bases of the parent tetragonal groups are admissible conventional bases of their monoclinic subgroups with the point groups C_{2hz}, C_{2hx}, C_{2hy}; C_{2z}, C_{2x}, C_{2y}; and C_{sz}, C_{sx}, C_{sy}. The tetragonal tP-type and tI-types are of the types mP and mS with reference to these subgroups and both lattice letters P, I as well as the conventional bases are retained.

Case (b1): The tetragonal lattice of the type tP is of the type mS with reference to monoclinic point groups C_{2hxy}, $C_{2hx\overline{y}}$; C_{2xy}, $C_{2x\overline{y}}$; and C_{sxy}, $C_{sx\overline{y}}$. We define the conventional monoclinic basis as above for the orthorhombic case (b) and distinguish the letter $\widehat{C}$ from the standard one again by a caret:

$$\widehat{C} = C[(\mathbf{a}-\mathbf{b})/2,(\mathbf{a}+\mathbf{b})/2,\mathbf{c}].$$

Case (b2): The tetragonal lattice of the type tI is again of the type mS with reference to monoclinic point groups C_{2hxy}, $C_{2hx\overline{y}}$; C_{2xy}, $C_{2x\overline{y}}$; and C_{sxy}, $C_{sx\overline{y}}$. We choose the monoclinic bases and lattice letters as follows:

$$\widehat{A} = A[(\mathbf{a}-\mathbf{b}+\mathbf{c})/2,(\mathbf{a}+\mathbf{b}),\mathbf{c}],$$

$$\widehat{B} = B[(\mathbf{a}-\mathbf{b}),(\mathbf{a}+\mathbf{b}+\mathbf{c})/2,\mathbf{c}].$$

Note that all these choices are subordinated to a rule that the tertiary directions $[1\overline{1}0]$ and $[110]$ correspond to the first and second positions, respectively, in the Hermann–Mauguin symbols of monoclinic subgroups.

Hexagonal Family of Parent Groups:

Let us recall that the hexagonal family splits into the trigonal and hexagonal system. Both lattice types hP and hR occur in the trigonal system while only the lattice type hP exists in the hexagonal system. The lattice type hR occurs only in groups of the trigonal system which have only monoclinic and triclinic subgroups.

Rhombohedral to Monoclinic Lattices:

In view of our choice of the relationship between crystallographic and Cartesian bases in combination with the obverse setting (used in Vol. A), we consider only those trigonal groups with a rhombohedral lattice which have the point groups C_{3i} $(\overline{3}_z)$, D_{3dx} $(\overline{3}_z m_x 1)$, D_{3x} $(3_z 2_x 1)$, or C_{3vx} $(3_z m_x 1)$. The lattice type hR turns into the type mS with reference to monoclinic subgroups, and we choose the lattice letters and conventional monoclinic bases as follows:

$$I_1 = I(\mathbf{a}, -\mathbf{c}_o, \mathbf{c}), \quad I_2 = I(\mathbf{b}, -\mathbf{a}_o, \mathbf{c}), \quad I_3 = I(-\mathbf{a} - \mathbf{b}, -\mathbf{b}_o, \mathbf{c}).$$

As a result of this choice, the orientation of the monoclinic axis corresponds to the first position in the Hermann–Mauguin symbols for the three conjugate monoclinic subgroups.

Hexagonal to Orthorhombic and Monoclinic Lattices:

The lattice type hP turns into the type mS for monoclinic subgroups of both trigonal and hexagonal groups and into the type oS for orthorhombic subgroups of hexagonal groups. In both cases we use the following lattice symbols with the well known *"ortho-hexagonal bases"*:

$$C_1 = C(\mathbf{a}, 2\mathbf{b} + \mathbf{a}, \mathbf{c}), \quad C_2 = C(\mathbf{b}, -2\mathbf{a} - \mathbf{b}, \mathbf{c}), \quad C_3 = C(-\mathbf{a} - \mathbf{b}, \mathbf{a} - \mathbf{b}, \mathbf{c}).$$

As a result, the two triplets of hexagonal directions, to which we assigned the axes x, x', x'' and y, y', y'', correspond to the first and second positions in Hermann–Mauguin symbols, while the z axis corresponds to the third position for orthorhombic as well as for monoclinic subgroups.

Cubic Family of Parent Groups:

We divide the subgroups of cubic groups into three categories:

1. Subgroups the main axis and one of the auxiliary axes (if present) of which are directed along the primary cubic direction.
2. Subgroups with two axes or with one main axis directed along the tertiary cubic direction.
3. Subgroups with main axes along the secondary cubic directions.

Below we consider these in more detail:

1. Subgroups with primary (and secondary, where applicable) directions along the primary cubic directions:

In this category we distinguish four cases:

Case (a): The lattices types cP, cF and cI turn into the types oP, oF and oI for the orthorhombic subgroups with point groups D_{2h} $(m_x m_y m_z)$, C_{2vz} $(m_x m_y 2_z)$, C_{2vx} $(2_x m_y m_z)$, C_{2vy} $(m_x 2_y m_z)$ and D_2 $(2_x 2_y 2_z)$. In all these cases we retain the original lattice symbol and the conventional basis.

Case (b): The lattice types cP and cI turn into the types tP and tI with reference to the tetragonal subgroups. However, the tetragonal conventional bases depend on the orientation of the tetragonal axis and two of the primary directions in cubic groups become secondary directions in tetragonal subgroups. To keep the order of elements in Hermann–Mauguin symbols of tetragonal subgroups, we choose the conventional tetragonal bases and supply the lattice letter P and I with subscripts c, a and b, so that we denote:

$$P_c = P(\mathbf{a}, \mathbf{b}, \mathbf{c}), \quad P_a = P(\mathbf{b}, \mathbf{c}, \mathbf{a}), \quad P_b = P(\mathbf{c}, \mathbf{a}, \mathbf{b})$$

$$I_c = I(\mathbf{a}, \mathbf{b}, \mathbf{c}), \quad I_a = I(\mathbf{b}, \mathbf{c}, \mathbf{a}), \quad I_b = I(\mathbf{c}, \mathbf{a}, \mathbf{b}).$$

Case (c): Cubic lattices of the type cF are of the type tI with reference to tetragonal subgroups. We use the following choice of lattice letters and of the tetragonal conventional bases:

$$\overline{I}_c = I[(\mathbf{a}-\mathbf{b})/2, (\mathbf{a}+\mathbf{b})/2, \mathbf{c}],$$

$$\overline{I}_a = I[(\mathbf{b}-\mathbf{c})/2, (\mathbf{b}+\mathbf{c})/2, \mathbf{a}] \quad \overline{I}_b = I[(\mathbf{c}-\mathbf{a})/2, (\mathbf{c}+\mathbf{a})/2, \mathbf{b}].$$

Note that the subscripts refer to the direction of the main tetragonal axis of the subgroup. It is worth mentioning that the origins of all standard cubic groups lie on the threefold axis 3_p (direction [111]). The rotations about this axis send the tetragonal subgroups to their conjugates by cyclic permutation of the vectors **a**, **b**, **c**. In terms of symbols this means cyclic permutation of indices a, b, c and of vectors **a**, **b**, **c** in the space shift after the symbol. It is therefore sufficient to give only one of the conjugate tetragonal subgroups. This is useful in the tabular presentation of results which lies behind the computerized presentation. There we use the tetragonal subgroup with the principal axis along c, *i.e.* along the [001] cubic direction. However, the program displays all cases.

Case (d): The cubic lattices of the types cP, cI are of the types mP and mI and the lattice type cF turns into the type mI for monoclinic subgroups with unique axis along the primary cubic direction. In the first two cases, we retain the lattice symbol and the conventional basis; in the last case we use the embellished lattices symbols

$$\widehat{I}_c = I[(\mathbf{a}-\mathbf{b})/2, (\mathbf{a}+\mathbf{b})/2, \mathbf{c}],$$

$$\widehat{I}_a = I[(\mathbf{a}, \mathbf{b}-\mathbf{c})/2, (\mathbf{b}+\mathbf{c})/2], \quad \widehat{I}_b = I[(\mathbf{c}+\mathbf{a})/2, \mathbf{b}, (\mathbf{c}-\mathbf{a})/2].$$

As a result, the positions in the Hermann–Mauguin symbols of monoclinic subgroups correspond to the cubic axes a, b and c, which turn into the monoclinic unique axes.

2. Subgroups with axes along tertiary cubic directions:

Case (a): Orthorhombic subgroups with one of the axes along primary and two axes along tertiary cubic directions appear either in triads of conjugate subgroups with point groups

$$\widehat{D}_{2hz}\ (m_{x\overline{y}}m_{xy}m_z),\ \widehat{D}_{2hx}\ (m_{y\overline{z}}m_{yz}m_x),\ \widehat{D}_{2hy}\ (m_{z\overline{x}}m_{zx}m_y);$$
$$\widehat{D}_{2z}\ (2_{x\overline{y}}2_{xy}2_z),\ \widehat{D}_{2x}\ (2_{y\overline{z}}2_{yz}2_x),\ \widehat{D}_{2y}\ (2_{z\overline{x}}2_{zx}2_y);$$

and

$$\widehat{C}_{2vz}\ (m_{x\overline{y}}m_{xy}2_z),\ \widehat{C}_{2vx}\ (m_{y\overline{z}}m_{yz}2_x),\ \widehat{C}_{2vy}\ (m_{z\overline{x}}m_{zx}2_y);$$

or in sixtuples of conjugate subgroups with point groups

$$\widehat{C}_{2vx\overline{y}}\ (2_{x\overline{y}}m_{xy}m_z),\ \widehat{C}_{2vy\overline{z}}\ (2_{y\overline{z}}m_{yz}m_x),\ \widehat{C}_{2vz\overline{x}}\ (2_{z\overline{x}}m_{zx}m_y),$$
$$\widehat{C}_{2vxy}\ (m_{x\overline{y}}2_{xy}m_z),\ \widehat{C}_{2vyz}\ (m_{y\overline{z}}2_{yz}m_x),\ \widehat{C}_{2vzx}\ (m_{z\overline{x}}2_{zx}m_y).$$

In all these cases we have one of the three following relationships to the original cubic lattices:

Case (a1): The cubic lattice of the type cP is of the type oS with reference to these point groups and we choose the conventional bases and lattice letters as follows:

$$\widehat{C}_c = C[(\mathbf{a}-\mathbf{b}), (\mathbf{a}+\mathbf{b}), \mathbf{c}],$$

$$\widehat{C}_a = C[(\mathbf{b}-\mathbf{c}),(\mathbf{b}+\mathbf{c}),\mathbf{a}], \quad \widehat{C}_b = C[(\mathbf{c}-\mathbf{a}),(\mathbf{c}+\mathbf{a}),\mathbf{b}].$$

Case (a2): The cubic lattice of the type cF is of the type oI with reference to these point groups and we choose the conventional bases and lattice letters as follows:

$$\overline{I}_c = I[(\mathbf{a}-\mathbf{b})/2,(\mathbf{a}+\mathbf{b})/2,\mathbf{c}],$$

$$\overline{I}_a = I[(\mathbf{b}-\mathbf{c})/2,(\mathbf{b}+\mathbf{c})/2,\mathbf{a}], \quad \overline{I}_b = I[(\mathbf{c}-\mathbf{a})/2,(\mathbf{c}+\mathbf{a})/2,\mathbf{b}].$$

Case (a3): The cubic lattice of the type cI is of the type oF with reference to these point groups and we choose the conventional bases and lattice letters as follows:

$$\widehat{F}_c = F[(\mathbf{a}-\mathbf{b})/2,(\mathbf{a}+\mathbf{b})/2,\mathbf{c}],$$

$$\widehat{F}_a = F[(\mathbf{b}-\mathbf{c})/2,(\mathbf{b}+\mathbf{c})/2,\mathbf{a}], \quad \widehat{F}_b = F[(\mathbf{c}-\mathbf{a})/2,(\mathbf{c}+\mathbf{a})/2,\mathbf{b}].$$

Case (b): Monoclinic subgroups with unique axis along the tertiary cubic direction appear in sixtuples of conjugate subgroups with point groups:

$$\widehat{C}_{2hxy}\ (12_{xy}/m_{xy}1),\ \widehat{C}_{2hyz}\ (12_{yz}/m_{yz}1),\ \widehat{C}_{2hzx}\ (12_{zx}/m_{zx}1),$$
$$\widehat{C}_{2hx\overline{y}}\ (2_{x\overline{y}}/m_{x\overline{y}}11),\ \widehat{C}_{2hy\overline{z}},\ (2_{y\overline{z}}/m_{yz\overline{y}}11),\ \widehat{C}_{2hz\overline{x}}\ (2_{z\overline{x}}/m_{z\overline{x}}11),$$

$$\widehat{C}_{2xy}\ (12_{xy}1),\ \widehat{C}_{2yz}\ (12_{yz}1),\ \widehat{C}_{2zx}\ (12_{zx}1),\ \widehat{C}_{2x\overline{y}}\ (2_{x\overline{y}}11),\ \widehat{C}_{2y\overline{z}},\ (2_{y\overline{z}}11),\ \widehat{C}_{2z\overline{x}}\ (2_{z\overline{x}}11),$$
and
$$\widehat{C}_{sxy}\ (1m_{xy}1),\ \widehat{C}_{syz}\ (1m_{yz}1),\ \widehat{C}_{szx}\ (1m_{zx}1),\ \widehat{C}_{sx\overline{y}}\ (m_{x\overline{y}}11),\ \widehat{C}_{sy\overline{z}},\ (m_{y\overline{z}}11),\ \widehat{C}_{sz\overline{x}}\ (m_{z\overline{x}}11),$$

Case (b1): The cubic lattices of types cP and cF turn, respectively, into types oS and oI in the orthorhombic case and both turn into type mS in the monoclinic case. The choice of lattice letters and of conventional bases

$$\widehat{C}_c = C[(\mathbf{a}-\mathbf{b}),(\mathbf{a}+\mathbf{b}),\mathbf{c}], \quad \widehat{C}_a = C[(\mathbf{b}-\mathbf{c}),(\mathbf{b}+\mathbf{c}),\mathbf{a}],$$

$$\widehat{C}_b = C[(\mathbf{c}-\mathbf{a}),(\mathbf{c}+\mathbf{a}),\mathbf{b}]$$

and

$$\overline{I}_c = I[(\mathbf{a}-\mathbf{b})/2,(\mathbf{a}+\mathbf{b})/2,\mathbf{c}], \quad \overline{I}_a = I[(\mathbf{b}-\mathbf{c})/2,(\mathbf{b}+\mathbf{c})/2,\mathbf{a}],$$

$$\overline{I}_b = I[(\mathbf{c}-\mathbf{a})/2,(\mathbf{c}+\mathbf{a})/2,\mathbf{b}]$$

is such that the directions $[1\overline{1}0]$ and $[110]$ correspond to the first and second positions in the Hermann–Mauguin symbols in both orthorhombic and monoclinic cases. So do the other pairs of directions obtained by threefold rotations.

Case (b1) and (b2): The cubic lattice types cP and cF turn into the types mP and mS for subgroups with these monoclinic point groups and we choose the embellished lattice letters $\widehat{C}_c$, $\widehat{C}_a$, $\widehat{C}_b$ and $\overline{I}_c$, $\overline{I}_a$, $\overline{I}_b$, and conventional bases as above in cases (a1) and (a2) of the orthorhombic subgroups.

Case (b3): The cubic lattice type cI becomes of the type mS with reference to these monoclinic subgroups. We choose the lattice letters and conventional bases as follows:

$$\widehat{A}_c = A[(\mathbf{a}-\mathbf{b}+\mathbf{c})/2,(\mathbf{a}+\mathbf{b}),\mathbf{c}], \quad \widehat{B}_c = B[(\mathbf{a}-\mathbf{b}),(\mathbf{a}+\mathbf{b}+\mathbf{c})/2,\mathbf{c}],$$

$$\widehat{A}_a = A[(\mathbf{b}-\mathbf{c}+\mathbf{a})/2,(\mathbf{b}+\mathbf{c}),\mathbf{a}], \quad \widehat{B}_a = B[(\mathbf{b}-\mathbf{c}),(\mathbf{b}+\mathbf{c}+\mathbf{a})/2,\mathbf{a}],$$

$$\widehat{A}_b = A[(\mathbf{c}-\mathbf{a}+\mathbf{b})/2, (\mathbf{c}+\mathbf{a}), \mathbf{b}], \quad \widehat{B}_b = B[(\mathbf{c}-\mathbf{a}), (\mathbf{c}+\mathbf{a}+\mathbf{b})/2, \mathbf{b}].$$

This is the same as in case (b2) of tetragonal to monoclinic groups with additional subscripts c, a, b.

3. Cubic to Trigonal Groups with a Rhombohedral Lattice:

All three types cP, cI and cF of cubic lattices correspond to rhombohedral lattices of the type R for the trigonal subgroups of geometric classes D_{3d}, D_3, C_{3v} and C_3. The threefold cubic axes turn into the trigonal axes distinguished by subscripts p, q, r and s for the directions [111], $[\overline{1}11]$, $[1\overline{1}1]$ and $[\overline{1}1\overline{1}]$, respectively. The trigonal subgroups are denoted by Hermann–Mauguin symbols embellished by superscripts which denote the original cubic type of the lattice and the orientation of the trigonal axis. The conventional bases of trigonal subgroups are then chosen as follows from the table below.

$$\begin{aligned} P \Longrightarrow \quad & R_{P,p} = T(\mathbf{a}, \mathbf{b}, \mathbf{c}) \\ & R_{P,q} = T(-\mathbf{a}, -\mathbf{b}, \mathbf{c}) \\ & R_{P,r} = T(\mathbf{a}, -\mathbf{b}, -\mathbf{c}) \\ & R_{P,s} = T(-\mathbf{a}, \mathbf{b}, -\mathbf{c}) \end{aligned}$$

$$\begin{aligned} I \Longrightarrow \quad & R_{I,p} = T[(\mathbf{a}+\mathbf{b}-\mathbf{c})/2, (\mathbf{b}+\mathbf{c}-\mathbf{a})/2, (\mathbf{c}+\mathbf{a}-\mathbf{b})/2] \\ & R_{I,q} = T[(-\mathbf{a}-\mathbf{b}-\mathbf{c})/2, (-\mathbf{b}+\mathbf{c}+\mathbf{a})/2, (\mathbf{c}-\mathbf{a}+\mathbf{b})/2] \\ & R_{I,r} = T[(\mathbf{a}-\mathbf{b}+\mathbf{c})/2, (-\mathbf{b}-\mathbf{c}-\mathbf{a})/2, (-\mathbf{c}+\mathbf{a}+\mathbf{b})/2] \\ & R_{I,s} = T[(-\mathbf{a}+\mathbf{b}+\mathbf{c})/2, (\mathbf{b}-\mathbf{c}+\mathbf{a})/2, (-\mathbf{c}-\mathbf{a}-\mathbf{b})/2] \end{aligned}$$

$$\begin{aligned} F \Longrightarrow \quad & R_{F,p} = T[(\mathbf{a}+\mathbf{b})/2, (\mathbf{b}+\mathbf{c})/2, (\mathbf{c}+\mathbf{a})/2] \\ & R_{F,q} = T[(-\mathbf{a}-\mathbf{b})/2, (-\mathbf{b}+\mathbf{c})/2, (\mathbf{c}-\mathbf{a})/2] \\ & R_{F,r} = T[(\mathbf{a}-\mathbf{b})/2, (-\mathbf{b}-\mathbf{c})/2, (-\mathbf{c}+\mathbf{a})/2] \\ & R_{F,s} = T[(-\mathbf{a}+\mathbf{b})/2, (\mathbf{b}-\mathbf{c})/2, (-\mathbf{c}-\mathbf{a})/2]. \end{aligned}$$

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Appendix A

Correlation of various notations and
Jones' faithful representation symbols:

Table A1: Cubic group $O_h - m\overline{3}m$ -
subgroup of proper rotations $O - 432$

Cubic system								
std.	B.C.	A.H.	Asch.	Kpts.	Kov.	$IT83$		Jon.
e	E	E	1	1	h_1	1		x,y,z
2_z		C_{2z}	2_z	4_3^2	h_4	2	$0,0,z$	$\overline{x},\overline{y},z$
2_x		C_{2x}	2_x	4_1^2	h_2	2	$x,0,0$	$x,\overline{y},\overline{z}$
2_y		C_{2y}	2_y	4_1^2	h_3	2	$0,y,0$	$\overline{x},y,\overline{z}$
3_p		C_{31}^+	3_δ	3_1	h_9	3^+	x,x,x	z,x,y
3_q		C_{32}^+	3_γ	3_2	h_{11}	3^+	$\overline{x},\overline{x},x$	$\overline{z},x,\overline{y}$
3_r		C_{33}^+	3_α	3_4	h_{12}	3^+	$x,\overline{x},\overline{x}$	$\overline{z},\overline{x},y$
3_s		C_{34}^+	3_β	3_3	h_{10}	3^+	$\overline{x},x,\overline{x}$	$z,\overline{x},\overline{y}$
3_p^2		C_{31}^-	3_δ^2	3_1^2	h_5	3^-	x,x,x	y,z,x
3_q^2		C_{32}^-	3_γ^2	3_2^2	h_6	3^-	$\overline{x},\overline{x},x$	$y,\overline{z},\overline{x}$
3_r^2		C_{33}^-	3_α^2	3_4^2	h_7	3^-	$x,\overline{x},\overline{x}$	$\overline{y},z,\overline{x}$
3_s^2		C_{34}^-	3_β^2	3_3^2	h_8	3^-	$\overline{x},x,\overline{x}$	$\overline{y},\overline{z},x$
4_z		C_{4z}^+	4_z	4_3	h_{14}	4^+	$0,0,z$	$\overline{y},x,z$
4_x		C_{4x}^+	4_x	4_1	h_{19}	4^+	$x,0,0$	$x,\overline{z},y$
4_y		C_{4y}^+	4_y	4_2	h_{24}	4^+	$0,y,0$	$z,y,\overline{x}$
4_z^3		C_{4z}^-	4_z^3	4_3^3	h_{15}	4^-	$0,0,z$	$y,\overline{x},z$
4_x^3		C_{4x}^-	4_x^3	4_1^3	h_{20}	4^-	$x,0,0$	$x,z,\overline{y}$
4_y^3		C_{4y}^-	4_y^3	4_2^3	h_{22}	4^-	$0,y,0$	$\overline{z},y,x$
2_{xy}	C_{2a}	C_{2a}'	2_e	2_1	h_{16}	2	$x,x,0$	$y,x,\overline{z}$
$2_{x\overline{y}}$	C_{2b}	C_{2b}'	2_f	2_2	h_{13}	2	$x,\overline{x},0$	$\overline{y},\overline{x},\overline{z}$
2_{zx}	C_{2c}	C_{2c}'	2_c	2_3	h_{23}	2	$x,0,x$	$z,\overline{y},x$
$2_{z\overline{x}}$	C_{2e}	C_{2e}'	2_d	2_4	h_{21}	2	$\overline{x},0,x$	$\overline{z},\overline{y},\overline{x}$
2_{yz}	C_{2d}	C_{2d}'	2_a	2_5	h_{18}	2	$0,y,y$	$\overline{x},z,y$
$2_{y\overline{z}}$	C_{2f}	C_{2f}'	2_b	2_6	h_{17}	2	$0,y,\overline{y}$	$\overline{x},\overline{z},\overline{y}$

Table A1 (cont.1/end): Cubic group $O_h - m\overline{3}m$ - coset of improper rotations $iO = Oi$

Cubic system								
std.	B.C.	A.H.	Asch.	Kpts.	Kov.	$IT83$		Jon.
i	I	i	$\overline{1}$	$\widetilde{2}$	h_{25}	$\overline{1}$	$0,0,0$	$\overline{x},\overline{y},\overline{z}$
m_z		σ_z	m_z	m_3	h_{28}	m	$x,y,0$	$x,y,\overline{z}$
m_x		σ_x	m_x	m_1	h_{26}	m	$0,y,z$	$\overline{x},y,z$
m_y		σ_y	m_y	m_2	h_{27}	m	$x,0,z$	$x,\overline{y},z$
$\overline{3}_p$		S_{61}^-	$\overline{3}_\delta$	$\widetilde{6}_1^5$	h_{33}	$\overline{3}^+$	x,x,x	$\overline{z},\overline{x},\overline{y}$
$\overline{3}_q$		S_{62}^-	$\overline{3}_\gamma$	$\widetilde{6}_2^5$	h_{35}	$\overline{3}^+$	$\overline{x},\overline{x},x$	$z,\overline{x},y$
$\overline{3}_r$		S_{63}^-	$\overline{3}_\alpha$	$\widetilde{6}_4^5$	h_{36}	$\overline{3}^+$	$x,\overline{x},\overline{x}$	$z,x,\overline{y}$
$\overline{3}_s$		S_{64}^-	$\overline{3}_\beta$	$\widetilde{6}_3^5$	h_{34}	$\overline{3}^+$	$\overline{x},x,\overline{x}$	$\overline{z},x,y$
$\overline{3}_p^5$		S_{61}^+	$\overline{3}_\delta^2$	$\widetilde{6}_1$	h_{29}	$\overline{3}^-$	x,x,x	$\overline{y},\overline{z},\overline{x}$
$\overline{3}_q^5$		S_{62}^+	$\overline{3}_\gamma^2$	$\widetilde{6}_2$	h_{30}	$\overline{3}^-$	$\overline{x},\overline{x},x$	$\overline{y},z,x$
$\overline{3}_r^5$		S_{63}^+	$\overline{3}_\alpha^2$	$\widetilde{6}_4$	h_{31}	$\overline{3}^-$	$x,\overline{x},\overline{x}$	$y,\overline{z},x$
$\overline{3}_s^5$		S_{64}^+	$\overline{3}_\beta^2$	$\widetilde{6}_3$	h_{32}	$\overline{3}^-$	$\overline{x},x,\overline{x}$	$y,z,\overline{x}$
$\overline{4}_z$		S_{4z}^-	$\overline{4}_z$	$\widetilde{4}_3^3$	h_{38}	$\overline{4}^+$	$0,0,z$	$y,\overline{x},\overline{z}$
$\overline{4}_x$		S_{4x}^-	$\overline{4}_x$	$\widetilde{4}_1^3$	h_{43}	$\overline{4}^+$	$x,0,0$	$\overline{x},z,\overline{y}$
$\overline{4}_y$		S_{4y}^-	$\overline{4}_y$	$\widetilde{4}_2$	h_{48}	$\overline{4}^+$	$0,y,0$	$\overline{z},\overline{y},x$
$\overline{4}_z^3$		S_{4z}^+	$\overline{4}_z^3$	$\widetilde{4}_3$	h_{39}	$\overline{4}^-$	$0,0,z$	$\overline{y},x,\overline{z}$
$\overline{4}_x^3$		S_{4x}^+	$\overline{4}_x^3$	$\widetilde{4}_1$	h_{44}	$\overline{4}^-$	$x,0,0$	$\overline{x},\overline{z},y$
$\overline{4}_y^3$		S_{4y}^+	$\overline{4}_y^3$	$\widetilde{4}_2$	h_{46}	$\overline{4}^-$	$0,y,0$	$z,\overline{y},\overline{x}$
m_{xy}	σ_{da}	σ_{d1}	m_e	m_5	h_{40}	m	$x,\overline{x},z$	$\overline{y},\overline{x},z$
$m_{x\overline{y}}$	σ_{db}	σ_{d2}	m_f	m_4	h_{37}	m	x,x,z	y,x,z
m_{zx}	σ_{dc}	σ_{d3}	m_c	m_7	h_{47}	m	$\overline{x},y,x$	$\overline{z},y,\overline{x}$
$m_{z\overline{x}}$	σ_{de}	σ_{d5}	m_d	m_6	h_{45}	m	x,y,x	z,y,x
m_{yz}	σ_{dd}	σ_{d4}	m_a	m_9	h_{42}	m	$x,y,\overline{y}$	$x,\overline{z},\overline{y}$
$m_{y\overline{z}}$	σ_{df}	σ_{d6}	m_b	m_8	h_{41}	m	x,y,y	x,z,y

Table A2: Hexagonal group $D_{6h} - 6_z/m_z m_x m_y$ - subgroup of proper rotations $D_6 - 6_z 2_x 2_y$

Hexagonal system							
std.	B.C.=A.H.	Asch.	Kpts.	Kov.	$IT83$		Jon.
e	E	1	1	h_1	1		x, y, z
6_z	C_6^+	6	6	h_2	6^+	$0, 0, z$	$x-y, x, z$
3_z	C_3^+	3	6^2	h_3	3^+	$0, 0, z$	$\overline{y}, x-y, z$
2_z	C_2	2	6^3	h_4	2	$0, 0, z$	$\overline{x}, \overline{y}, z$
3_z^2	C_3^-	3^2	6^4	h_5	3^-	$0, 0, z$	$y-x, \overline{x}, z$
6_z^5	C_6^-	6^5	6^5	h_6	6^-	$0, 0, z$	$y, y-x, z$
2_x	C_{21}''	2_1	2_1	h_9	2	$x, 0, 0$	$x-y, \overline{y}, \overline{z}$
$2_{x'}$	C_{22}''	2_3	2_3	h_7	2	$0, y, 0$	$\overline{x}, y-x, \overline{z}$
$2_{x''}$	C_{23}''	2_5	2_5	h_{11}	2	$x, x, 0$	$y, x, \overline{z}$
2_y	C_{21}'	2_2	2_4	h_{12}	2	$x, 2x, 0$	$y-x, y, \overline{z}$
$2_{y'}$	C_{22}'	2_4	2_6	h_{10}	2	$2x, x, 0$	$x, x-y, \overline{z}$
$2_{y''}$	C_{23}'	2_6	2_2	h_8	2	$x, \overline{x}, 0$	$\overline{y}, \overline{x}, \overline{z}$

Hexagonal group $D_{6h} - 6_z/m_z m_x m_y$ - coset of improper rotations $iD_6 = D_6 i$

Hexagonal system							
std.	B.C.=A.H.	Asch.	Kpts.	Kov.	$IT83$		Jon.
i	I	$\overline{1}$	$\widetilde{2}$	h_{13}	$\overline{1}$	$0, 0, 0$	$\overline{x}, \overline{y}, \overline{z}$
$\overline{6}_z$	S_3^-	$\overline{6}$	$\widetilde{3}^5$	h_{14}	$\overline{6}^+$	$0, 0, z$	$y-x, \overline{x}, \overline{z}$
$\overline{3}_z$	S_6^-	$\overline{3}$	$\widetilde{6}^5$	h_{15}	$\overline{3}^+$	$0, 0, z$	$y, y-x, \overline{z}$
m_z	σ_h	m	m	h_{16}	m	$x, y, 0$	$x, y, \overline{z}$
$\overline{3}_z^5$	S_6^+	$\overline{3}^2$	$\widetilde{6}$	h_{17}	$\overline{3}^-$	$0, 0, z$	$x-y, x, \overline{z}$
$\overline{6}_z^5$	S_3^+	$\overline{6}^5$	$\widetilde{3}$	h_{18}	$\overline{6}^-$	$0, 0, z$	$\overline{y}, x-y, \overline{z}$
m_x	σ_{v1}	m_1	m_1	h_{21}	m	$x, 2x, z$	$y-x, y, z$
$m_{x'}$	σ_{v2}	m_3	m_3	h_{19}	m	$2x, x, z$	$x, x-y, z$
$m_{x''}$	σ_{v3}	m_5	m_5	h_{23}	m	$x, \overline{x}, z$	$\overline{y}, \overline{x}, z$
m_y	σ_{d1}	m_2	m_4	h_{24}	m	$x, 0, z$	$x-y, \overline{y}, z$
$m_{y'}$	σ_{d2}	m_4	m_6	h_{22}	m	$0, y, z$	$\overline{x}, y-x, z$
$m_{y''}$	σ_{d3}	m_6	m_4	h_{20}	m	x, x, z	y, x, z

Some relations between powers of elements

We use throughout only those elements or their powers which are listed in Tables A1, A2 under the heading std. with various subscripts indicating directions of axes. These are listed below as the first ones with a common subscript z in relations to valid but unused powers. The relations on the left-hand side show powers of elements which have the same meaning, the relations on the right-hand side show the inverses in terms of used symbols.

$$
\begin{array}{ll}
2_z = 4_z^2 = \overline{4}_z^2 = 6_z^3 & 4_z^3 = 4_z^{-1}, \quad \overline{4}_z^3 = \overline{4}_z^{-1} \\
3_z = 6_z^2 = \overline{6}_z^2 = \overline{3}_z^4 & 3_z^2 = 3_z^{-1}, \quad 6_z^5 = 6_z^{-1} \\
3_z^2 = 6_z^4 = \overline{6}_z^4 = \overline{3}_z^2 & \overline{3}_z^5 = \overline{3}_z^{-1}, \quad \overline{6}_z^5 = \overline{6}_z^{-1} \\
i = \overline{3}_z^3; \quad m_z = \overline{6}_z^3 &
\end{array}
$$

References from which symbols are taken and comments

std. This manual and software

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Asch. Ascher, E., **Properties of Shubnikov point groups. Part 1.** Battelle Report, Geneva.

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Jon. Jones' faithful symbols (see Bradley & Cracknell, 1972).

Comments: The standard symbols belong to a variety of symbols, used, for example, by Ascher or by Koptsik; other symbols of this type are scattered in the literature with different subscripts (crystallographers would probably prefer subscripts [111], $[\overline{1}11]$, $[\overline{1}1\overline{1}]$, $[1\overline{1}1]$ to our p, q, r, s and even worse for x, x', x'' and y, y', y''). Spectroscopic symbols, though rather widely used, are not completely compatible even in the two main cited sources; some of them are too close to Schönflies symbols for point groups. Symbols by Kovalev do not bear any explicit information with the exception of h_1 which is the unit element. In addition, the letters h_i with the same index i have different meaning in cubic and hexagonal groups. The symbols used in *International Tables* (Tables 11.2 and 11.3 for our Tables A1 and A2) are the most complicated and least suitable for further handling; for example, it is quite out of question to use them in Seitz symbols.

Appendix B

Schönflies and Hermann-Mauguin Symbols of Groups in Standard Orientations and of their Subgroups

Cubic system

	$O_h - m\overline{3}m$	
$T_h - m\overline{3}$	$O - 432$	$T_d - \overline{4}3m$
	$T - 23$	

Tetragonal system

$D_{4hz} - 4_z/m_z m_x m_{xy}$	$D_{4hx} - 4_x/m_x m_y m_{yz}$	$D_{4hy} - 4_y/m_y m_z m_{zx}$
$D_{4z} - 4_z 2_x 2_{xy}$	$D_{4x} - 4_x 2_y 2_{yz}$	$D_{4y} - 4_y 2_z 2_{zx}$
$C_{4vz} - 4_z m_x m_{xy}$	$C_{4vx} - 4_x m_y m_{yz}$	$C_{4vy} - 4_y m_z m_{zx}$
$D_{2dz} - \overline{4}_z 2_x m_{xy}$	$D_{2dx} - \overline{4}_x 2_y m_{yz}$	$D_{2dy} - \overline{4}_y 2_z m_{zx}$
$\widehat{D}_{2dz} - \overline{4}_z m_x 2_{xy}$	$\widehat{D}_{2dx} - \overline{4}_x m_y 2_{yz}$	$\widehat{D}_{2dy} - \overline{4}_y m_z 2_{zx}$
$C_{4hz} - 4_z/m_z$	$C_{4hx} - 4_x/m_x$	$C_{4hy} - 4_y/m_y$
$C_{4z} - 4_z$	$C_{4x} - 4_x$	$C_{4y} - 4_y$
$S_{4z} - \overline{4}_z$	$S_{4x} - \overline{4}_x$	$S_{4y} - \overline{4}_y$

Trigonal system

Cubic branch

$D_{3dp} - \overline{3}_p m_{x\overline{y}}$	$D_{3dq} - \overline{3}_q m_{x\overline{y}}$	$D_{3dr} - \overline{3}_r m_{xy}$	$D_{3ds} - \overline{3}_s m_{xy}$
$D_{3p} - 3_p 2_{x\overline{y}}$	$D_{3q} - 3_q 2_{x\overline{y}}$	$D_{3r} - 3_r 2_{xy}$	$D_{3s} - 3_s 2_{xy}$
$C_{3vp} - 3_p m_{x\overline{y}}$	$C_{3vq} - 3_q m_{x\overline{y}}$	$C_{3vr} - 3_r m_{xy}$	$C_{3vs} - 3_s m_{xy}$
$C_{3ip} - \overline{3}_p$	$C_{3iq} - \overline{3}_q$	$C_{3ir} - \overline{3}_r$	$C_{3is} - \overline{3}_s$
$C_{3p} - 3_p$	$C_{3q} - 3_q$	$C_{3r} - 3_r$	$C_{3s} - 3_s$

Hexagonal branch

$D_{3dx} - \overline{3}_z m_x 1$	$D_{3dy} - \overline{3}_z 1 m_y$
$D_{3x} - 3_z 2_x 1$	$D_{3y} - 3_z 12_y$
$C_{3vx} - 3_z m_x 1$	$C_{3vy} - 3_z 1 m_y$
$C_{3i} - \overline{3}_z$	
$C_3 - 3_z$	

Hexagonal family

Hexagonal system

$D_{6h} - 6_z/m_z m_x m_y$
$D_6 - 6_z 2_x 2_y$
$C_{6v} - 6_z m_x m_y$
$D_{3h} - \overline{6}_z 2_x m_y$
$\widehat{D}_{3h} - \overline{6}_z m_x 2_y$
$C_{6h} - 6_z/m_z$
$C_6 - 6_z$
$C_{3h} - \overline{6}_z$

Orthorhombic system

Cubic branch			Common	Hexagonal branch	
$\widehat{D}_{2hz} - m_{x\overline{y}} m_{xy} m_z$	$\widehat{D}_{2hx} - m_{y\overline{z}} m_{yz} m_x$	$\widehat{D}_{2hy} - m_{z\overline{x}} m_{zx} m_y$	$D_{2h} - m_x m_y m_z$	$D_{2h'} - m_{x'} m_{y'} m_z$	$D_{2h''} - m_{x''} m_{y''} m_z$
$\widehat{D}_{2z} - 2_{x\overline{y}} 2_{xy} 2_z$	$\widehat{D}_{2x} - 2_{y\overline{z}} 2_{yz} 2_x$	$\widehat{D}_{2y} - 2_{z\overline{x}} 2_{zx} 2_y$	$D_2 - 2_x 2_y 2_z$	$D_{2'} - 2_{x'} 2_{y'} 2_z$	$D_{2''} - 2_{x''} 2_{y''} 2_z$
$\widehat{C}_{2vz} - m_{x\overline{y}} m_{xy} 2_z$	$\widehat{C}_{2vxy} - m_{x\overline{y}} 2_{xy} m_z$	$\widehat{C}_{2vx\overline{y}} - 2_{x\overline{y}} m_{xy} m_z$	$C_{2vz} - m_x m_y 2_z$	$C_{2vz'} - m_{x'} m_{y'} 2_z$	$C_{2vz''} - m_{x''} m_{y''} 2_z$
$\widehat{C}_{2vx} - m_{y\overline{z}} m_{yz} 2_x$	$\widehat{C}_{2vyz} - m_{y\overline{z}} 2_{yz} m_x$	$\widehat{C}_{2vy\overline{z}} - 2_{y\overline{z}} m_{yz} m_x$	$C_{2vx} - 2_x m_y m_z$	$C_{2vx'} - 2_{x'} m_{y'} m_z$	$C_{2vx''} - 2_{x''} m_{y''} m_z$
$\widehat{C}_{2vy} - m_{z\overline{x}} m_{zx} 2_y$	$\widehat{C}_{2vzx} - m_{z\overline{x}} 2_{zx} m_y$	$\widehat{C}_{2vz\overline{x}} - 2_{z\overline{x}} m_{zx} m_y$	$C_{2vy} - m_x 2_y m_z$	$C_{2vy'} - m_{x'} 2_{y'} m_z$	$C_{2vy''} - m_{x''} 2_{y''} m_z$

Monoclinic system

Cubic branch		Common	Hexagonal branch	
$C_{2hxy} - 2_{xy}/m_{xy}$	$C_{2hx\overline{y}} - 2_{x\overline{y}}/m_{x\overline{y}}$	$C_{2hz} - 2_z/m_z$		
$C_{2hyz} - 2_{yz}/m_{yz}$	$C_{2hy\overline{z}} - 2_{y\overline{z}}/m_{y\overline{z}}$	$C_{2hx} - 2_x/m_x$	$C_{2hx'} - 2_{x'}/m_{x'}$	$C_{2hx''} - 2_{x''}/m_{x''}$
$C_{2hzx} - 2_{zx}/m_{zx}$	$C_{2hz\overline{x}} - 2_{z\overline{x}}/m_{z\overline{x}}$	$C_{2hy} - 2_y/m_y$	$C_{2hy'} - 2_{y'}/m_{y'}$	$C_{2hy''} - 2_{y''}/m_{y''}$
$C_{2xy} - 2_{xy}$	$C_{2x\overline{y}} - 2_{x\overline{y}}$	$C_{2z} - 2_z$		
$C_{2yz} - 2_{yz}$	$C_{2y\overline{z}} - 2_{y\overline{z}}$	$C_{2x} - 2_x$	$C_{2x'} - 2_{x'}$	$C_{2x''} - 2_{x''}$
$C_{2zx} - 2_{zx}$	$C_{2z\overline{x}} - 2_{z\overline{x}}$	$C_{2y} - 2_y$	$C_{2y'} - 2_{y'}$	$C_{2y''} - 2_{y''}$
$C_{sxy} - m_{xy}$	$C_{sx\overline{y}} - m_{x\overline{y}}$	$C_{sz} - m_z$		
$C_{syz} - m_{yz}$	$C_{sy\overline{z}} - m_{y\overline{z}}$	$C_{sx} - m_x$	$C_{sx'} - m_{x'}$	$C_{sx''} - m_{x''}$
$C_{szx} - m_{zx}$	$C_{sz\overline{x}} - m_{z\overline{x}}$	$C_{sy} - m_y$	$C_{sy'} - m_{y'}$	$C_{sy''} - m_{y''}$

Inversion group $C_i - \overline{1}$
Common to all centrosymmetric groups

Identity group $C_1 - 1$
Common to all groups

Appendix C

Isomorphisms used for defining irreducible representations

Triclinic groups

Isomorphism class $1 \approx C_1 \quad e = 1$

Isomorphism class $\overline{1} \approx C_i \quad e = 1 \quad i = \overline{1}$

Monoclinic groups

Isomorphism class $2 \approx C_2$

C_{2z}	(2_z)	e	2_z	C_{sz}	(m_z)	e	m_z
C_{2x}	(2_x)	e	2_x	C_{sx}	(m_x)	e	m_x
C_{2y}	(2_y)	e	2_y	C_{sy}	(m_y)	e	m_y
C_{2xy}	(2_{xy})	e	2_{xy}	C_{sxy}	(m_{xy})	e	m_{xy}
$C_{2x\overline{y}}$	$(2_{x\overline{y}})$	e	$2_{x\overline{y}}$	$C_{sx\overline{y}}$	$(m_{x\overline{y}})$	e	$m_{x\overline{y}}$
C_{2yz}	(2_{yz})	e	2_{yz}	C_{syz}	(m_{yz})	e	m_{yz}
$C_{2y\overline{z}}$	$(2_{y\overline{z}})$	e	$2_{y\overline{z}}$	$C_{sy\overline{z}}$	$(m_{y\overline{z}})$	e	$m_{y\overline{z}}$
C_{2zx}	(2_{zx})	e	2_{zx}	C_{szx}	(m_{zx})	e	m_{zx}
$C_{2z\overline{x}}$	$(2_{z\overline{x}})$	e	$2_{z\overline{x}}$	$C_{sz\overline{x}}$	$(m_{z\overline{x}})$	e	$m_{z\overline{x}}$
$C_{2x'}$	$(2_{x'})$	e	$2_{x'}$	$C_{sx'}$	$(m_{x'})$	e	$m_{x'}$
$C_{2x''}$	$(2_{x''})$	e	$2_{x''}$	$C_{sx''}$	$(m_{x''})$	e	$m_{x''}$
$C_{2y'}$	$(2_{y'})$	e	$2_{y'}$	$C_{sy'}$	$(m_{y'})$	e	$m_{y'}$
$C_{2y''}$	$(2_{y''})$	e	$2_{y''}$	$C_{sy''}$	$(m_{y''})$	e	$m_{y''}$

Isomorphism class $2/m \approx C_{2h}$

C_{2hz}	$(2_z/m_z)$	e	2_z	i	m_z
C_{2hx}	$(2_x/m_x)$	e	2_x	i	m_x
C_{2hy}	$(2_y/m_y)$	e	2_y	i	m_y
C_{2hxy}	$(2_{xy}/m_{xy})$	e	2_{xy}	i	m_{xy}
$C_{2hx\overline{y}}$	$(2_{x\overline{y}}/m_{x\overline{y}})$	e	$2_{x\overline{y}}$	i	$m_{x\overline{y}}$
C_{2hyz}	$(2_{yz}/m_{yz})$	e	2_{yz}	i	m_{yz}
$C_{2hy\overline{z}}$	$(2_{y\overline{z}}/m_{y\overline{z}})$	e	$2_{y\overline{z}}$	i	$m_{y\overline{z}}$
C_{2hzx}	$(2_{zx}/m_{zx})$	e	2_{zx}	i	m_{zx}
$C_{2hz\overline{x}}$	$(2_{z\overline{x}}/m_{z\overline{x}})$	e	$2_{z\overline{x}}$	i	$m_{z\overline{x}}$
$C_{2hx'}$	$(2_{x'}/m_{x'})$	e	$2_{x'}$	i	$m_{x'}$
$C_{2hx''}$	$(2_{x''}/m_{x''})$	e	$2_{x''}$	i	$m_{x''}$
$C_{2hy'}$	$(2_{y'}/m_{y'})$	e	$2_{y'}$	i	$m_{y'}$
$C_{2hy''}$	$(2_{y''}/m_{y''})$	e	$2_{y''}$	i	$m_{y''}$

Isomorphism class $222 \approx D_2$

D_2	$(2_x 2_y 2_z)$	e	2_z	2_x	2_y
C_{2vz}	$(m_x m_y 2_z)$	e	2_z	m_x	m_y
C_{2vx}	$(2_x m_y m_z)$	e	m_z	2_x	m_y
C_{2vy}	$(m_x 2_y m_z)$	e	m_z	m_x	2_y
$\widehat{D}_{2z}$	$(2_{x\overline{y}} 2_{xy} 2_z)$	e	2_z	$2_{x\overline{y}}$	2_{xy}
$\widehat{C}_{2vz}$	$(m_{x\overline{y}} m_{xy} 2_z)$	e	2_z	$m_{x\overline{y}}$	m_{xy}
$\widehat{C}_{2vxy}$	$(m_{x\overline{y}} 2_{xy} m_z)$	e	m_z	$m_{x\overline{y}}$	2_{xy}
$\widehat{C}_{2vx\overline{y}}$	$(2_{x\overline{y}} m_{xy} m_z)$	e	m_z	$2_{x\overline{y}}$	m_{xy}
$\widehat{D}_{2x}$	$(2_{y\overline{z}} 2_{yz} 2_x)$	e	2_x	$2_{y\overline{z}}$	2_{yz}
$\widehat{C}_{2vx}$	$(m_{y\overline{z}} m_{yz} 2_x)$	e	2_x	$m_{y\overline{z}}$	m_{yz}
$\widehat{C}_{2vyz}$	$(m_{y\overline{z}} 2_{yz} m_x)$	e	m_x	$m_{y\overline{z}}$	2_{yz}
$\widehat{C}_{2vy\overline{z}}$	$(2_{y\overline{z}} m_{yz} m_x)$	e	m_x	$2_{y\overline{z}}$	m_{yz}
$\widehat{D}_{2y}$	$(2_{z\overline{x}} 2_{zx} 2_y)$	e	2_y	$2_{z\overline{x}}$	2_{zx}
$\widehat{C}_{2vy}$	$(m_{z\overline{x}} m_{zx} 2_y)$	e	2_y	$m_{z\overline{x}}$	m_{zx}
$\widehat{C}_{2vzx}$	$(m_{z\overline{x}} 2_{zx} m_y)$	e	m_y	$m_{z\overline{x}}$	2_{zx}
$\widehat{C}_{2vz\overline{x}}$	$(2_{z\overline{x}} m_{zx} m_y)$	e	m_y	$2_{z\overline{x}}$	m_{zx}
$D_{2'}$	$(2_{x'} 2_{y'} 2_z)$	e	2_z	$2_{x'}$	$2_{y'}$
$C_{2vz'}$	$(m_{x'} m_{y'} 2_z)$	e	2_z	$m_{x'}$	$m_{y'}$
$C_{2vx'}$	$(2_{x'} m_{y'} m_z)$	e	m_z	$2_{x'}$	$m_{y'}$
$C_{2vy'}$	$(m_{x'} 2_{y'} m_z)$	e	m_z	$m_{x'}$	$2_{y'}$
$D_{2''}$	$(2_{x''} 2_{y''} 2_z)$	e	2_z	$2_{x''}$	$2_{y''}$
$C_{2vz''}$	$(m_{x''} m_{y''} 2_z)$	e	2_z	$m_{x''}$	$m_{y''}$
$C_{2vx''}$	$(2_{x''} m_{y''} m_z)$	e	m_z	$2_{x''}$	$m_{y''}$
$C_{2vy''}$	$(m_{x''} 2_{y''} m_z)$	e	m_z	$m_{x''}$	$2_{y''}$

Isomorphism class $mmm \approx D_{2h}$

D_{2h}	$(m_x m_y m_z)$	e	2_z	2_x	2_y	i	m_z	m_x	m_y
$\widehat{D}_{2hz}$	$(m_{x\overline{y}} m_{xy} m_z)$	e	2_z	$2_{x\overline{y}}$	2_{xy}	i	m_z	$m_{x\overline{y}}$	m_{xy}
$\widehat{D}_{2hx}$	$(m_{y\overline{z}} m_{yz} m_x)$	e	2_x	$2_{y\overline{z}}$	2_{yz}	i	m_x	$m_{y\overline{z}}$	m_{yz}
$\widehat{D}_{2hy}$	$(m_{z\overline{x}} m_{zx} m_y)$	e	2_y	$2_{z\overline{x}}$	2_{zx}	i	m_y	$m_{z\overline{x}}$	m_{zx}
$D_{2h'}$	$(m_{x'} m_{y'} m_z)$	e	2_z	$2_{x'}$	$2_{y'}$	i	m_z	$m_{x'}$	$m_{y'}$
$D_{2h''}$	$(m_{x''} m_{y''} m_z)$	e	2_z	$2_{x''}$	$2_{y''}$	i	m_z	$m_{x''}$	$m_{y''}$

Isomorphism class $4 \approx C_4$

C_{4z} (4_z)	e	4_z	2_z	4_z^{-1}
S_{4z} $(\overline{4}_z)$	e	$\overline{4}_z$	2_z	$\overline{4}_z^{-1}$
C_{4x} (4_x)	e	4_x	2_x	4_x^{-1}
S_{4x} $(\overline{4}_x)$	e	$\overline{4}_x$	2_x	$\overline{4}_x^{-1}$
C_{4y} (4_y)	e	4_y	2_y	4_y^{-1}
S_{4y} $(\overline{4}_y)$	e	$\overline{4}_y$	2_y	$\overline{4}_y^{-1}$

Isomorphism class $422 \approx D_4$

D_{4z} $(4_z 2_x 2_{xy})$	e	4_z	2_z	4_z^{-1}	2_x	2_{xy}	2_y	$2_{x\overline{y}}$
C_{4vz} $(4_z m_x m_{xy})$	e	4_z	2_z	4_z^{-1}	m_x	m_{xy}	m_y	$m_{x\overline{y}}$
D_{2dz} $(\overline{4}_z 2_x m_{xy})$	e	$\overline{4}_z$	2_z	$\overline{4}_z^{-1}$	2_x	m_{xy}	2_y	$m_{x\overline{y}}$
$\widehat{D}_{2dz}$ $(\overline{4}_z m_x 2_{xy})$	e	$\overline{4}_z$	2_z	$\overline{4}_z^{-1}$	m_x	2_{xy}	m_y	$2_{x\overline{y}}$
D_{4x} $(4_x 2_y 2_{yz})$	e	4_x	2_x	4_x^{-1}	2_y	2_{yz}	2_z	$2_{y\overline{z}}$
C_{4vx} $(4_x m_y m_{yz})$	e	4_x	2_x	4_x^{-1}	m_y	m_{yz}	m_z	$m_{y\overline{z}}$
D_{2dx} $(\overline{4}_x 2_y m_{yz})$	e	$\overline{4}_x$	2_x	$\overline{4}_x^{-1}$	2_y	m_{yz}	2_z	$m_{y\overline{z}}$
$\widehat{D}_{2dx}$ $(\overline{4}_x m_y 2_{yz})$	e	$\overline{4}_x$	2_x	$\overline{4}_x^{-1}$	m_y	2_{yz}	m_z	$2_{y\overline{z}}$
D_{4y} $(4_y 2_z 2_{zx})$	e	4_y	2_y	4_y^{-1}	2_z	2_{zx}	2_x	$2_{z\overline{x}}$
C_{4vy} $(4_y m_z m_{zx})$	e	4_y	2_y	4_y^{-1}	m_z	m_{zx}	m_x	$m_{z\overline{x}}$
D_{2dy} $(\overline{4}_y 2_z m_{zx})$	e	$\overline{4}_y$	2_y	$\overline{4}_y^{-1}$	2_z	m_{zx}	2_x	$m_{z\overline{x}}$
$\widehat{D}_{2dy}$ $(\overline{4}_y m_z 2_{zx})$	e	$\overline{4}_y$	2_y	$\overline{4}_y^{-1}$	m_z	2_{zx}	m_x	$2_{z\overline{x}}$

Isomorphism class $4/mmm \approx D_{4h}$

D_{4hz} $(4_z/m_z m_x m_{xy})$	e	4_z	2_z	4_z^{-1}	2_x	2_{xy}	2_y	$2_{x\overline{y}}$	i	$\overline{4}_z$	m_z	$\overline{4}_z^{-1}$	m_x	m_{xy}	m_y	$m_{x\overline{y}}$
D_{4hx} $(4_x/m_x m_y m_{yz})$	e	4_x	2_x	4_x^{-1}	2_y	2_{yz}	2_z	$2_{y\overline{z}}$	i	$\overline{4}_x$	m_x	$\overline{4}_x^{-1}$	m_y	m_{yz}	m_z	$m_{y\overline{z}}$
D_{4hy} $(4_y/m_y m_z m_{zx})$	e	4_y	2_y	4_y^{-1}	2_z	2_{zx}	2_x	$2_{z\overline{x}}$	i	$\overline{4}_y$	m_y	$\overline{4}_y^{-1}$	m_z	m_{zx}	m_x	$m_{z\overline{x}}$

Isomorphism class $3 \approx C_3$

C_3	(3)	e	3	3^2
C_{3p}	(3_p)	e	3_p	3_p^2
C_{3q}	(3_q)	e	3_q	3_q^2
C_{3r}	(3_r)	e	3_r	3_r^2
C_{3s}	(3_s)	e	3_s	3_s^2

Isomorphism class $\overline{3} \approx C_{3i}$

C_{3i}	$(\overline{3})$	e	$\overline{3}$	3^2	i	3	$\overline{3}^5$
C_{3ip}	$(\overline{3}_p)$	e	$\overline{3}_p$	3_p^2	i	3_p	$\overline{3}_p^5$
C_{3iq}	$(\overline{3}_q)$	e	$\overline{3}_q$	3_q^2	i	3_q	$\overline{3}_q^5$
C_{3ir}	$(\overline{3}_r)$	e	$\overline{3}_r$	3_r^2	i	3_r	$\overline{3}_r^5$
C_{3is}	$(\overline{3}_s)$	e	$\overline{3}_s$	3_s^2	i	3_s	$\overline{3}_s^5$

Isomorphism class $32 \approx D_3$

D_{3x}	$(3_z 2_x 1)$	e	3_z	3_z^2	2_x	$2_{x''}$	$2_{x'}$
C_{3vx}	$(3_z m_x 1)$	e	3_z	3_z^2	m_x	$m_{x''}$	$m_{x'}$
D_{3y}	$(3_z 1 2_y)$	e	3_z	3_z^2	2_y	$2_{y''}$	$2_{y'}$
C_{3vy}	$(3_z 1 m_y)$	e	3_z	3_z^2	m_y	$m_{y''}$	$m_{y'}$
D_{3p}	$(3_p 2_{x\overline{y}})$	e	3_p	3_p^2	$2_{x\overline{y}}$	$2_{y\overline{z}}$	$2_{z\overline{x}}$
D_{3q}	$(3_q 2_{x\overline{y}})$	e	3_q	3_q^2	$2_{x\overline{y}}$	2_{yz}	2_{zx}
D_{3r}	$(3_r 2_{xy})$	e	3_r	3_r^2	2_{xy}	$2_{y\overline{z}}$	2_{zx}
D_{3s}	$(3_s 2_{xy})$	e	3_s	3_s^2	2_{xy}	2_{yz}	$2_{z\overline{x}}$
C_{3vp}	$(3_p m_{x\overline{y}})$	e	3_p	3_p^2	$m_{x\overline{y}}$	$m_{y\overline{z}}$	$m_{z\overline{x}}$
C_{3vq}	$(3_q m_{x\overline{y}})$	e	3_q	3_q^2	$m_{x\overline{y}}$	m_{yz}	m_{zx}
C_{3vr}	$(3_r m_{xy})$	e	3_r	3_r^2	m_{xy}	$m_{y\overline{z}}$	m_{zx}
C_{3vs}	$(3_s m_{xy})$	e	3_s	3_s^2	m_{xy}	m_{yz}	$m_{z\overline{x}}$

Isomorphism class $\overline{3}2 \approx D_{3d}$

D_{3dx}	$(\overline{3}_z m_x 1)$	e	3_z	3_z^2	2_x	$2_{x''}$	$2_{x'}$	i	$\overline{3}_z$	$\overline{3}_z^5$	m_x	$m_{x''}$	$m_{x'}$
D_{3dy}	$(\overline{3}_z 1 m_y)$	e	3_z	3_z^2	2_y	$2_{y''}$	$2_{y'}$	i	$\overline{3}_z$	$\overline{3}_z^5$	m_y	$m_{y''}$	$m_{y'}$
D_{3dp}	$(\overline{3}_p m_{x\overline{y}})$	e	3_p	3_p^2	$2_{x\overline{y}}$	$2_{y\overline{z}}$	$2_{z\overline{x}}$	i	$\overline{3}_p$	$\overline{3}_p^5$	$m_{x\overline{y}}$	$m_{y\overline{z}}$	$m_{z\overline{x}}$
D_{3dq}	$(\overline{3}_q m_{x\overline{y}})$	e	3_q	3_q^2	$2_{x\overline{y}}$	2_{yz}	2_{zx}	i	$\overline{3}_q$	$\overline{3}_q^5$	$m_{x\overline{y}}$	m_{yz}	m_{zx}
D_{3dr}	$(\overline{3}_r m_{xy})$	e	3_r	3_r^2	2_{xy}	$2_{y\overline{z}}$	2_{zx}	i	$\overline{3}_r$	$\overline{3}_r^5$	m_{xy}	$m_{y\overline{z}}$	m_{zx}
D_{3ds}	$(\overline{3}_s m_{xy})$	e	3_s	3_s^2	2_{xy}	2_{yz}	$2_{z\overline{x}}$	i	$\overline{3}_s$	$\overline{3}_s^5$	m_{xy}	m_{yz}	$m_{z\overline{x}}$

Hexagonal groups

Isomorphism class $6 \approx C_6$

C_6 (6_z)	e	6_z	3_z	2_z	3_z^2	6_z^5
C_{3h} $(\overline{6}_z)$	e	$\overline{6}_z$	3_z	m_z	3_z^2	$\overline{6}_z^5$

Isomorphism class $622 \approx D_6$

D_6 $(6_z 2_x 2_y)$	e	6_z	3_z	2_z	3_z^2	6_z^5	2_x	$2_{y'}$	$2_{x''}$	2_y	$2_{x'}$	$2_{y''}$
C_{6v} $(6_z m_x m_y)$	e	6_z	3_z	2_z	3_z^2	6_z^5	m_x	$m_{y'}$	$m_{x''}$	m_y	$m_{x'}$	$m_{y''}$
D_{3h} $(\overline{6}_z 2_x m_y)$	e	$\overline{6}_z$	3_z	m_z	3_z^2	$\overline{6}_z^5$	2_x	$m_{y'}$	$2_{x''}$	m_y	$2_{x'}$	$m_{y''}$
$\widehat{D}_{3h}$ $(\overline{6}_z m_x 2_y)$	e	$\overline{6}_z$	3_z	m_z	3_z^2	$\overline{6}_z^5$	m_x	$2_{y'}$	$m_{x''}$	2_y	$m_{x'}$	$2_{y''}$

Cubic groups

Isomorphism class $432 \approx O$

O (432)	T	$4_z T$
T_d $(\overline{4}32)$	T	$\overline{4}_z T$

Note: Trigonal subgroups of cubic groups are defined as follows:

Subscripts p, q, r and s correspond to rotations about threefold axes with directions [111], $[\overline{1}\overline{1}1]$, $[1\overline{1}\overline{1}]$ and $[\overline{1}1\overline{1}]$, respectively.

The group D_{3p} with main axis along [111] therefore has elements:
e, 3_p, 3_p^2, $2_{x\overline{y}}$, $2_{y\overline{z}}$ and $2_{z\overline{x}}$.
Groups D_{3q}, D_{3r} and D_{3s} are, respectively, obtained by conjugations *via* 2_z, 2_x and 2_y, respectively, so that:
$D_{3q} = 2_z D_{3p} 2_z$, $D_{3r} = 2_x D_{3p} 2_x$ and $D_{3s} = 2_y D_{3p} 2_y$.

Appendix D

Standard polynomials:

$\xi = \frac{1}{\sqrt{2}}(x+iy)$	$\eta = \frac{1}{\sqrt{2}}(x-iy)$
$\xi^n = (\frac{1}{\sqrt{2}})^n[R_n(x,y) + iI_n(x,y)]$	$\eta^n = (\frac{1}{\sqrt{2}})^n[R_n(x,y) - iI_n(x,y)]$
$x = R_1(x,y)$	$I_1(x,y) = y$
$x^2 - y^2 = R_2(x,y)$	$I_2(x,y) = 2xy$
$x^3 - 3xy^2 = R_3(x,y)$	$I_3(x,y) = 3x^2y - y^3$
$x^4 - 6x^2y^2 + y^4 = R_4(x,y)$	$I_4(x,y) = 4xy(x^2 - y^2)$
$x^5 - 10x^3y^2 + 5xy^4 = R_5(x,y)$	$I_5(x,y) = 5x^4y - 10x^2y^3 + y^5$
$x^6 - 15x^2y^4 + 15x^2y^4 - y^6 = R_6(x,y)$	$I_6(x,y) = 2xy(x^2 - 3y^2)(3x^2 - y^2)$

$$Q(x,y,z) = x^2(z^4 - y^4) + y^2(x^4 - z^4) + z^2(y^4 - x^4)$$

Some useful relations:

$$R_2(y,x) = -R_2(x,y) \quad I_2(y,x) = I_2(x,y)$$

$$R_3(y,x) = I_3(x,y)$$
$$R_3(x,-y) = R_3(x,y) \quad I_3(x,-y) = -I_3(x,y)$$
$$R_3(-x,y) = -R_3(x,y) \quad I_3(-x,y) = I_3(x,y)$$

$$R_4(y,x) = R_4(x,y) \quad I_4(y,x) = -I_4(x,y)$$
$$R_4(x,-y) = R_4(-x,y) = R_4(x,y) \quad I_4(x,-y) = I_4(-x,y) = -I_4(x,y)$$

$$R_5(y,x) = I_5(x,y)$$
$$R_5(x,-y) = -R_5(-x,y) = R_4(x,y) \quad I_5(x,-y) = -I_5(-x,y) = -I_5(x,y)$$

$$R_6(y,x) = -R_6(x,y) \quad I_6(y,x) = -I_6(x,y)$$
$$R_6(x,-y) = R_6(-x,y) = R_4(x,y) \quad I_6(x,-y) = I_6(-x,y) = -I_6(x,y)$$

$$Q(x,y,z) = Q(y,z,x) = Q(z,x,y) =$$
$$-Q(x,z,y) = -Q(z,x,y) = -Q(y,z,x)$$

Appendix E: Labelling of Covariants and Conversion Equations

The tables in this part are given only for the following groups of proper rotations:

tetragonal	trigonal	hexagonal	cubic
$4_z \ - \ C_{4z}$	$3_z \ - \ C_3$	$6_z \ - \ C_6$	$23 \ - \ T$
$4_z 2_x 2_{xy} \ - \ D_{4z}$	$3_z 2_x \ - \ D_{3x} \quad 3_z 2_y \ - \ D_{3y}$	$6_z 2_x 2_y \ - \ D_6$	$432 \ - \ O$

and for tensors $\mathbf{u}$, $\mathbf{A}$, $\mathbf{s}$ and $\mathbf{q}$, all of which are of even parity with respect to space inversion i.

To each group there are assigned two tables on facing pages. The first table, called Labelling of Covariants, assigns numerical labels to linearly independent $D^{(\alpha)}(G)$-covariants in cases where more than one covariant of a given tensor to this irep exist. We shall illustrate it for the case of the tensor $\mathbf{A}$. One-dimensional covariants, including invariants, are denoted by the sans-serif letter A with two indices, the first of which is the numerical label of an irep and the second of which is the number of the covariant. If only one covariant of the type exists, we drop the second index. Thus A_1 means an invariant, A_3 means a $\chi_3(G)$-covariant but $\mathsf{A}_{1,1}$, $\mathsf{A}_{1,2}$, $\mathsf{A}_{1,3}$ mean the first, second and third invariant and $\mathsf{A}_{3,1}$, $\mathsf{A}_{3,2}$ mean the first and second $\chi_3(G)$-covariant. The two-dimensional $D^{(2)}(G)$-covariants are expressed as $\mathbf{A}_1^{(2)} = (A_{2x,1}, A_{2y,1})$, $\mathbf{A}_2^{(2)} = (A_{2x,2}, A_{2y,2})$, $\mathbf{A}_3^{(2)} = (A_{2x,3}, A_{2y,3})$, and so on if more than three linearly independent $D^{(2)}(G)$-covariants exist, while $\mathbf{A}^{(2)} = (A_{2x}, A_{2y})$ signals that there is no other $D^{(2)}(G)$-covariant. In cubic groups we use only the components of covariants.

The table on each facing page bears the title Conversion Equations and contains Cartesian tensor components expressed in terms of the covariant components. If all noninvariant components are set to zero, we get the tensor form, invariant under the group G. By comparison with the main tables we can see which covariant components onset at each transition from the parent group G. Thus these components can be described as the tensor parameters of the transition. Conversion equations are a convenient platform from which to launch the detailed investigation of domain pairs and domain walls. The results of such an investigation in a form which an experimentalist can use directly are in preparation as a continuation of this work.

Conversion equations are not necessary for parent groups up to $m_x m_y m_z - D_{2h}$ because Cartesian components are themselves relative invariants (this is, however, due to the choice of group orientations). Labelling of covariants and solution of conversion equations for other tensors and for other groups can be performed by rewriting the results of Table E with the use of Opechowski's magic relations, which will be considered in detail elsewhere because they enable us to extend the current results to magnetic groups and properties. The relations between covariants of tensors which differ only by parities with respect to various groups of the same Laue class have already been discussed by Kopský (1979*b*). These relations can also be seen from tables of covariants (Kopský, 1979*a*, 2001*b*).

Group $4_z/m_z$ - (C_{4hz})

Labelling of Covariants

$\mathsf{u}_{1,1} = u_1 + u_2$
$\mathsf{u}_{1,2} = u_3$

$\mathsf{u}_{3,1} = u_1 - u_2$
$\mathsf{u}_{3,2} = u_6$
$\mathbf{u}^{(1)} = (u_{1x}, u_{1y}) = (u_4, -u_5)$

$\mathsf{A}_{1,1} = A_{14} - A_{25}$
$\mathsf{A}_{1,2} = A_{31} + A_{32}$
$\mathsf{A}_{1,3} = A_{15} + A_{24}$
$\mathsf{A}_{1,4} = A_{33}$

$\mathsf{A}_{3,1} = A_{14} + A_{25}$
$\mathsf{A}_{3,2} = A_{31} - A_{32}$
$\mathsf{A}_{3,3} = A_{15} - A_{24}$
$\mathsf{A}_{3,4} = A_{36}$

$\mathbf{A}_1^{(1)} = (A_{1x,1}, A_{1y,1}) = (A_{11}, A_{22})$
$\mathbf{A}_2^{(1)} = (A_{1x,2}, A_{1y,2}) = (A_{12}, A_{21})$

$\mathbf{A}_3^{(1)} = (A_{1x,3}, A_{1y,3}) = (A_{13}, A_{23})$
$\mathbf{A}_4^{(1)} = (A_{1x,4}, A_{1y,4}) = (A_{26}, A_{16})$
$\mathbf{A}_5^{(1)} = (A_{1x,5}, A_{1y,5}) = (A_{35}, A_{34})$

$\mathsf{s}_{1,1} = s_{11} + s_{22}$
$\mathsf{s}_{1,2} = s_{13} + s_{23}$
$\mathsf{s}_{1,3} = s_{44} + s_{55}$
$\mathsf{s}_{1,4} = s_{16} - s_{26}$
$\mathsf{s}_{1,5} = s_{12}$
$\mathsf{s}_{1,6} = s_{33}$
$\mathsf{s}_{1,7} = s_{66}$

$\mathsf{s}_{3,1} = s_{11} - s_{22}$
$\mathsf{s}_{3,2} = s_{13} - s_{23}$
$\mathsf{s}_{3,3} = s_{44} - s_{55}$
$\mathsf{s}_{3,4} = s_{16} + s_{26}$
$\mathsf{s}_{3,5} = s_{36}$
$\mathsf{s}_{3,6} = s_{45}$

$\mathbf{s}_1^{(1)} = (s_{1x,1}, s_{1y,1}) = (s_{14}, -s_{25})$
$\mathbf{s}_2^{(1)} = (s_{1x,2}, s_{1y,2}) = (s_{24}, -s_{15})$

$\mathbf{s}_3^{(1)} = (s_{1x,3}, s_{1y,3}) = (s_{34}, -s_{35})$
$\mathbf{s}_4^{(1)} = (s_{1x,4}, s_{1y,4}) = (s_{56}, -s_{46})$

$\mathsf{q}_{1,1} = q_{13} + q_{23}$
$\mathsf{q}_{1,2} = q_{16} - q_{26}$
$\mathsf{q}_{1,3} = q_{45}$

$\mathsf{q}_{3,1} = q_{13} - q_{23}$
$\mathsf{q}_{3,2} = q_{16} + q_{26}$
$\mathsf{q}_{3,3} = q_{12}$
$\mathsf{q}_{3,4} = q_{36}$

$\mathbf{q}_1^{(1)} = (q_{1x,1}, q_{1y,1}) = (q_{14}, -q_{25})$
$\mathbf{q}_2^{(1)} = (q_{1x,2}, q_{1y,2}) = (q_{24}, -q_{15})$

$\mathbf{q}_3^{(1)} = (q_{1x,3}, q_{1y,3}) = (q_{34}, -q_{35})$
$\mathbf{q}_4^{(1)} = (q_{1x,4}, q_{1y,4}) = (q_{56}, -q_{46})$

Conversion Equations

$$u_1 = \tfrac{1}{2}(\mathsf{u}_{1,1} + \mathsf{u}_{3,1}) \qquad u_2 = \tfrac{1}{2}(\mathsf{u}_{1,1} - \mathsf{u}_{3,1}) \qquad u_3 = \mathsf{u}_{1,2}$$
$$u_4 = u_{1x} \qquad u_5 = -u_{1y} \qquad u_6 = \mathsf{u}_{3,2}$$

$$A_{11} = A_{1x,1} \quad A_{22} = A_{1y,1} \quad A_{12} = A_{1x,2} \quad A_{21} = A_{1y,2}$$
$$A_{13} = A_{1x,3} \quad A_{23} = A_{1y,3} \quad A_{26} = A_{1x,4} \quad A_{16} = A_{1y,4}$$
$$A_{35} = A_{1x,5} \quad A_{34} = A_{1y,5} \quad A_{33} = \mathsf{A}_{1,4} \quad A_{36} = \mathsf{A}_{3,4}$$
$$A_{14} = \tfrac{1}{2}(\mathsf{A}_{1,1} + \mathsf{A}_{3,1}) \quad A_{25} = \tfrac{1}{2}(-\mathsf{A}_{1,1} + \mathsf{A}_{3,1})$$
$$A_{31} = \tfrac{1}{2}(\mathsf{A}_{1,2} + \mathsf{A}_{3,2}) \quad A_{32} = \tfrac{1}{2}(\mathsf{A}_{1,2} - \mathsf{A}_{3,2})$$
$$A_{15} = \tfrac{1}{2}(\mathsf{A}_{1,3} + \mathsf{A}_{3,3}) \quad A_{24} = \tfrac{1}{2}(\mathsf{A}_{1,3} - \mathsf{A}_{3,3})$$

$$s_{11} = \tfrac{1}{2}(\mathsf{s}_{1,1} + \mathsf{s}_{3,1}) \quad s_{22} = \tfrac{1}{2}(\mathsf{s}_{1,1} - \mathsf{s}_{3,1}) \quad s_{13} = \tfrac{1}{2}(\mathsf{s}_{1,2} + \mathsf{s}_{3,2}) \quad s_{23} = \tfrac{1}{2}(\mathsf{s}_{1,2} - \mathsf{s}_{3,2})$$
$$s_{44} = \tfrac{1}{2}(\mathsf{s}_{1,3} + \mathsf{s}_{3,3}) \quad s_{55} = \tfrac{1}{2}(\mathsf{s}_{1,3} - \mathsf{s}_{3,3}) \quad s_{16} = \tfrac{1}{2}(\mathsf{s}_{1,4} + \mathsf{s}_{3,4}) \quad s_{26} = \tfrac{1}{2}(-\mathsf{s}_{1,4} + \mathsf{s}_{3,4})$$
$$s_{12} = \mathsf{s}_{1,5} \quad s_{33} = \mathsf{s}_{1,6} \quad s_{66} = \mathsf{s}_{1,7} \quad s_{36} = \mathsf{s}_{3,5} \quad s_{45} = \mathsf{s}_{3,6}$$
$$s_{14} = s_{1x,1} \quad s_{25} = -s_{1y,1} \quad s_{24} = s_{1x,2} \quad s_{15} = -s_{1y,2}$$
$$s_{34} = s_{1x,3} \quad s_{35} = -s_{1y,3} \quad s_{56} = s_{1x,4} \quad s_{46} = -s_{1y,4}$$

$$q_{13} = \tfrac{1}{2}(\mathsf{q}_{1,1} + \mathsf{q}_{3,1}) \quad q_{23} = \tfrac{1}{2}(\mathsf{q}_{1,1} - \mathsf{q}_{3,1}) \quad q_{16} = \tfrac{1}{2}(\mathsf{q}_{1,2} + \mathsf{q}_{3,2}) \quad q_{26} = \tfrac{1}{2}(-\mathsf{q}_{1,2} + \mathsf{q}_{3,2})$$
$$q_{45} = \mathsf{q}_{1,3} \quad q_{12} = \mathsf{q}_{3,3} \quad q_{36} = \mathsf{q}_{3,4}$$
$$q_{14} = q_{1x,1} \quad q_{25} = -q_{1y,1} \quad q_{24} = q_{1x,2} \quad q_{15} = -q_{1y,2}$$
$$q_{34} = q_{1x,3} \quad q_{35} = -q_{1y,3} \quad q_{56} = q_{1x,4} \quad q_{46} = -q_{1y,4}$$

Group $4_z2_x2_{xy}$ - (D_{4z})

Labelling of Covariants

$\mathsf{u}_{1,1} = u_1 + u_2$ $\quad \mathsf{u}_3 = u_1 - u_2$ $\quad \mathsf{u}_4 = u_6$

$\mathsf{u}_{1,2} = u_3$ $\quad \mathbf{u}^{(1)} = (u_{1x}, u_{1y}) = (u_4, -u_5)$

$\mathsf{A}_1 = A_{14} - A_{25}$ $\quad \mathsf{A}_{2,1} = A_{31} + A_{32}$ $\quad \mathsf{A}_{3,1} = A_{14} + A_{25}$ $\quad \mathsf{A}_{4,1} = A_{31} - A_{32}$

$\mathsf{A}_{2,2} = A_{15} + A_{24}$ $\quad \mathsf{A}_{3,2} = A_{36}$ $\quad \mathsf{A}_{4,2} = A_{15} - A_{24}$

$\mathsf{A}_{2,3} = A_{33}$

$\mathbf{A}_1^{(1)} = (A_{1x,1}, A_{1y,1}) = (A_{11}, A_{22})$ $\quad \mathbf{A}_3^{(1)} = (A_{1x,3}, A_{1y,3}) = (A_{13}, A_{23})$

$\mathbf{A}_2^{(1)} = (A_{1x,2}, A_{1y,2}) = (A_{12}, A_{21})$ $\quad \mathbf{A}_4^{(1)} = (A_{1x,4}, A_{1y,4}) = (A_{26}, A_{16})$

$\mathbf{A}_5^{(1)} = (A_{1x,5}, A_{1y,5}) = (A_{35}, A_{34})$

$\mathsf{s}_{1,1} = s_{11} + s_{22}$ $\quad \mathsf{s}_{2,1} = s_{16} - s_{26}$ $\quad \mathsf{s}_{3,1} = s_{11} - s_{22}$ $\quad \mathsf{s}_{4,1} = s_{16} + s_{26}$

$\mathsf{s}_{1,2} = s_{13} + s_{23}$ $\quad \mathsf{s}_{3,2} = s_{13} - s_{23}$ $\quad \mathsf{s}_{4,2} = s_{36}$

$\mathsf{s}_{1,3} = s_{44} + s_{55}$ $\quad \mathsf{s}_{3,3} = s_{44} - s_{55}$ $\quad \mathsf{s}_{4,3} = s_{45}$

$\mathsf{s}_{1,4} = s_{12}$

$\mathsf{s}_{1,5} = s_{33}$ $\quad \mathbf{s}_1^{(1)} = (s_{1x,1}, s_{1y,1}) = (s_{14}, -s_{25})$

$\mathsf{s}_{1,6} = s_{66}$ $\quad \mathbf{s}_2^{(1)} = (s_{1x,2}, s_{1y,2}) = (s_{24}, -s_{15})$

$\mathbf{s}_3^{(1)} = (s_{1x,3}, s_{1y,3}) = (s_{34}, -s_{35})$

$\mathbf{s}_4^{(1)} = (s_{1x,4}, s_{1y,4}) = (s_{56}, -s_{46})$

$\mathsf{q}_{1,1} = q_{13} + q_{23}$ $\quad \mathsf{q}_{2,1} = q_{16} - q_{26}$ $\quad \mathsf{q}_{3,1} = q_{13} - q_{23}$ $\quad \mathsf{q}_{4,1} = q_{16} + q_{26}$

$\mathsf{q}_{2,2} = q_{45}$ $\quad \mathsf{q}_{3,2} = q_{12}$ $\quad \mathsf{q}_{4,2} = q_{36}$

$\mathbf{q}_1^{(1)} = (q_{1x,1}, q_{1y,1}) = (q_{14}, -q_{25})$

$\mathbf{q}_2^{(1)} = (q_{1x,2}, q_{1y,2}) = (q_{24}, -q_{15})$

$\mathbf{q}_3^{(1)} = (q_{1x,3}, q_{1y,3}) = (q_{34}, -q_{35})$

$\mathbf{q}_4^{(1)} = (q_{1x,4}, q_{1y,4}) = (q_{56}, -q_{46})$

Conversion Equations

$$u_1 = \tfrac{1}{2}(\mathsf{u}_{1,1} + \mathsf{u}_3) \quad u_2 = \tfrac{1}{2}(\mathsf{u}_{1,1} - \mathsf{u}_3) \quad u_3 = \mathsf{u}_{1,2}$$
$$u_4 = u_{1x} \quad u_5 = -u_{1y} \quad u_6 = \mathsf{u}_4$$

$$A_{11} = A_{1x,1} \quad A_{22} = A_{1y,1} \quad A_{12} = A_{1x,2} \quad A_{21} = A_{1y,2}$$
$$A_{13} = A_{1x,3} \quad A_{23} = A_{1y,3} \quad A_{26} = A_{1x,4} \quad A_{16} = A_{1y,4}$$
$$A_{35} = A_{1x,5} \quad A_{34} = A_{1y,5} \quad A_{33} = \mathsf{A}_{2,3} \quad A_{36} = \mathsf{A}_{3,2}$$
$$A_{14} = \tfrac{1}{2}(\mathsf{A}_1 + \mathsf{A}_{3,1}) \quad A_{25} = \tfrac{1}{2}(-\mathsf{A}_1 + \mathsf{A}_{3,1})$$
$$A_{31} = \tfrac{1}{2}(\mathsf{A}_{2,1} + \mathsf{A}_{4,1}) \quad A_{32} = \tfrac{1}{2}(\mathsf{A}_{2,1} - \mathsf{A}_{4,1})$$
$$A_{15} = \tfrac{1}{2}(\mathsf{A}_{2,2} + \mathsf{A}_{4,2}) \quad A_{24} = \tfrac{1}{2}(\mathsf{A}_{2,2} - \mathsf{A}_{4,2})$$

$$s_{11} = \tfrac{1}{2}(\mathsf{s}_{1,1} + \mathsf{s}_{3,1}) \quad s_{22} = \tfrac{1}{2}(\mathsf{s}_{1,1} - \mathsf{s}_{3,1}) \quad s_{13} = \tfrac{1}{2}(\mathsf{s}_{1,2} + \mathsf{s}_{3,2}) \quad s_{23} = \tfrac{1}{2}(\mathsf{s}_{1,2} - \mathsf{s}_{3,2})$$
$$s_{44} = \tfrac{1}{2}(\mathsf{s}_{1,3} + \mathsf{s}_{3,3}) \quad s_{55} = \tfrac{1}{2}(\mathsf{s}_{1,3} - \mathsf{s}_{3,3}) \quad s_{16} = \tfrac{1}{2}(\mathsf{s}_{2,1} + \mathsf{s}_{4,1}) \quad s_{26} = \tfrac{1}{2}(-\mathsf{s}_{2,1} + \mathsf{s}_{4,1})$$
$$s_{12} = \mathsf{s}_{1,4} \quad s_{33} = \mathsf{s}_{1,5} \quad s_{66} = \mathsf{s}_{1,6} \quad s_{36} = \mathsf{s}_{4,2} \quad s_{45} = \mathsf{s}_{4,3}$$
$$s_{14} = s_{1x,1} \quad s_{25} = -s_{1y,1} \quad s_{24} = s_{1x,2} \quad s_{15} = -s_{1y,2}$$
$$s_{34} = s_{1x,3} \quad s_{35} = -s_{1y,3} \quad s_{56} = s_{1x,4} \quad s_{46} = -s_{1y,4}$$

$$q_{13} = \tfrac{1}{2}(\mathsf{q}_{1,1} + \mathsf{q}_{3,1}) \quad q_{23} = \tfrac{1}{2}(\mathsf{q}_{1,1} - \mathsf{q}_{3,1}) \quad q_{16} = \tfrac{1}{2}(\mathsf{q}_{2,1} + \mathsf{q}_{4,1}) \quad q_{26} = \tfrac{1}{2}(-\mathsf{q}_{2,1} + \mathsf{q}_{4,1})$$
$$q_{45} = \mathsf{q}_{2,2} \quad q_{12} = \mathsf{q}_{3,2} \quad q_{36} = \mathsf{q}_{4,2}$$
$$q_{14} = q_{1x,1} \quad q_{25} = -q_{1y,1} \quad q_{24} = q_{1x,2} \quad q_{15} = -q_{1y,2}$$
$$q_{34} = q_{1x,3} \quad q_{35} = -q_{1y,3} \quad q_{56} = q_{1x,4} \quad q_{46} = -q_{1y,4}$$

Group 3_z - (C_3)

Labelling of Covariants

$\mathsf{u}_{o,1} = u_1 + u_2$ $\qquad$ $\mathbf{u}_1^{(1)} = (u_{1x,1}, u_{1y,1}) = (u_1 - u_2, -2u_6)$

$\mathsf{u}_{o,2} = u_3$ $\qquad$ $\mathbf{u}_2^{(1)} = (u_{1x,2}, u_{1y,2}) = (u_4, -u_5)$

$\mathsf{A}_{1,1} = A_{14} - A_{25}$ $\qquad$ $\mathbf{A}_1^{(1)} = (A_{1x,1}, A_{1y,1}) = (A_{11} + A_{12}, A_{22} + A_{21})$

$\mathsf{A}_{1,2} = A_{31} + A_{32}$ $\qquad$ $\mathbf{A}_2^{(1)} = (A_{1x,2}, A_{1y,2}) = (A_{11} + A_{26}, A_{22} + A_{16})$

$\mathsf{A}_{1,3} = A_{15} + A_{24}$ $\qquad$ $\mathbf{A}_3^{(1)} = (A_{1x,3}, A_{1y,3}) = (A_{13}, A_{23})$

$\mathsf{A}_{1,4} = A_{33}$ $\qquad$ $\mathbf{A}_4^{(1)} = (A_{1x,4}, A_{1y,4}) = (A_{35}, A_{34})$

$\mathsf{A}_{1,5} = A_{11} - A_{12} - 2A_{26}$ $\qquad$ $\mathbf{A}_5^{(1)} = (A_{1x,5}, A_{1y,5}) = (2A_{36}, A_{31} - A_{32})$

$\mathsf{A}_{1,6} = A_{22} - A_{21} - 2A_{16}$ $\qquad$ $\mathbf{A}_6^{(1)} = (A_{1x,6}, A_{1y,6}) = (A_{14} + A_{25}, A_{15} - A_{24})$

$\mathsf{s}_{1,1} = s_{11} + s_{22} + 2s_{12}$ $\qquad$ $\mathbf{s}_1^{(1)} = (s_{1x,1}, s_{1y,1}) = (s_{14} + s_{24}, -s_{15} - s_{25})$

$\mathsf{s}_{1,2} = s_{11} + s_{22} + 2s_{66}$ $\qquad$ $\mathbf{s}_2^{(1)} = (s_{1x,2}, s_{1y,2}) = (s_{14} - s_{56}, s_{46} - s_{25})$

$\mathsf{s}_{1,3} = s_{13} + s_{23}$ $\qquad$ $\mathbf{s}_3^{(1)} = (s_{1x,3}, s_{1y,3}) = (s_{34}, -s_{35})$

$\mathsf{s}_{1,4} = s_{44} + s_{55}$ $\qquad$ $\mathbf{s}_4^{(1)} = (s_{1x,4}, s_{1y,4}) = [s_{11} - s_{22}, -2(s_{16} + s_{26})]$

$\mathsf{s}_{1,5} = s_{33}$ $\qquad$ $\mathbf{s}_5^{(1)} = (s_{1x,5}, s_{1y,5}) = [s_{11} + s_{22} - 2s_{12} - 4s_{66}, 4(s_{16} - s_{26})]$

$\mathsf{s}_{1,6} = s_{14} - s_{24} + 2s_{56}$ $\qquad$ $\mathbf{s}_6^{(1)} = (s_{1x,6}, s_{1y,6}) = (s_{13} - s_{23}, -2s_{36})$

$\mathsf{s}_{1,7} = s_{15} - s_{25} - 2s_{46}$ $\qquad$ $\mathbf{s}_7^{(1)} = (s_{1x,7}, s_{1y,7}) = (s_{44} - s_{55}, 2s_{45})$

$\mathsf{q}_{1,1} = q_{13} + q_{23}$ $\qquad$ $\mathbf{q}_1^{(1)} = (q_{1x,1}, q_{1y,1}) = (q_{34}, -q_{35})$

$\mathsf{q}_{1,2} = q_{16} - q_{26}$ $\qquad$ $\mathbf{q}_2^{(1)} = (q_{1x,2}, q_{1y,2}) = (q_{14} + q_{24}, -q_{15} - q_{25})$

$\mathsf{q}_{1,3} = q_{45}$ $\qquad$ $\mathbf{q}_3^{(1)} = (q_{1x,3}, q_{1y,3}) = (q_{14} + q_{56}, -q_{46} - q_{25})$

$\mathsf{q}_{1,4} = q_{14} - q_{24} - 2q_{56}$ $\qquad$ $\mathbf{q}_4^{(4)} = (q_{1x,4}, q_{1y,4}) = (q_{12}, q_{16} + q_{26})$

$\mathsf{q}_{1,5} = q_{15} - q_{25} + 2q_{46}$ $\qquad$ $\mathbf{q}_5^{(1)} = (q_{1x,5}, q_{1y,5}) = (q_{13} - q_{23}, 2q_{36})$

Conversion Equations

$$u_1 = \tfrac{1}{2}(\mathsf{u}_{o,1} + u_{1x,1}) \quad u_2 = \tfrac{1}{2}(\mathsf{u}_{o,1} - u_{1x,1}) \quad u_3 = \mathsf{u}_{o,2}$$
$$u_4 = u_{1x,2} \quad u_5 = -u_{1y,2} \quad u_6 = -\tfrac{1}{2}u_{1y,1}$$

$$\begin{aligned}
A_{11} &= \tfrac{1}{4}\mathsf{A}_{1,5} + \tfrac{1}{4}A_{1x,1} + \tfrac{1}{2}A_{1x,2} & A_{22} &= \tfrac{1}{4}\mathsf{A}_{1,6} + \tfrac{1}{4}A_{1y,1} + \tfrac{1}{2}A_{1y,2}\\
A_{12} &= -\tfrac{1}{4}\mathsf{A}_{1,5} + \tfrac{3}{4}A_{1x,1} - \tfrac{1}{2}A_{1x,2} & A_{21} &= -\tfrac{1}{4}\mathsf{A}_{1,6} + \tfrac{3}{4}A_{1y,1} - \tfrac{1}{2}A_{1y,2}\\
A_{26} &= -\tfrac{1}{4}\mathsf{A}_{1,5} - \tfrac{1}{4}A_{1x,1} + \tfrac{1}{2}A_{1x,2} & A_{16} &= -\tfrac{1}{4}\mathsf{A}_{1,6} - \tfrac{1}{4}A_{1y,1} + \tfrac{1}{2}A_{1y,2}
\end{aligned}$$

$$A_{14} = \tfrac{1}{2}(\mathsf{A}_{1,1} + A_{1x,6}) \quad A_{31} = \tfrac{1}{2}(\mathsf{A}_{1,2} + A_{1y,5}) \quad A_{15} = \tfrac{1}{2}(\mathsf{A}_{1,3} + A_{1y,6})$$
$$A_{25} = \tfrac{1}{2}(-\mathsf{A}_{1,1} + A_{1x,6}) \quad A_{32} = \tfrac{1}{2}(\mathsf{A}_{1,2} - A_{1y,5}) \quad A_{24} = \tfrac{1}{2}(\mathsf{A}_{1,3} - A_{1y,6})$$

$$A_{33} = \mathsf{A}_{1,4} \quad A_{36} = \tfrac{1}{2}A_{1x,5} \quad A_{13} = A_{1x,3} \quad A_{23} = A_{1y,3} \quad A_{35} = A_{1x,4} \quad A_{34} = A_{1y,4}$$

$$\begin{aligned}
s_{11} &= \tfrac{1}{8}\mathsf{s}_{1,1} + \tfrac{1}{4}\mathsf{s}_{1,2} + \tfrac{1}{2}s_{1x,4} + \tfrac{1}{8}s_{1x,5}\\
s_{22} &= \tfrac{1}{8}\mathsf{s}_{1,1} + \tfrac{1}{4}\mathsf{s}_{1,2} - \tfrac{1}{2}s_{1x,4} + \tfrac{1}{8}s_{1x,5}\\
s_{12} &= \tfrac{3}{8}\mathsf{s}_{1,1} - \tfrac{1}{4}\mathsf{s}_{1,2} - \tfrac{1}{8}s_{1x,5}\\
s_{66} &= -\tfrac{1}{8}\mathsf{s}_{1,1} + \tfrac{1}{4}\mathsf{s}_{1,2} - \tfrac{1}{8}s_{1x,5}
\end{aligned}$$

$$\begin{aligned}
s_{14} &= \tfrac{1}{4}\mathsf{s}_{1,6} + \tfrac{1}{4}s_{1x,1} + \tfrac{1}{2}s_{1x,2} & s_{15} &= \tfrac{1}{4}\mathsf{s}_{1,7} - \tfrac{3}{4}s_{1y,1} + \tfrac{1}{2}s_{1y,2}\\
s_{24} &= -\tfrac{1}{4}\mathsf{s}_{1,6} + \tfrac{3}{4}s_{1x,1} - \tfrac{1}{2}s_{1x,2} & s_{25} &= -\tfrac{1}{4}\mathsf{s}_{1,7} - \tfrac{1}{4}s_{1y,1} - \tfrac{1}{2}s_{1y,2}\\
s_{56} &= \tfrac{1}{4}\mathsf{s}_{1,6} + \tfrac{1}{4}s_{1x,1} - \tfrac{1}{2}s_{1x,2} & s_{46} &= -\tfrac{1}{4}\mathsf{s}_{1,7} - \tfrac{1}{4}s_{1y,1} + \tfrac{1}{2}s_{1y,2}
\end{aligned}$$

$$\begin{aligned}
s_{13} &= \tfrac{1}{2}(\mathsf{s}_{1,3} + s_{1x,6}) & s_{23} &= \tfrac{1}{2}(\mathsf{s}_{1,3} - s_{1x,6})\\
s_{44} &= \tfrac{1}{2}(\mathsf{s}_{1,4} + s_{1x,7}) & s_{55} &= \tfrac{1}{2}(\mathsf{s}_{1,4} - s_{1x,7})\\
s_{16} &= -\tfrac{1}{4}s_{1y,4} + \tfrac{1}{8}s_{1y,5} & s_{26} &= -\tfrac{1}{4}s_{1y,4} - \tfrac{1}{8}s_{1y,5}
\end{aligned}$$

$$s_{33} = \mathsf{s}_{1,5} \quad s_{34} = s_{1x,3} \quad s_{35} = -s_{1y,3} \quad s_{36} = -\tfrac{1}{2}s_{1y,6} \quad s_{45} = \tfrac{1}{2}s_{1y,7}$$

$$\begin{aligned}
q_{13} &= \tfrac{1}{2}(\mathsf{q}_{1,1} + q_{1x,5}) & q_{16} &= \tfrac{1}{2}(\mathsf{q}_{1,2} + q_{1y,4})\\
q_{23} &= \tfrac{1}{2}(\mathsf{q}_{1,1} - q_{1x,5}) & q_{26} &= -\tfrac{1}{2}(\mathsf{q}_{1,2} - q_{1y,4})
\end{aligned}$$

$$\begin{aligned}
q_{14} &= \tfrac{1}{4}\mathsf{q}_{1,4} + \tfrac{1}{4}q_{1x,2} + \tfrac{1}{2}q_{1x,3} & q_{15} &= \tfrac{1}{4}\mathsf{q}_{1,5} - \tfrac{3}{4}q_{1y,2} + \tfrac{1}{2}q_{1y,3}\\
q_{24} &= -\tfrac{1}{4}\mathsf{q}_{1,4} + \tfrac{3}{4}q_{1x,2} - \tfrac{1}{2}q_{1x,3} & q_{25} &= -\tfrac{1}{4}\mathsf{q}_{1,5} - \tfrac{1}{4}q_{1y,2} - \tfrac{1}{2}q_{1y,3}\\
q_{56} &= -\tfrac{1}{4}\mathsf{q}_{1,4} - \tfrac{1}{4}q_{1x,2} + \tfrac{1}{2}q_{1x,3} & q_{46} &= \tfrac{1}{4}\mathsf{q}_{1,5} + \tfrac{1}{4}q_{1y,2} - \tfrac{1}{2}q_{1y,3}
\end{aligned}$$

$$q_{45} = \mathsf{q}_{1,3} \quad q_{34} = q_{1x,1} \quad q_{35} = -q_{1y,1} \quad q_{12} = q_{1x,4} \quad q_{36} = \tfrac{1}{2}q_{1y,5}$$

Group $3_z 2_x$ - (D_{3x})

Labelling of Covariants

$\mathsf{u}_{o,1} = u_1 + u_2$	$\mathbf{u}_1^{(1)} = (u_{1x,1}, u_{1y,1}) = (u_4, -u_5)$
$\mathsf{u}_{o,2} = u_3$	$\mathbf{u}_2^{(1)} = (u_{1x,2}, u_{1y,2}) = (u_1 - u_2, -2u_6)$
$\mathsf{A}_{1,1} = A_{14} - A_{25}$	$\mathbf{A}_1^{(1)} = (A_{1x,1}, A_{1y,1}) = (A_{11} + A_{12}, A_{22} + A_{21})$
$\mathsf{A}_{1,2} = A_{11} - A_{12} - 2A_{26}$	$\mathbf{A}_2^{(1)} = (A_{1x,2}, A_{1y,2}) = (A_{11} + A_{26}, A_{22} + A_{16})$
	$\mathbf{A}_3^{(1)} = (A_{1x,3}, A_{1y,3}) = (A_{13}, A_{23})$
$\mathsf{A}_{2,1} = A_{31} + A_{32}$	$\mathbf{A}_4^{(1)} = (A_{1x,4}, A_{1y,4}) = (A_{35}, A_{34})$
$\mathsf{A}_{2,2} = A_{15} + A_{24}$	
$\mathsf{A}_{2,3} = A_{33}$	$\mathbf{A}_5^{(1)} = (A_{1x,5}, A_{1y,5}) = (2A_{36}, A_{31} - A_{32})$
$\mathsf{A}_{2,4} = A_{22} - A_{21} - 2A_{16}$	$\mathbf{A}_6^{(1)} = (A_{1x,6}, A_{1y,6}) = (A_{14} + A_{25}, A_{15} - A_{24})$
$\mathsf{s}_{1,1} = s_{11} + s_{22} + 2s_{12}$	$\mathbf{s}_1^{(1)} = (s_{1x,1}, s_{1y,1}) = (s_{14} + s_{24}, -s_{15} - s_{25})$
$\mathsf{s}_{1,2} = s_{11} + s_{22} + 2s_{66}$	$\mathbf{s}_2^{(1)} = (s_{1x,2}, s_{1y,2}) = (s_{14} - s_{56}, s_{46} - s_{25})$
$\mathsf{s}_{1,3} = s_{13} + s_{23}$	$\mathbf{s}_3^{(1)} = (s_{1x,3}, s_{1y,3}) = (s_{34}, -s_{35})$
$\mathsf{s}_{1,4} = s_{44} + s_{55}$	
$\mathsf{s}_{1,5} = s_{33}$	$\mathbf{s}_4^{(1)} = (s_{1x,4}, s_{1y,4}) = [s_{11} - s_{22}, -2(s_{16} + s_{26})]$
$\mathsf{s}_{1,6} = s_{14} - s_{24} + 2s_{56}$	$\mathbf{s}_5^{(1)} = (s_{1x,5}, s_{1y,5}) = [s_{11} + s_{22} - 2s_{12} - 4s_{66}, 4(s_{16} - s_{26})]$
	$\mathbf{s}_6^{(1)} = (s_{1x,6}, s_{1y,6}) = (s_{13} - s_{23}, -2s_{36})$
$\mathsf{s}_2 = s_{15} - s_{25} - 2s_{46}$	$\mathbf{s}_7^{(1)} = (s_{1x,7}, s_{1y,7}) = (s_{44} - s_{55}, 2s_{45})$
$\mathsf{q}_{1,1} = q_{13} + q_{23}$	$\mathbf{q}_1^{(1)} = (q_{1x,1}, q_{1y,1}) = (q_{34}, -q_{35})$
$\mathsf{q}_{1,2} = q_{14} - q_{24} - 2q_{56}$	$\mathbf{q}_2^{(1)} = (q_{1x,2}, q_{1y,2}) = (q_{14} + q_{24}, -q_{15} - q_{25})$
	$\mathbf{q}_3^{(1)} = (q_{1x,3}, q_{1y,3}) = (q_{14} + q_{56}, -q_{46} - q_{25})$
$\mathsf{q}_{2,1} = q_{16} - q_{26}$	
$\mathsf{q}_{2,2} = q_{45}$	$\mathbf{q}_4^{(1)} = (q_{1x,4}, q_{1y,4}) = (q_{12}, q_{16} + q_{26})$
$\mathsf{q}_{2,3} = q_{15} - q_{25} + 2q_{46}$	$\mathbf{q}_5^{(1)} = (q_{1x,5}, q_{1y,5}) = (q_{13} - q_{23}, 2q_{36})$

Conversion Equations

$$u_1 = \tfrac{1}{2}(\mathsf{u}_{o,1} + u_{1x,2}) \quad u_2 = \tfrac{1}{2}(\mathsf{u}_{o,1} - u_{1x,2}) \quad u_3 = \mathsf{u}_{o,2}$$
$$u_4 = u_{1x,1} \quad u_5 = -u_{1y,1} \quad u_6 = -\tfrac{1}{2}u_{1y,2}$$

$$\begin{aligned}
A_{11} &= \tfrac{1}{4}\mathsf{A}_{1,2} + \tfrac{1}{4}A_{1x,1} + \tfrac{1}{2}A_{1x,2} & A_{22} &= \tfrac{1}{4}\mathsf{A}_{2,4} + \tfrac{1}{4}A_{1y,1} + \tfrac{1}{2}A_{1y,2}\\
A_{12} &= -\tfrac{1}{4}\mathsf{A}_{1,2} + \tfrac{3}{4}A_{1x,1} - \tfrac{1}{2}A_{1x,2} & A_{21} &= -\tfrac{1}{4}\mathsf{A}_{2,4} + \tfrac{3}{4}A_{1y,1} - \tfrac{1}{2}A_{1y,2}\\
A_{26} &= -\tfrac{1}{4}\mathsf{A}_{1,2} - \tfrac{1}{4}A_{1x,1} + \tfrac{1}{2}A_{1x,2} & A_{16} &= -\tfrac{1}{4}\mathsf{A}_{2,4} - \tfrac{1}{4}A_{1y,1} + \tfrac{1}{2}A_{1y,2}
\end{aligned}$$

$$A_{14} = \tfrac{1}{2}(\mathsf{A}_{1,1} + A_{1x,6}) \quad A_{31} = \tfrac{1}{2}(\mathsf{A}_{2,1} + A_{1y,5}) \quad A_{15} = \tfrac{1}{2}(\mathsf{A}_{2,2} + A_{1y,6})$$
$$A_{25} = \tfrac{1}{2}(-\mathsf{A}_{1,1} + A_{1x,6}) \quad A_{32} = \tfrac{1}{2}(\mathsf{A}_{2,1} - A_{1y,5}) \quad A_{24} = \tfrac{1}{2}(\mathsf{A}_{2,2} - A_{1y,6})$$

$$A_{33} = \mathsf{A}_{2,3} \quad A_{36} = \tfrac{1}{2}A_{1x,5} \quad A_{13} = A_{1x,3} \quad A_{23} = A_{1y,3} \quad A_{35} = A_{1x,4} \quad A_{34} = A_{1y,4}$$

$$\begin{aligned}
s_{11} &= \tfrac{1}{8}\mathsf{s}_{1,1} + \tfrac{1}{4}\mathsf{s}_{1,2} + \tfrac{1}{2}s_{1x,4} + \tfrac{1}{8}s_{1x,5}\\
s_{22} &= \tfrac{1}{8}\mathsf{s}_{1,1} + \tfrac{1}{4}\mathsf{s}_{1,2} - \tfrac{1}{2}s_{1x,4} + \tfrac{1}{8}s_{1x,5}\\
s_{12} &= \tfrac{3}{8}\mathsf{s}_{1,1} - \tfrac{1}{4}\mathsf{s}_{1,2} - \tfrac{1}{8}s_{1x,5}\\
s_{66} &= -\tfrac{1}{8}\mathsf{s}_{1,1} + \tfrac{1}{4}\mathsf{s}_{1,2} - \tfrac{1}{8}s_{1x,5}
\end{aligned}$$

$$\begin{aligned}
s_{14} &= \tfrac{1}{4}\mathsf{s}_{1,6} + \tfrac{1}{4}s_{1x,1} + \tfrac{1}{2}s_{1x,2} & s_{15} &= \tfrac{1}{4}\mathsf{s}_{2} - \tfrac{3}{4}s_{1y,1} + \tfrac{1}{2}s_{1y,2}\\
s_{24} &= -\tfrac{1}{4}\mathsf{s}_{1,6} + \tfrac{3}{4}s_{1x,1} - \tfrac{1}{2}s_{1x,2} & s_{25} &= -\tfrac{1}{4}\mathsf{s}_{2} - \tfrac{1}{4}s_{1y,1} - \tfrac{1}{2}s_{1y,2}\\
s_{56} &= \tfrac{1}{4}\mathsf{s}_{1,6} + \tfrac{1}{4}s_{1x,1} - \tfrac{1}{2}s_{1x,2} & s_{46} &= -\tfrac{1}{4}\mathsf{s}_{2} - \tfrac{1}{4}s_{1y,1} + \tfrac{1}{2}s_{1y,2}
\end{aligned}$$

$$\begin{aligned}
s_{13} &= \tfrac{1}{2}(\mathsf{s}_{1,3} + s_{1x,6}) & s_{23} &= \tfrac{1}{2}(\mathsf{s}_{1,3} - s_{1x,6})\\
s_{44} &= \tfrac{1}{2}(\mathsf{s}_{1,4} + s_{1x,7}) & s_{55} &= \tfrac{1}{2}(\mathsf{s}_{1,4} - s_{1x,7})\\
s_{16} &= -\tfrac{1}{4}s_{1y,4} + \tfrac{1}{8}s_{1y,5} & s_{26} &= -\tfrac{1}{4}s_{1y,4} - \tfrac{1}{8}s_{1y,5}
\end{aligned}$$

$$s_{33} = \mathsf{s}_{1,5} \quad s_{34} = s_{1x,3} \quad s_{35} = -s_{1y,3} \quad s_{36} = -\tfrac{1}{2}s_{1y,6} \quad s_{45} = \tfrac{1}{2}s_{1y,7}$$

$$\begin{aligned}
q_{13} &= \tfrac{1}{2}(\mathsf{q}_{1,1} + q_{1x,5}) & q_{16} &= \tfrac{1}{2}(\mathsf{q}_{2,1} + q_{1y,4})\\
q_{23} &= \tfrac{1}{2}(\mathsf{q}_{1,1} - q_{1x,5}) & q_{26} &= -\tfrac{1}{2}(\mathsf{q}_{2,1} - q_{1y,4})
\end{aligned}$$

$$\begin{aligned}
q_{14} &= \tfrac{1}{4}\mathsf{q}_{1,2} + \tfrac{1}{4}q_{1x,2} + \tfrac{1}{2}q_{1x,3} & q_{15} &= \tfrac{1}{4}\mathsf{q}_{2,3} - \tfrac{3}{4}q_{1y,2} + \tfrac{1}{2}q_{1y,3}\\
q_{24} &= -\tfrac{1}{4}\mathsf{q}_{1,2} + \tfrac{3}{4}q_{1x,2} - \tfrac{1}{2}q_{1x,3} & q_{25} &= -\tfrac{1}{4}\mathsf{q}_{2,3} - \tfrac{1}{4}q_{1y,2} - \tfrac{1}{2}q_{1y,3}\\
q_{56} &= -\tfrac{1}{4}\mathsf{q}_{1,2} - \tfrac{1}{4}q_{1x,2} + \tfrac{1}{2}q_{1x,3} & q_{46} &= \tfrac{1}{4}\mathsf{q}_{2,3} + \tfrac{1}{4}q_{1y,2} - \tfrac{1}{2}q_{1y,3}
\end{aligned}$$

$$q_{45} = \mathsf{q}_{2,2} \quad q_{34} = q_{1x,1} \quad q_{35} = -q_{1y,1} \quad q_{12} = q_{1x,4} \quad q_{36} = \tfrac{1}{2}q_{1y,5}$$

Group $3_z 2_y$ - (D_{3y})

Labelling of Covariants

$\mathsf{u}_{o,1} = u_1 + u_2$	$\mathbf{u}_1^{(1)} = (u_{1x,1}, u_{1y,1}) = (u_4, -u_5)$
$\mathsf{u}_{o,2} = u_3$	$\mathbf{u}_2^{(1)} = (u_{1x,2}, u_{1y,2}) = (2u_6, u_1 - u_2)$
$\mathsf{A}_{1,1} = A_{14} - A_{25}$	$\mathbf{A}_1^{(1)} = (A_{1x,1}, A_{1y,1}) = (A_{11} + A_{12}, A_{22} + A_{21})$
$\mathsf{A}_{1,2} = A_{22} - A_{21} - 2A_{16}$	$\mathbf{A}_2^{(1)} = (A_{1x,2}, A_{1y,2}) = (A_{11} + A_{26}, A_{22} + A_{16})$
	$\mathbf{A}_3^{(1)} = (A_{1x,3}, A_{1y,3}) = (A_{13}, A_{23})$
$\mathsf{A}_{2,1} = A_{31} + A_{32}$	$\mathbf{A}_4^{(1)} = (A_{1x,4}, A_{1y,4}) = (A_{35}, A_{34})$
$\mathsf{A}_{2,2} = A_{15} + A_{24}$	
$\mathsf{A}_{2,3} = A_{33}$	$\mathbf{A}_5^{(1)} = (A_{1x,5}, A_{1y,5}) = (A_{32} - A_{31}, 2A_{36})$
$\mathsf{A}_{2,4} = A_{11} - A_{12} - 2A_{26}$	$\mathbf{A}_6^{(1)} = (A_{1x,6}, A_{1y,6}) = (A_{24} - A_{15}, A_{14} + A_{25})$
$\mathsf{s}_{1,1} = s_{11} + s_{22} + 2s_{12}$	$\mathbf{s}_1^{(1)} = (s_{1x,1}, s_{1y,1}) = (s_{14} + s_{24}, -s_{15} - s_{25})$
$\mathsf{s}_{1,2} = s_{11} + s_{22} + 2s_{66}$	$\mathbf{s}_2^{(1)} = (s_{1x,2}, s_{1y,2}) = (s_{14} - s_{56}, s_{46} - s_{25})$
$\mathsf{s}_{1,3} = s_{13} + s_{23}$	$\mathbf{s}_3^{(1)} = (s_{1x,3}, s_{1y,3}) = (s_{34}, -s_{35})$
$\mathsf{s}_{1,4} = s_{44} + s_{55}$	
$\mathsf{s}_{1,5} = s_{33}$	$\mathbf{s}_4^{(1)} = (s_{1x,4}, s_{1y,4}) = [2(s_{16} + s_{26}), s_{11} - s_{22}]$
$\mathsf{s}_{1,6} = s_{15} - s_{25} - 2s_{46}$	$\mathbf{s}_5^{(1)} = (s_{1x,5}, s_{1y,5}) = [4(s_{26} - s_{16}), s_{11} + s_{22} - 2s_{12} - 4s_{66}]$
	$\mathbf{s}_6^{(1)} = (s_{1x,6}, s_{1y,6}) = (2s_{36}, s_{13} - s_{23})$
$\mathsf{s}_2 = s_{14} - s_{24} + 2s_{56}$	$\mathbf{s}_7^{(1)} = (s_{1x,7}, s_{1y,7}) = (2s_{45}, s_{55} - s_{44})$
$\mathsf{q}_{1,1} = q_{13} + q_{23}$	$\mathbf{q}_1^{(1)} = (q_{1x,1}, q_{1y,1}) = (q_{34}, -q_{35})$
$\mathsf{q}_{1,2} = q_{15} - q_{25} + 2q_{46}$	$\mathbf{q}_2^{(1)} = (q_{1x,2}, q_{1y,2}) = (q_{14} + q_{24}, -q_{15} - q_{25})$
	$\mathbf{q}_3^{(1)} = (q_{1x,3}, q_{1y,3}) = (q_{14} + q_{56}, -q_{46} - q_{25})$
$\mathsf{q}_{2,1} = q_{16} - q_{26}$	
$\mathsf{q}_{2,2} = q_{45}$	$\mathbf{q}_4^{(1)} = (q_{1x,4}, q_{1y,4}) = (q_{16} + q_{26}, -q_{12})$
$\mathsf{q}_{2,3} = q_{14} - q_{24} - 2q_{56}$	$\mathbf{q}_5^{(1)} = (q_{1x,5}, q_{1y,5}) = (2q_{36}, q_{23} - q_{13})$

Conversion Equations

$$u_1 = \tfrac{1}{2}(\mathsf{u}_{o,1} + u_{1y,2}) \quad u_2 = \tfrac{1}{2}(\mathsf{u}_{o,1} - u_{1y,2}) \quad u_3 = \mathsf{u}_{o,2}$$
$$u_4 = u_{1x,1} \quad u_5 = -u_{1y,1} \quad u_6 = \tfrac{1}{2}u_{1x,2}$$

$$\begin{aligned}
A_{11} &= \tfrac{1}{4}\mathsf{A}_{2,4} + \tfrac{1}{4}A_{1x,1} + \tfrac{1}{2}A_{1x,2} & A_{22} &= \tfrac{1}{4}\mathsf{A}_{1,2} + \tfrac{1}{4}A_{1y,1} + \tfrac{1}{2}A_{1y,2}\\
A_{12} &= -\tfrac{1}{4}\mathsf{A}_{2,4} + \tfrac{3}{4}A_{1x,1} - \tfrac{1}{2}A_{1x,2} & A_{21} &= -\tfrac{1}{4}\mathsf{A}_{1,2} + \tfrac{3}{4}A_{1y,1} - \tfrac{1}{2}A_{1y,2}\\
A_{26} &= -\tfrac{1}{4}\mathsf{A}_{2,4} - \tfrac{1}{4}A_{1x,1} + \tfrac{1}{2}A_{1x,2} & A_{16} &= -\tfrac{1}{4}\mathsf{A}_{1,2} - \tfrac{1}{4}A_{1y,1} + \tfrac{1}{2}A_{1y,2}
\end{aligned}$$

$$A_{14} = \tfrac{1}{2}(\mathsf{A}_{1,1} + A_{1y,6}) \quad A_{31} = \tfrac{1}{2}(\mathsf{A}_{2,1} - A_{1x,5}) \quad A_{15} = \tfrac{1}{2}(\mathsf{A}_{2,2} - A_{1x,6})$$
$$A_{25} = \tfrac{1}{2}(-\mathsf{A}_{1,1} + A_{1y,6}) \quad A_{32} = \tfrac{1}{2}(\mathsf{A}_{2,1} + A_{1x,5}) \quad A_{24} = \tfrac{1}{2}(\mathsf{A}_{2,2} + A_{1x,6})$$

$$A_{33} = \mathsf{A}_{2,3} \quad A_{36} = \tfrac{1}{2}A_{1y,5} \quad A_{13} = A_{1x,3} \quad A_{23} = A_{1y,3} \quad A_{35} = A_{1x,4} \quad A_{34} = A_{1y,4}$$

$$\begin{aligned}
s_{11} &= \tfrac{1}{8}\mathsf{s}_{1,1} + \tfrac{1}{4}\mathsf{s}_{1,2} + \tfrac{1}{2}s_{1y,4} + \tfrac{1}{8}s_{1y,5}\\
s_{22} &= \tfrac{1}{8}\mathsf{s}_{1,1} + \tfrac{1}{4}\mathsf{s}_{1,2} - \tfrac{1}{2}s_{1y,4} + \tfrac{1}{8}s_{1y,5}\\
s_{12} &= \tfrac{3}{8}\mathsf{s}_{1,1} - \tfrac{1}{4}\mathsf{s}_{1,2} - \tfrac{1}{8}s_{1y,5}\\
s_{66} &= -\tfrac{1}{8}\mathsf{s}_{1,1} + \tfrac{1}{4}\mathsf{s}_{1,2} - \tfrac{1}{8}s_{1y,5}
\end{aligned}$$

$$\begin{aligned}
s_{14} &= \tfrac{1}{4}\mathsf{s}_{2} + \tfrac{1}{4}s_{1x,1} + \tfrac{1}{2}s_{1x,2} & s_{15} &= \tfrac{1}{4}\mathsf{s}_{1,6} - \tfrac{3}{4}s_{1y,1} + \tfrac{1}{2}s_{1y,2}\\
s_{24} &= -\tfrac{1}{4}\mathsf{s}_{2} + \tfrac{3}{4}s_{1x,1} - \tfrac{1}{2}s_{1x,2} & s_{25} &= -\tfrac{1}{4}\mathsf{s}_{1,6} - \tfrac{1}{4}s_{1y,1} - \tfrac{1}{2}s_{1y,2}\\
s_{56} &= \tfrac{1}{4}\mathsf{s}_{2} + \tfrac{1}{4}s_{1x,1} - \tfrac{1}{2}s_{1x,2} & s_{46} &= -\tfrac{1}{4}\mathsf{s}_{1,6} - \tfrac{1}{4}s_{1y,1} + \tfrac{1}{2}s_{1y,2}
\end{aligned}$$

$$\begin{aligned}
s_{13} &= \tfrac{1}{2}(\mathsf{s}_{1,3} + s_{1y,6}) & s_{23} &= \tfrac{1}{2}(\mathsf{s}_{1,3} - s_{1y,6})\\
s_{44} &= \tfrac{1}{2}(\mathsf{s}_{1,4} - s_{1y,7}) & s_{55} &= \tfrac{1}{2}(\mathsf{s}_{1,4} + s_{1y,7})\\
s_{16} &= \tfrac{1}{4}s_{1x,4} - \tfrac{1}{8}s_{1x,5} & s_{26} &= \tfrac{1}{4}s_{1x,4} + \tfrac{1}{8}s_{1x,5}
\end{aligned}$$

$$s_{33} = \mathsf{s}_{1,5} \quad s_{34} = s_{1x,3} \quad s_{35} = -s_{1y,3} \quad s_{36} = \tfrac{1}{2}s_{1x,6} \quad s_{45} = \tfrac{1}{2}s_{1x,7}$$

$$\begin{aligned}
q_{13} &= \tfrac{1}{2}(\mathsf{q}_{1,1} - q_{1y,5}) & q_{16} &= \tfrac{1}{2}(\mathsf{q}_{2,1} + q_{1x,4})\\
q_{23} &= \tfrac{1}{2}(\mathsf{q}_{1,1} + q_{1y,5}) & q_{26} &= -\tfrac{1}{2}(\mathsf{q}_{2,1} - q_{1x,4})
\end{aligned}$$

$$\begin{aligned}
q_{14} &= \tfrac{1}{4}\mathsf{q}_{2,3} + \tfrac{1}{4}q_{1x,2} + \tfrac{1}{2}q_{1x,3} & q_{15} &= \tfrac{1}{4}\mathsf{q}_{1,2} - \tfrac{3}{4}q_{1y,2} + \tfrac{1}{2}q_{1y,3}\\
q_{24} &= -\tfrac{1}{4}\mathsf{q}_{2,3} + \tfrac{3}{4}q_{1x,2} - \tfrac{1}{2}q_{1x,3} & q_{25} &= -\tfrac{1}{4}\mathsf{q}_{1,2} - \tfrac{1}{4}q_{1y,2} - \tfrac{1}{2}q_{1y,3}\\
q_{56} &= -\tfrac{1}{4}\mathsf{q}_{2,3} - \tfrac{1}{4}q_{1x,2} + \tfrac{1}{2}q_{1x,3} & q_{46} &= \tfrac{1}{4}\mathsf{q}_{1,2} + \tfrac{1}{4}q_{1y,2} - \tfrac{1}{2}q_{1y,3}
\end{aligned}$$

$$q_{45} = \mathsf{q}_{2,2} \quad q_{34} = q_{1x,1} \quad q_{35} = -q_{1y,1} \quad q_{12} = -q_{1y,4} \quad q_{36} = \tfrac{1}{2}q_{1x,5}$$

Group 6_z - (C_6)

Labelling of Covariants

$\mathsf{u}_{o,1} = u_1 + u_2$	$\mathbf{u}^{(1)} = (u_{1x}, u_{1y}) = (u_4, -u_5)$
$\mathsf{u}_{o,2} = u_3$	$\mathbf{u}^{(2)} = (u_{2x}, u_{2y}) = (u_1 - u_2, 2u_6)$
$\mathsf{A}_{1,1} = A_{14} - A_{25}$	$\mathbf{A}_1^{(1)} = (A_{1x,1}, A_{1y,1}) = (A_{11} + A_{12}, A_{22} + A_{21})$
$\mathsf{A}_{1,2} = A_{31} + A_{32}$	$\mathbf{A}_2^{(1)} = (A_{1x,2}, A_{1y,2}) = (A_{11} + A_{26}, A_{22} + A_{16})$
$\mathsf{A}_{1,3} = A_{15} + A_{24}$	$\mathbf{A}_3^{(1)} = (A_{1x,3}, A_{1y,3}) = (A_{13}, A_{23})$
$\mathsf{A}_{1,4} = A_{33}$	$\mathbf{A}_4^{(1)} = (A_{1x,4}, A_{1y,4}) = (A_{35}, A_{34})$
$\mathsf{A}_{3,1} = A_{11} - A_{12} - 2A_{26}$	$\mathbf{A}_1^{(2)} = (A_{2x,1}, A_{2y,1}) = (2A_{36}, A_{32} - A_{31})$
$\mathsf{A}_{3,2} = A_{22} - A_{21} - 2A_{16}$	$\mathbf{A}_2^{(2)} = (A_{2x,2}, A_{2y,2}) = (A_{14} + A_{25}, A_{24} - A_{15})$
$\mathsf{s}_{1,1} = s_{11} + s_{22} + 2s_{12}$	$\mathbf{s}_1^{(1)} = (s_{1x,1}, s_{1y,1}) = (s_{14} + s_{24}, -s_{15} - s_{25})$
$\mathsf{s}_{1,2} = s_{11} + s_{22} + 2s_{66}$	$\mathbf{s}_2^{(1)} = (s_{1x,2}, s_{1y,2}) = (s_{14} - s_{56}, s_{46} - s_{25})$
$\mathsf{s}_{1,3} = s_{13} + s_{23}$	$\mathbf{s}_3^{(1)} = (s_{1x,3}, s_{1y,3}) = (s_{34}, -s_{35})$
$\mathsf{s}_{1,4} = s_{44} + s_{55}$	
$\mathsf{s}_{1,5} = s_{33}$	$\mathbf{s}_1^{(2)} = (s_{2x,1}, s_{2y,1}) = [s_{11} - s_{22}, 2(s_{16} + s_{26})]$
	$\mathbf{s}_2^{(2)} = (s_{2x,2}, s_{2y,2}) = [s_{11} + s_{22} - 2s_{12} - 4s_{66}, 4(s_{26} - s_{16})]$
$\mathsf{s}_{3,1} = s_{14} - s_{24} + 2s_{56}$	$\mathbf{s}_3^{(2)} = (s_{2x,3}, s_{2y,3}) = (s_{13} - s_{23}, 2s_{36})$
$\mathsf{s}_{3,2} = s_{15} - s_{25} - 2s_{46}$	$\mathbf{s}_4^{(2)} = (s_{2x,4}, s_{2y,4}) = (s_{44} - s_{55}, -2s_{45})$
$\mathsf{q}_{1,1} = q_{13} + q_{23}$	$\mathbf{q}_1^{(1)} = (q_{1x,1}, q_{1y,1}) = (q_{34}, -q_{35})$
$\mathsf{q}_{1,2} = q_{16} - q_{26}$	$\mathbf{q}_2^{(1)} = (q_{1x,2}, q_{1y,2}) = (q_{14} + q_{24}, -q_{15} - q_{25})$
$\mathsf{q}_{1,3} = q_{45}$	$\mathbf{q}_3^{(1)} = (q_{1x,3}, q_{1y,3}) = (q_{14} + q_{56}, -q_{46} - q_{25})$
$\mathsf{q}_{3,1} = q_{14} - q_{24} - 2q_{56}$	$\mathbf{q}_1^{(2)} = (q_{2x,1}, q_{2y,1}) = (q_{12}, -q_{16} - q_{26})$
$\mathsf{q}_{3,2} = q_{15} - q_{25} + 2q_{46}$	$\mathbf{q}_2^{(2)} = (q_{2x,2}, q_{2y,2}) = (q_{13} - q_{23}, -2q_{36})$

Conversion Equations

$$u_1 = \tfrac{1}{2}(\mathsf{u}_{o,1} + u_{2x}) \quad u_2 = \tfrac{1}{2}(\mathsf{u}_{o,1} - u_{2x}) \quad u_3 = \mathsf{u}_{o,2}$$
$$u_4 = u_{1x} \quad u_5 = -u_{1y} \quad u_6 = \tfrac{1}{2}u_{2y}$$

$$\begin{aligned}
A_{11} &= \tfrac{1}{4}\mathsf{A}_{3,1} + \tfrac{1}{4}A_{1x,1} + \tfrac{1}{2}A_{1x,2} & A_{22} &= \tfrac{1}{4}\mathsf{A}_{3,2} + \tfrac{1}{4}A_{1y,1} + \tfrac{1}{2}A_{1y,2}\\
A_{12} &= -\tfrac{1}{4}\mathsf{A}_{3,1} + \tfrac{3}{4}A_{1x,1} - \tfrac{1}{2}A_{1x,2} & A_{21} &= -\tfrac{1}{4}\mathsf{A}_{3,2} + \tfrac{3}{4}A_{1y,1} - \tfrac{1}{2}A_{1y,2}\\
A_{26} &= -\tfrac{1}{4}\mathsf{A}_{3,1} - \tfrac{1}{4}A_{1x,1} + \tfrac{1}{2}A_{1x,2} & A_{16} &= -\tfrac{1}{4}\mathsf{A}_{3,2} - \tfrac{1}{4}A_{1y,1} + \tfrac{1}{2}A_{1y,2}
\end{aligned}$$

$$A_{14} = \tfrac{1}{2}(\mathsf{A}_{1,1} + A_{2x,2}) \quad A_{31} = \tfrac{1}{2}(\mathsf{A}_{1,2} - A_{2y,1}) \quad A_{15} = \tfrac{1}{2}(\mathsf{A}_{1,3} - A_{2y,2})$$
$$A_{25} = \tfrac{1}{2}(-\mathsf{A}_{1,1} + A_{2x,2}) \quad A_{32} = \tfrac{1}{2}(\mathsf{A}_{1,2} + A_{2y,1}) \quad A_{24} = \tfrac{1}{2}(\mathsf{A}_{1,3} + A_{2y,2})$$

$$A_{33} = \mathsf{A}_{1,4} \quad A_{36} = \tfrac{1}{2}A_{2x,1} \quad A_{13} = A_{1x,3} \quad A_{23} = A_{1y,3} \quad A_{35} = A_{1x,4} \quad A_{34} = A_{1y,4}$$

$$\begin{aligned}
s_{11} &= \tfrac{1}{8}\mathsf{s}_{1,1} + \tfrac{1}{4}\mathsf{s}_{1,2} + \tfrac{1}{2}s_{2x,1} + \tfrac{1}{8}s_{2x,2}\\
s_{22} &= \tfrac{1}{8}\mathsf{s}_{1,1} + \tfrac{1}{4}\mathsf{s}_{1,2} - \tfrac{1}{2}s_{2x,1} + \tfrac{1}{8}s_{2x,2}\\
s_{12} &= \tfrac{3}{8}\mathsf{s}_{1,1} - \tfrac{1}{4}\mathsf{s}_{1,2} - \tfrac{1}{8}s_{2x,2}\\
s_{66} &= -\tfrac{1}{8}\mathsf{s}_{1,1} + \tfrac{1}{4}\mathsf{s}_{1,2} - \tfrac{1}{8}s_{2x,2}
\end{aligned}$$

$$\begin{aligned}
s_{14} &= \tfrac{1}{4}\mathsf{s}_{3,1} + \tfrac{1}{4}s_{1x,1} + \tfrac{1}{2}s_{1x,2} & s_{15} &= \tfrac{1}{4}\mathsf{s}_{3,2} - \tfrac{3}{4}s_{1y,1} + \tfrac{1}{2}s_{1y,2}\\
s_{24} &= -\tfrac{1}{4}\mathsf{s}_{3,1} + \tfrac{3}{4}s_{1x,1} - \tfrac{1}{2}s_{1x,2} & s_{25} &= -\tfrac{1}{4}\mathsf{s}_{3,2} - \tfrac{1}{4}s_{1y,1} - \tfrac{1}{2}s_{1y,2}\\
s_{56} &= \tfrac{1}{4}\mathsf{s}_{3,1} + \tfrac{1}{4}s_{1x,1} - \tfrac{1}{2}s_{1x,2} & s_{46} &= -\tfrac{1}{4}\mathsf{s}_{3,2} - \tfrac{1}{4}s_{1y,1} + \tfrac{1}{2}s_{1y,2}
\end{aligned}$$

$$\begin{aligned}
s_{13} &= \tfrac{1}{2}(\mathsf{s}_{1,3} + s_{2x,3}) & s_{23} &= \tfrac{1}{2}(\mathsf{s}_{1,3} - s_{2x,3})\\
s_{44} &= \tfrac{1}{2}(\mathsf{s}_{1,4} + s_{2x,4}) & s_{55} &= \tfrac{1}{2}(\mathsf{s}_{1,4} - s_{2x,4})\\
s_{16} &= \tfrac{1}{4}s_{2y,1} - \tfrac{1}{8}s_{2y,2} & s_{26} &= \tfrac{1}{4}s_{2y,1} + \tfrac{1}{8}s_{2y,2}
\end{aligned}$$

$$s_{33} = \mathsf{s}_{1,5} \quad s_{34} = s_{1x,3} \quad s_{35} = -s_{1y,3} \quad s_{36} = \tfrac{1}{2}s_{2y,3} \quad s_{45} = -\tfrac{1}{2}s_{2y,4}$$

$$\begin{aligned}
q_{13} &= \tfrac{1}{2}(\mathsf{q}_{1,1} + q_{2x,2}) & q_{16} &= \tfrac{1}{2}(\mathsf{q}_{1,2} - q_{2y,1})\\
q_{23} &= \tfrac{1}{2}(\mathsf{q}_{1,1} - q_{2x,2}) & q_{26} &= -\tfrac{1}{2}(\mathsf{q}_{1,2} + q_{2y,1})
\end{aligned}$$

$$\begin{aligned}
q_{14} &= \tfrac{1}{4}\mathsf{q}_{3,1} + \tfrac{1}{4}q_{1x,2} + \tfrac{1}{2}q_{1x,3} & q_{15} &= \tfrac{1}{4}\mathsf{q}_{3,2} - \tfrac{3}{4}q_{1y,2} + \tfrac{1}{2}q_{1y,3}\\
q_{24} &= -\tfrac{1}{4}\mathsf{q}_{3,1} + \tfrac{3}{4}q_{1x,2} - \tfrac{1}{2}q_{1x,3} & q_{25} &= -\tfrac{1}{4}\mathsf{q}_{3,2} - \tfrac{1}{4}q_{1y,2} - \tfrac{1}{2}q_{1y,3}\\
q_{56} &= -\tfrac{1}{4}\mathsf{q}_{3,1} - \tfrac{1}{4}q_{1x,2} + \tfrac{1}{2}q_{1x,3} & q_{46} &= \tfrac{1}{4}\mathsf{q}_{3,2} + \tfrac{1}{4}q_{1y,2} - \tfrac{1}{2}q_{1y,3}
\end{aligned}$$

$$q_{45} = \mathsf{q}_{1,3} \quad q_{34} = q_{1x,1} \quad q_{35} = -q_{1y,1} \quad q_{12} = q_{2x,1} \quad q_{36} = -\tfrac{1}{2}q_{2y,2}$$

Group $6_z 2_x 2_y$ - (D_6)

Labelling of Covariants

$\mathsf{u}_{o,1} = u_1 + u_2$	$\mathbf{u}^{(1)} = (u_{1x}, u_{1y}) = (u_4, -u_5)$
$\mathsf{u}_{o,2} = u_3$	$\mathbf{u}^{(2)} = (u_{2x}, u_{2y}) = (u_1 - u_2, 2u_6)$
$\mathsf{A}_1 = A_{14} - A_{25}$	$\mathbf{A}_1^{(1)} = (A_{1x,1}, A_{1y,1}) = (A_{11} + A_{12}, A_{22} + A_{21})$
	$\mathbf{A}_2^{(1)} = (A_{1x,2}, A_{1y,2}) = (A_{11} + A_{26}, A_{22} + A_{16})$
$\mathsf{A}_{2,1} = A_{31} + A_{32}$	$\mathbf{A}_3^{(1)} = (A_{1x,3}, A_{1y,3}) = (A_{13}, A_{23})$
$\mathsf{A}_{2,2} = A_{15} + A_{24}$	$\mathbf{A}_4^{(1)} = (A_{1x,4}, A_{1y,4}) = (A_{35}, A_{34})$
$\mathsf{A}_{2,3} = A_{33}$	
$\mathsf{A}_3 = A_{11} - A_{12} - 2A_{26}$	$\mathbf{A}_1^{(2)} = (A_{2x,1}, A_{2y,1}) = (2A_{36}, A_{32} - A_{31})$
$\mathsf{A}_4 = A_{22} - A_{21} - 2A_{16}$	$\mathbf{A}_2^{(2)} = (A_{2x,2}, A_{2y,2}) = (A_{14} + A_{25}, A_{24} - A_{15})$
$\mathsf{s}_{1,1} = s_{11} + s_{22} + 2s_{12}$	$\mathbf{s}_1^{(1)} = (s_{1x,1}, s_{1y,1}) = (s_{14} + s_{24}, -s_{15} - s_{25})$
$\mathsf{s}_{1,2} = s_{11} + s_{22} + 2s_{66}$	$\mathbf{s}_2^{(1)} = (s_{1x,2}, s_{1y,2}) = (s_{14} - s_{56}, s_{46} - s_{25})$
$\mathsf{s}_{1,3} = s_{13} + s_{23}$	$\mathbf{s}_3^{(1)} = (s_{1x,3}, s_{1y,3}) = (s_{34}, -s_{35})$
$\mathsf{s}_{1,4} = s_{44} + s_{55}$	
$\mathsf{s}_{1,5} = s_{33}$	$\mathbf{s}_1^{(2)} = (s_{2x,1}, s_{2y,1}) = [s_{11} - s_{22}, 2(s_{16} + s_{26})]$
	$\mathbf{s}_2^{(2)} = (s_{2x,2}, s_{2y,2}) = [s_{11} + s_{22} - 2s_{12} - 4s_{66}, 4(s_{26} - s_{16})]$
$\mathsf{s}_3 = s_{14} - s_{24} + 2s_{56}$	$\mathbf{s}_3^{(2)} = (s_{2x,3}, s_{2y,3}) = (s_{13} - s_{23}, 2s_{36})$
$\mathsf{s}_4 = s_{15} - s_{25} - 2s_{46}$	$\mathbf{s}_4^{(2)} = (s_{2x,4}, s_{2y,4}) = (s_{44} - s_{55}, -2s_{45})$
$\mathsf{q}_1 = q_{13} + q_{23}$	$\mathbf{q}_1^{(1)} = (q_{1x,1}, q_{1y,1}) = (q_{34}, -q_{35})$
	$\mathbf{q}_2^{(1)} = (q_{1x,2}, q_{1y,2}) = (q_{14} + q_{24}, -q_{15} - q_{25})$
$\mathsf{q}_{2,1} = q_{16} - q_{26}$	$\mathbf{q}_3^{(1)} = (q_{1x,3}, q_{1y,3}) = (q_{14} + q_{56}, -q_{46} - q_{25})$
$\mathsf{q}_{2,2} = q_{45}$	
$\mathsf{q}_3 = q_{14} - q_{24} - 2q_{56}$	$\mathbf{q}_1^{(2)} = (q_{2x,1}, q_{2y,1}) = (q_{12}, -q_{16} - q_{26})$
$\mathsf{q}_4 = q_{15} - q_{25} + 2q_{46}$	$\mathbf{q}_2^{(2)} = (q_{2x,2}, q_{2y,2}) = (q_{13} - q_{23}, -2q_{36})$

Conversion Equations

$$u_1 = \tfrac{1}{2}(\mathsf{u}_{o,1} + u_{2x}) \quad u_2 = \tfrac{1}{2}(\mathsf{u}_{o,1} - u_{2x}) \quad u_3 = \mathsf{u}_{o,2}$$
$$u_4 = u_{1x} \quad u_5 = -u_{1y} \quad u_6 = \tfrac{1}{2}u_{2y}$$

$$\begin{aligned}
A_{11} &= \tfrac{1}{4}\mathsf{A}_3 + \tfrac{1}{4}A_{1x,1} + \tfrac{1}{2}A_{1x,2} & A_{22} &= \tfrac{1}{4}\mathsf{A}_4 + \tfrac{1}{4}A_{1y,1} + \tfrac{1}{2}A_{1y,2}\\
A_{12} &= -\tfrac{1}{4}\mathsf{A}_3 + \tfrac{3}{4}A_{1x,1} - \tfrac{1}{2}A_{1x,2} & A_{21} &= -\tfrac{1}{4}\mathsf{A}_4 + \tfrac{3}{4}A_{1y,1} - \tfrac{1}{2}A_{1y,2}\\
A_{26} &= -\tfrac{1}{4}\mathsf{A}_3 - \tfrac{1}{4}A_{1x,1} + \tfrac{1}{2}A_{1x,2} & A_{16} &= -\tfrac{1}{4}\mathsf{A}_4 - \tfrac{1}{4}A_{1y,1} + \tfrac{1}{2}A_{1y,2}
\end{aligned}$$

$$A_{14} = \tfrac{1}{2}(\mathsf{A}_1 + A_{2x,2}) \quad A_{31} = \tfrac{1}{2}(\mathsf{A}_{2,1} - A_{2y,1}) \quad A_{15} = \tfrac{1}{2}(\mathsf{A}_{2,2} - A_{2y,2})$$
$$A_{25} = \tfrac{1}{2}(-\mathsf{A}_1 + A_{2x,2}) \quad A_{32} = \tfrac{1}{2}(\mathsf{A}_{2,1} + A_{2y,1}) \quad A_{24} = \tfrac{1}{2}(\mathsf{A}_{2,2} + A_{2y,2})$$

$$A_{33} = \mathsf{A}_{2,3} \quad A_{36} = \tfrac{1}{2}A_{2x,1} \quad A_{13} = A_{1x,3} \quad A_{23} = A_{1y,3} \quad A_{35} = A_{1x,4} \quad A_{34} = A_{1y,4}$$

$$\begin{aligned}
s_{11} &= \tfrac{1}{8}\mathsf{s}_{1,1} + \tfrac{1}{4}\mathsf{s}_{1,2} + \tfrac{1}{2}s_{2x,1} + \tfrac{1}{8}s_{2x,2}\\
s_{22} &= \tfrac{1}{8}\mathsf{s}_{1,1} + \tfrac{1}{4}\mathsf{s}_{1,2} - \tfrac{1}{2}s_{2x,1} + \tfrac{1}{8}s_{2x,2}\\
s_{12} &= \tfrac{3}{8}\mathsf{s}_{1,1} - \tfrac{1}{4}\mathsf{s}_{1,2} - \tfrac{1}{8}s_{2x,2}\\
s_{66} &= -\tfrac{1}{8}\mathsf{s}_{1,1} + \tfrac{1}{4}\mathsf{s}_{1,2} - \tfrac{1}{8}s_{2x,2}
\end{aligned}$$

$$\begin{aligned}
s_{14} &= \tfrac{1}{4}\mathsf{s}_3 + \tfrac{1}{4}s_{1x,1} + \tfrac{1}{2}s_{1x,2} & s_{15} &= \tfrac{1}{4}\mathsf{s}_4 - \tfrac{3}{4}s_{1y,1} + \tfrac{1}{2}s_{1y,2}\\
s_{24} &= -\tfrac{1}{4}\mathsf{s}_3 + \tfrac{3}{4}s_{1x,1} - \tfrac{1}{2}s_{1x,2} & s_{25} &= -\tfrac{1}{4}\mathsf{s}_4 - \tfrac{1}{4}s_{1y,1} - \tfrac{1}{2}s_{1y,2}\\
s_{56} &= \tfrac{1}{4}\mathsf{s}_3 + \tfrac{1}{4}s_{1x,1} - \tfrac{1}{2}s_{1x,2} & s_{46} &= -\tfrac{1}{4}\mathsf{s}_4 - \tfrac{1}{4}s_{1y,1} + \tfrac{1}{2}s_{1y,2}
\end{aligned}$$

$$\begin{aligned}
s_{13} &= \tfrac{1}{2}(\mathsf{s}_{1,3} + s_{2x,3}) & s_{23} &= \tfrac{1}{2}(\mathsf{s}_{1,3} - s_{2x,3})\\
s_{44} &= \tfrac{1}{2}(\mathsf{s}_{1,4} + s_{2x,4}) & s_{55} &= \tfrac{1}{2}(\mathsf{s}_{1,4} - s_{2x,4})\\
s_{16} &= \tfrac{1}{4}s_{2y,1} - \tfrac{1}{8}s_{2y,2} & s_{26} &= \tfrac{1}{4}s_{2y,1} + \tfrac{1}{8}s_{2y,2}
\end{aligned}$$

$$s_{33} = \mathsf{s}_{1,5} \quad s_{34} = s_{1x,3} \quad s_{35} = -s_{1y,3} \quad s_{36} = \tfrac{1}{2}s_{2y,3} \quad s_{45} = -\tfrac{1}{2}s_{2y,4}$$

$$\begin{aligned}
q_{13} &= \tfrac{1}{2}(\mathsf{q}_1 + q_{2x,2}) & q_{16} &= \tfrac{1}{2}(\mathsf{q}_{2,1} - q_{2y,1})\\
q_{23} &= \tfrac{1}{2}(\mathsf{q}_1 - q_{2x,2}) & q_{26} &= -\tfrac{1}{2}(\mathsf{q}_{2,1} + q_{2y,1})
\end{aligned}$$

$$\begin{aligned}
q_{14} &= \tfrac{1}{4}\mathsf{q}_3 + \tfrac{1}{4}q_{1x,2} + \tfrac{1}{2}q_{1x,3} & q_{15} &= \tfrac{1}{4}\mathsf{q}_4 - \tfrac{3}{4}q_{1y,2} + \tfrac{1}{2}q_{1y,3}\\
q_{24} &= -\tfrac{1}{4}\mathsf{q}_3 + \tfrac{3}{4}q_{1x,2} - \tfrac{1}{2}q_{1x,3} & q_{25} &= -\tfrac{1}{4}\mathsf{q}_4 - \tfrac{1}{4}q_{1y,2} - \tfrac{1}{2}q_{1y,3}\\
q_{56} &= -\tfrac{1}{4}\mathsf{q}_3 - \tfrac{1}{4}q_{1x,2} + \tfrac{1}{2}q_{1x,3} & q_{46} &= \tfrac{1}{4}\mathsf{q}_4 + \tfrac{1}{4}q_{1y,2} - \tfrac{1}{2}q_{1y,3}
\end{aligned}$$

$$q_{45} = \mathsf{q}_{2,2} \quad q_{34} = q_{1x,1} \quad q_{35} = -q_{1y,1} \quad q_{12} = q_{2x,1} \quad q_{36} = -\tfrac{1}{2}q_{2y,2}$$

Group 23 - (T)

Labelling of Covariants

$$\mathsf{u}_o = u_1 + u_2 + u_3 \quad \mathbf{u}^{(3)} = (u_{3x}, u_{3y}) = [u_3 - \tfrac{1}{2}(u_1 + u_2), \tfrac{\sqrt{3}}{2}(u_1 - u_2)]$$
$$\mathbf{u}^{(1)} = (u_{1x}, u_{1y}, u_{1z}) = (u_4, u_5, u_6)$$

$$\mathsf{A}_1 = A_{14} + A_{25} + A_{36} \qquad \mathbf{A}^{(3)} = (A_{3x}, A_{3y}) = [\tfrac{\sqrt{3}}{2}(A_{14} - A_{25}), \tfrac{1}{2}(A_{14} + A_{25}) - A_{36}]$$

$$\mathbf{A}_1^{(1)} = (A_{1x,1}, A_{1y,1}, A_{1z,1}) = (A_{13}, A_{21}, A_{32})$$
$$\mathbf{A}_2^{(1)} = (A_{1x,2}, A_{1y,2}, A_{1z,2}) = (A_{35}, A_{16}, A_{24})$$
$$\mathbf{A}_3^{(1)} = (A_{1x,3}, A_{1y,3}, A_{1z,3}) = (A_{11}, A_{22}, A_{33})$$
$$\mathbf{A}_4^{(1)} = (A_{1x,4}, A_{1y,4}, A_{1z,4}) = (A_{12}, A_{23}, A_{31})$$
$$\mathbf{A}_5^{(1)} = (A_{1x,5}, A_{1y,5}, A_{1z,5}) = (A_{26}, A_{34}, A_{15})$$

$$\mathsf{s}_{1,1} = s_{11} + s_{22} + s_{33} \qquad \mathbf{s}_1^{(3)} = (s_{3x,1}, s_{3y,1}) = [s_{33} - \tfrac{1}{2}(s_{11} + s_{22}), \tfrac{\sqrt{3}}{2}(s_{11} - s_{22})]$$
$$\mathsf{s}_{1,2} = s_{23} + s_{13} + s_{12} \qquad \mathbf{s}_2^{(3)} = (s_{3x,2}, s_{3y,2}) = [s_{12} - \tfrac{1}{2}(s_{23} + s_{13}), \tfrac{\sqrt{3}}{2}(s_{23} - s_{13})]$$
$$\mathsf{s}_{1,3} = s_{44} + s_{55} + s_{66} \qquad \mathbf{s}_3^{(3)} = (s_{3x,3}, s_{3y,3}) = [s_{66} - \tfrac{1}{2}(s_{44} + s_{55}), \tfrac{\sqrt{3}}{2}(s_{44} - s_{55})]$$

$$\mathbf{s}_1^{(1)} = (s_{1x,1}, s_{1y,1}, s_{1z,1}) = (s_{34}, s_{15}, s_{26})$$
$$\mathbf{s}_2^{(1)} = (s_{1x,2}, s_{1y,2}, s_{1z,2}) = (s_{24}, s_{35}, s_{16})$$
$$\mathbf{s}_3^{(1)} = (s_{1x,3}, s_{1y,3}, s_{1z,3}) = (s_{14}, s_{25}, s_{36})$$
$$\mathbf{s}_4^{(1)} = (s_{1x,4}, s_{1y,4}, s_{1z,4}) = (s_{56}, s_{46}, s_{45})$$

$$\mathsf{q}_1 = q_{23} + q_{31} + q_{12} \qquad \mathbf{q}^{(3)} = (q_{3x}, q_{3y}) = [\tfrac{\sqrt{3}}{2}(q_{23} - q_{31}), \tfrac{1}{2}(q_{23} + q_{31}) - q_{12}]$$

$$\mathbf{q}_1^{(1)} = (q_{1x,1}, q_{1y,1}, q_{1z,1}) = (q_{34}, q_{15}, q_{26})$$
$$\mathbf{q}_2^{(1)} = (q_{1x,2}, q_{1y,2}, q_{1z,2}) = (q_{24}, q_{35}, q_{16})$$
$$\mathbf{q}_3^{(1)} = (q_{1x,3}, q_{1y,3}, q_{1z,3}) = (q_{14}, q_{25}, q_{36})$$
$$\mathbf{q}_4^{(1)} = (q_{1x,4}, q_{1y,4}, q_{1z,4}) = (q_{56}, q_{64}, q_{45})$$

Conversion Equations:

$$u_1 = \tfrac{1}{3}\mathsf{u}_o - \tfrac{1}{3}u_{3x} + \tfrac{1}{\sqrt{3}}u_{3y} \qquad u_2 = \tfrac{1}{3}\mathsf{u}_o - \tfrac{1}{3}u_{3x} - \tfrac{1}{\sqrt{3}}u_{3y} \qquad u_3 = \tfrac{1}{3}\mathsf{u}_o + \tfrac{2}{3}u_{3x}$$
$$u_4 = u_{1x} \qquad u_5 = u_{1y} \qquad u_6 = u_{1z}$$

$$A_{14} = \tfrac{1}{3}\mathsf{A}_1 + \tfrac{1}{\sqrt{3}}A_{3x} + \tfrac{1}{3}A_{3y} \qquad A_{25} = \tfrac{1}{3}\mathsf{A}_1 - \tfrac{1}{\sqrt{3}}A_{3x} + \tfrac{1}{3}A_{3y} \qquad A_{36} = \tfrac{1}{3}\mathsf{A}_1 - \tfrac{2}{3}A_{3y}$$
$$A_{13} = A_{1x,1} \qquad A_{21} = A_{1y,1} \qquad A_{32} = A_{1z,1}$$
$$A_{35} = A_{1x,2} \qquad A_{16} = A_{1y,2} \qquad A_{24} = A_{1z,2}$$
$$A_{11} = A_{1x,3} \qquad A_{22} = A_{1y,3} \qquad A_{33} = A_{1z,3}$$
$$A_{12} = A_{1x,4} \qquad A_{23} = A_{1y,4} \qquad A_{31} = A_{1z,4}$$
$$A_{26} = A_{1x,5} \qquad A_{34} = A_{1y,5} \qquad A_{15} = A_{1z,5}$$

$$s_{11} = \tfrac{1}{3}\mathsf{s}_{1,1} - \tfrac{1}{3}s_{3x,1} + \tfrac{1}{\sqrt{3}}s_{3y,1} \qquad s_{22} = \tfrac{1}{3}\mathsf{s}_{1,1} - \tfrac{1}{3}s_{3x,1} - \tfrac{1}{\sqrt{3}}s_{3y,1} \qquad s_{33} = \tfrac{1}{3}\mathsf{s}_{1,1} + \tfrac{2}{3}s_{3x,1}$$
$$s_{23} = \tfrac{1}{3}\mathsf{s}_{1,2} - \tfrac{1}{3}s_{3x,2} + \tfrac{1}{\sqrt{3}}s_{3y,2} \qquad s_{13} = \tfrac{1}{3}\mathsf{s}_{1,2} - \tfrac{1}{3}s_{3x,2} - \tfrac{1}{\sqrt{3}}s_{3y,2} \qquad s_{12} = \tfrac{1}{3}\mathsf{s}_{1,2} + \tfrac{2}{3}s_{3x,2}$$
$$s_{44} = \tfrac{1}{3}\mathsf{s}_{1,3} - \tfrac{1}{3}s_{3x,3} + \tfrac{1}{\sqrt{3}}s_{3y,3} \qquad s_{55} = \tfrac{1}{3}\mathsf{s}_{1,3} - \tfrac{1}{3}s_{3x,3} - \tfrac{1}{\sqrt{3}}s_{3y,3} \qquad s_{66} = \tfrac{1}{3}\mathsf{s}_{1,3} + \tfrac{2}{3}s_{3x,3}$$

$$s_{34} = s_{1x,1} \qquad s_{15} = s_{1y,1} \qquad s_{26} = s_{1z,1}$$
$$s_{24} = s_{1x,2} \qquad s_{35} = s_{1y,2} \qquad s_{16} = s_{1z,2}$$
$$s_{14} = s_{1x,3} \qquad s_{25} = s_{1y,3} \qquad s_{36} = s_{1z,3}$$
$$s_{56} = s_{1x,4} \qquad s_{46} = s_{1y,4} \qquad s_{45} = s_{1z,4}$$

$$q_{23} = \tfrac{1}{3}\mathsf{q}_1 + \tfrac{1}{\sqrt{3}}q_{3x} + \tfrac{1}{3}q_{3y} \qquad q_{31} = \tfrac{1}{3}\mathsf{q}_1 - \tfrac{1}{\sqrt{3}}q_{3x} + \tfrac{1}{3}q_{3y} \qquad q_{12} = \tfrac{1}{3}\mathsf{q}_1 - \tfrac{2}{3}q_{3y}$$
$$q_{34} = q_{1x,1} \qquad q_{15} = q_{1y,1} \qquad q_{26} = q_{1z,1}$$
$$q_{24} = q_{1x,2} \qquad q_{35} = q_{1y,2} \qquad q_{46} = q_{1z,2}$$
$$q_{14} = q_{1x,3} \qquad q_{25} = q_{1y,3} \qquad q_{36} = q_{1z,3}$$
$$q_{56} = q_{1x,4} \qquad q_{64} = q_{1y,4} \qquad q_{45} = q_{1z,4}$$

Group 432 - (O)

Labelling of Covariants

$$\mathsf{u}_o = u_1 + u_2 + u_3 \quad \mathbf{u}^{(3)} = (u_{3x}, u_{3y}) = [u_3 - \tfrac{1}{2}(u_1 + u_2), \tfrac{\sqrt{3}}{2}(u_1 - u_2)]$$
$$\mathbf{u}^{(2)} = (u_{2x}, u_{2y}, u_{2z}) = (u_4, u_5, u_6)$$

$$\mathsf{A}_2 = A_{14} + A_{25} + A_{36} \qquad \mathbf{A}^{(3)} = (A_{3x}, A_{3y}) = [\tfrac{\sqrt{3}}{2}(A_{14} - A_{25}), \tfrac{1}{2}(A_{14} + A_{25}) - A_{36}]$$

$$\mathbf{A}_1^{(1)} = (A_{1x,1}, A_{1y,1}, A_{1z,1}) = (A_{13} + A_{12}, A_{21} + A_{23}, A_{32} + A_{31})$$
$$\mathbf{A}_1^{(2)} = (A_{1x,2}, A_{1y,2}, A_{1z,2}) = (A_{35} + A_{26}, A_{16} + A_{34}, A_{24} + A_{15})$$
$$\mathbf{A}_1^{(3)} = (A_{1x,3}, A_{1y,3}, A_{1z,3}) = (A_{11}, A_{22}, A_{33})$$

$$\mathbf{A}_2^{(1)} = (A_{2x,1}, A_{2y,1}, A_{2z,1}) = (A_{13} - A_{12}, A_{21} - A_{23}, A_{32} - A_{31})$$
$$\mathbf{A}_2^{(2)} = (A_{2x,2}, A_{2y,2}, A_{2z,2}) = (A_{36} - A_{26}, A_{16} - A_{34}, A_{24} - A_{15})$$

$$\mathsf{s}_{1,1} = s_{11} + s_{22} + s_{33} \qquad \mathbf{s}_1^{(3)} = (s_{3x,1}, s_{3y,1}) = [s_{33} - \tfrac{1}{2}(s_{11} + s_{22}), \tfrac{\sqrt{3}}{2}(s_{11} - s_{22})]$$
$$\mathsf{s}_{1,2} = s_{23} + s_{13} + s_{12} \qquad \mathbf{s}_2^{(3)} = (s_{3x,2}, s_{3y,2}) = [s_{12} - \tfrac{1}{2}(s_{23} + s_{13}), \tfrac{\sqrt{3}}{2}(s_{23} - s_{13})]$$
$$\mathsf{s}_{1,3} = s_{44} + s_{55} + s_{66} \qquad \mathbf{s}_3^{(3)} = (s_{3x,3}, s_{3y,3}) = [s_{66} - \tfrac{1}{2}(s_{44} + s_{55}), \tfrac{\sqrt{3}}{2}(s_{44} - s_{55})]$$

$$\mathbf{s}_1^{(1)} = (s_{1x,1}, s_{1y,1}, s_{1z,1}) = (s_{34} - s_{24}, s_{15} - s_{35}, s_{26} - s_{16})$$

$$\mathbf{s}_1^{(2)} = (s_{1x,2}, s_{1y,2}, s_{1z,2}) = (s_{34} + s_{24}, s_{15} + s_{35}, s_{26} + s_{16})$$
$$\mathbf{s}_2^{(2)} = (s_{1x,3}, s_{1y,3}, s_{1z,3}) = (s_{14}, s_{25}, s_{36})$$
$$\mathbf{s}_3^{(2)} = (s_{1x,4}, s_{1y,4}, s_{1z,4}) = (s_{56}, s_{46}, s_{45})$$

$$\mathsf{q}_2 = q_{23} + q_{31} + q_{12} \qquad \mathbf{q}^{(3)} = (q_{3x}, q_{3y}) = [\tfrac{\sqrt{3}}{2}(q_{23} - q_{31}), \tfrac{1}{2}(q_{23} + q_{31}) - q_{12}]$$

$$\mathbf{q}_1^{(1)} = (q_{1x,1}, q_{1y,1}, q_{1z,1}) = (q_{34} - q_{24}, q_{15} - q_{35}, q_{26} - q_{26})$$
$$\mathbf{q}_2^{(1)} = (q_{1x,2}, q_{1y,2}, q_{1z,2}) = (q_{56}, q_{64}, q_{45})$$

$$\mathbf{q}_1^{(2)} = (q_{2x,1}, q_{2y,1}, q_{2z,1}) = (q_{34} + q_{24}, q_{15} + q_{35}, q_{26} + q_{16})$$
$$\mathbf{q}_2^{(2)} = (q_{2x,2}, q_{2y,2}, q_{2z,2}) = (q_{14}, q_{25}, q_{36})$$

Conversion Equations:

$u_1 = \frac{1}{3}\mathsf{u}_o - \frac{1}{3}u_{3x} + \frac{1}{\sqrt{3}}u_{3y}$ $\quad u_2 = \frac{1}{3}\mathsf{u}_o - \frac{1}{3}u_{3x} - \frac{1}{\sqrt{3}}u_{3y}$ $\quad u_3 = \frac{1}{3}\mathsf{u}_o + \frac{2}{3}u_{3x}$

$u_4 = u_{2x}$ $\quad u_5 = u_{2y}$ $\quad u_6 = u_{2z}$

$A_{14} = \frac{1}{3}\mathsf{A}_2 + \frac{1}{\sqrt{3}}A_{3x} + \frac{1}{3}A_{3y}$ $\quad A_{25} = \frac{1}{3}\mathsf{A}_2 - \frac{1}{\sqrt{3}}A_{3x} + \frac{1}{3}A_{3y}$ $\quad A_{36} = \frac{1}{3}\mathsf{A}_2 - \frac{2}{3}A_{3y}$

$A_{13} = \frac{1}{2}(A_{1x,1} + A_{2x,1})$ $\quad A_{21} = \frac{1}{2}(A_{1y,1} + A_{2y,1})$ $\quad A_{32} = \frac{1}{2}(A_{1z,1} + A_{2z,1})$

$A_{12} = \frac{1}{2}(A_{1x,1} - A_{2x,1})$ $\quad A_{23} = \frac{1}{2}(A_{1y,1} - A_{2y,1})$ $\quad A_{31} = \frac{1}{2}(A_{1z,1} - A_{2z,1})$

$A_{35} = \frac{1}{2}(A_{1x,2} + A_{2x,2})$ $\quad A_{16} = \frac{1}{2}(A_{1y,2} + A_{2y,2})$ $\quad A_{24} = \frac{1}{2}(A_{1z,2} + A_{2z,2})$

$A_{26} = \frac{1}{2}(A_{1x,2} - A_{2x,2})$ $\quad A_{34} = \frac{1}{2}(A_{1y,2} - A_{2y,2})$ $\quad A_{15} = \frac{1}{2}(A_{1z,2} - A_{2z,2})$

$A_{11} = A_{1x,3}$ $\quad A_{22} = A_{1y,3}$ $\quad A_{33} = A_{1z,3}$

$s_{11} = \frac{1}{3}\mathsf{s}_{1,1} - \frac{1}{3}s_{3x,1} + \frac{1}{\sqrt{3}}s_{3y,1}$ $\quad s_{22} = \frac{1}{3}\mathsf{s}_{1,1} - \frac{1}{3}s_{3x,1} - \frac{1}{\sqrt{3}}s_{3y,1}$ $\quad s_{33} = \frac{1}{3}\mathsf{s}_{1,1} + \frac{2}{3}s_{3x,1}$

$s_{23} = \frac{1}{3}\mathsf{s}_{1,2} - \frac{1}{3}s_{3x,2} + \frac{1}{\sqrt{3}}s_{3y,2}$ $\quad s_{13} = \frac{1}{3}\mathsf{s}_{1,2} - \frac{1}{3}s_{3x,2} - \frac{1}{\sqrt{3}}s_{3y,2}$ $\quad s_{12} = \frac{1}{3}\mathsf{s}_{1,2} + \frac{2}{3}s_{3x,2}$

$s_{44} = \frac{1}{3}\mathsf{s}_{1,3} - \frac{1}{3}s_{3x,3} + \frac{1}{\sqrt{3}}s_{3y,3}$ $\quad s_{55} = \frac{1}{3}\mathsf{s}_{1,3} - \frac{1}{3}s_{3x,3} - \frac{1}{\sqrt{3}}s_{3y,3}$ $\quad s_{66} = \frac{1}{3}\mathsf{s}_{1,3} + \frac{2}{3}s_{3x,3}$

$s_{34} = \frac{1}{2}(s_{1x,1} + s_{2x,1})$ $\quad s_{15} = \frac{1}{2}(s_{1y,1} + s_{2y,1})$ $\quad s_{26} = \frac{1}{2}(s_{1z,1} + s_{2z,1})$

$s_{24} = \frac{1}{2}(-s_{1x,1} + s_{2x,1})$ $\quad s_{35} = \frac{1}{2}(-s_{1y,1} + s_{2y,1})$ $\quad s_{16} = \frac{1}{2}(-s_{1z,1} + s_{2z,1})$

$s_{14} = s_{2x,2}$ $\quad s_{25} = s_{2y,2}$ $\quad s_{36} = s_{2z,2}$

$s_{56} = s_{2x,3}$ $\quad s_{46} = s_{2y,3}$ $\quad s_{45} = s_{2z,3}$

$q_{23} = \frac{1}{3}\mathsf{q}_2 + \frac{1}{\sqrt{3}}q_{3x} + \frac{1}{3}q_{3y}$ $\quad q_{31} = \frac{1}{3}\mathsf{q}_2 - \frac{1}{\sqrt{3}}q_{3x} + \frac{1}{3}q_{3y}$ $\quad q_{12} = \frac{1}{3}\mathsf{q}_2 - \frac{2}{3}q_{3y}$

$q_{34} = \frac{1}{2}(q_{1x,1} + q_{2x,1})$ $\quad q_{15} = \frac{1}{2}(q_{1y,1} + q_{2y,1})$ $\quad q_{26} = \frac{1}{2}(q_{1z,1} + q_{2z,1})$

$q_{24} = \frac{1}{2}(-q_{1x,1} + q_{2x,1})$ $\quad q_{35} = \frac{1}{2}(-q_{1y,1} + q_{2y,1})$ $\quad q_{46} = \frac{1}{2}(-q_{1z,1} + q_{2z,1})$

$q_{14} = q_{1x,2}$ $\quad q_{25} = q_{1y,2}$ $\quad q_{36} = q_{1z,2}$

$q_{56} = q_{2x,2}$ $\quad q_{64} = q_{2y,2}$ $\quad q_{45} = q_{2z,2}$

Appendix F: List of symmetry descents

Parent symmetry	Ferroic symmetry	Type of descent	Exomorphic type
Triclinic parent group			
$\overline{1}\ (C_i) \Downarrow$	$1\ (C_1)$	A0	1. $C_2 \Downarrow C_1$
Monoclinic parent group			
$2_z\ (C_{2z}) \Downarrow$	$1\ (C_1)$	A0	1. $C_2 \Downarrow C_1$
$m_z\ (C_{sz}) \Downarrow$	$1\ (C_1)$	A0	1. $C_2 \Downarrow C_1$
$2_z/m_z\ (C_{2hz}) \Downarrow$	$\overline{1}\ (C_i)$	A0	1. $C_2 \Downarrow C_1$
	$2_z\ (C_{2z})$	A0	1. $C_2 \Downarrow C_1$
	$m_z\ (C_{sz})$	A0	1. $C_2 \Downarrow C_1$
	$1\ (C_1)$	A2	5. $D_2 \Downarrow C_1$
Orthorhombic parent group			
$2_x2_y2_z\ (D_2) \Downarrow$	$2_z\ (C_{2z})$	A0	1. $C_2 \Downarrow C_1$
	$2_x\ (C_{2x})$	A0	1. $C_2 \Downarrow C_1$
	$2_y\ (C_{2y})$	A0	1. $C_2 \Downarrow C_1$
	$1\ (C_1)$	A2	5. $D_2 \Downarrow C_1$
$m_xm_y2_z\ (C_{2vz}) \Downarrow$	$2_z\ (C_{2z})$	A0	1. $C_2 \Downarrow C_1$
	$m_x\ (C_{sx})$	A0	1. $C_2 \Downarrow C_1$
	$m_y\ (C_{sy})$	A0	1. $C_2 \Downarrow C_1$
	$1\ (C_1)$	A2	5. $D_2 \Downarrow C_1$
$m_xm_ym_z\ (D_{2h}) \Downarrow$	$2_z/m_z\ (C_{2hz})$	A0	1. $C_2 \Downarrow C_1$
	$2_x/m_x\ (C_{2hx})$	A0	1. $C_2 \Downarrow C_1$
	$2_y/m_y\ (C_{2hy})$	A0	1. $C_2 \Downarrow C_1$
	$2_x2_y2_z\ (D_2)$	A0	1. $C_2 \Downarrow C_1$
	$m_xm_y2_z\ (C_{2vz})$	A0	1. $C_2 \Downarrow C_1$
	$2_xm_ym_z\ (C_{2vx})$	A0	1. $C_2 \Downarrow C_1$
	$m_x2_ym_z\ (C_{2vy})$	A0	1. $C_2 \Downarrow C_1$
	$\overline{1}\ (C_i)$	A2	5. $D_2 \Downarrow C_1$
	$2_z\ (C_{2z})$	A2	5. $D_2 \Downarrow C_1$
	$2_x\ (C_{2x})$	A2	5. $D_2 \Downarrow C_1$
	$2_y\ (C_{2y})$	A2	5. $D_2 \Downarrow C_1$
	$m_z\ (C_{sz})$	A2	5. $D_2 \Downarrow C_1$
	$m_x\ (C_{sx})$	A2	5. $D_2 \Downarrow C_1$
	$m_y\ (C_{sy})$	A2	5. $D_2 \Downarrow C_1$
	$1\ (C_1)$	A2	11. $D_{2h} \Downarrow C_1$

Parent symmetry	Ferroic symmetry	Type of descent	Exomorphic type
Tetragonal parent group			
$4_z\ (C_{4z}) \Downarrow$	$2_z\ (C_{2z})$	A0	1. $C_2 \Downarrow C_1$
	$1\ (C_1)$	A1b	3. $C_4 \Downarrow C_1$
$\overline{4}_z\ (S_{4z}) \Downarrow$	$2_z\ (C_{2z})$	A0	1. $C_2 \Downarrow C_1$
	$1\ (C_1)$	A1b	3. $C_4 \Downarrow C_1$
$4_z/m_z\ (C_{4hz}) \Downarrow$	$2_z/m_z\ (C_{2hz})$	A0	1. $C_2 \Downarrow C_1$
	$4_z\ (C_{4z})$	A0	1. $C_2 \Downarrow C_1$
	$\overline{4}_z\ (S_{4z})$	A0	1. $C_2 \Downarrow C_1$
	$2_z\ (C_{2z})$	A2	5. $D_2 \Downarrow C_1$
	$\overline{1}\ (C_i)$	A1b	3. $C_4 \Downarrow C_1$
	$m_z\ (C_{sz})$	A1b	3. $C_4 \Downarrow C_1$
	$1\ (C_1)$	A2	12. $C_{4h} \Downarrow C_1$
$4_z2_x2_{xy}\ (D_{4z}) \Downarrow$	$4_z\ (C_{4z})$	A0	1. $C_2 \Downarrow C_1$
	$2_x2_y2_z\ (D_2)$	A0	1. $C_2 \Downarrow C_1$
	$2_{x\overline{y}}2_{xy}2_z\ (\widehat{D}_{2z})$	A0	1. $C_2 \Downarrow C_1$
	$2_z\ (C_{2z})$	A2	5. $D_2 \Downarrow C_1$
	$2_x, 2_y\ (C_{2x}, C_{2y})$	B1b	7b. $D_4 \Downarrow C_{2i}$
	$2_{xy}, 2_{x\overline{y}}\ (C_{2xy}, C_{2x\overline{y}})$	B1b	7b. $D_4 \Downarrow C_{2i}$
	$1\ (C_1)$	A1b	7a. $D_4 \Downarrow C_1$
$4_zm_xm_{xy}\ (C_{4vz}) \Downarrow$	$4_z\ (C_{4z})$	A0	1. $C_2 \Downarrow C_1$
	$m_xm_y2_z\ (C_{2vz})$	A0	1. $C_2 \Downarrow C_1$
	$m_{x\overline{y}}m_{xy}2_z\ (\widehat{C}_{2vz})$	A0	1. $C_2 \Downarrow C_1$
	$2_z\ (C_{2z})$	A2	5. $D_2 \Downarrow C_1$
	$m_x, m_y\ (C_{sx}, C_{sy})$	B1b	7b. $D_4 \Downarrow C_{2i}$
	$m_{xy}, m_{x\overline{y}}\ (C_{sxy}, C_{sx\overline{y}})$	B1b	7b. $D_4 \Downarrow C_{2i}$
	$1\ (C_1)$	A1b	7a. $D_4 \Downarrow C_1$
$\overline{4}_z2_xm_{xy}\ (D_{2dz}) \Downarrow$	$\overline{4}_z\ (S_{4z})$	A0	1. $C_2 \Downarrow C_1$
	$2_x2_y2_z\ (D_2)$	A0	1. $C_2 \Downarrow C_1$
	$m_{x\overline{y}}m_{xy}2_z\ (\widehat{C}_{2vz})$	A0	1. $C_2 \Downarrow C_1$
	$2_z\ (C_{2z})$	A2	5. $D_2 \Downarrow C_1$
	$2_x, 2_y\ (C_{2x}, C_{2y})$	B1b	7b. $D_4 \Downarrow C_{2i}$
	$m_{xy}, m_{x\overline{y}}\ (C_{sxy}, C_{sx\overline{y}})$	B1b	7b. $D_4 \Downarrow C_{2i}$
	$1\ (C_1)$	A1b	7a. $D_4 \Downarrow C_1$
$\overline{4}_zm_x2_{xy}\ (\widehat{D}_{2dz}) \Downarrow$	$\overline{4}_z\ (S_{4z})$	A0	1. $C_2 \Downarrow C_1$
	$m_xm_y2_z\ (C_{2vz})$	A0	1. $C_2 \Downarrow C_1$
	$2_{x\overline{y}}2_{xy}2_z\ (\widehat{D}_{2z})$	A0	1. $C_2 \Downarrow C_1$
	$2_z\ (C_{2z})$	A2	5. $D_2 \Downarrow C_1$
	$m_x, m_y\ (C_{sx}, C_{sy})$	B1b	7b. $D_4 \Downarrow C_{2i}$
	$2_{xy}, 2_{x\overline{y}}\ (C_{2xy}, C_{2x\overline{y}})$	B1b	7b. $D_4 \Downarrow C_{2i}$
	$1\ (C_1)$	A1b	7a. $D_4 \Downarrow C_1$

Parent symmetry	Ferroic symmetry	Type of descent	Exomorphic type
Tetragonal parent group			
$4_z/m_z m_x m_{xy}$ $(D_{4hz}) \Downarrow$			
	$4_z/m_z$ (C_{4hz})	A0	1. $C_2 \Downarrow C_1$
	$m_x m_y m_z$ (D_{2h})	A0	1. $C_2 \Downarrow C_1$
	$m_{x\overline{y}} m_{xy} m_z$ $(\widehat{D}_{2hz})$	A0	1. $C_2 \Downarrow C_1$
	$4_z 2_x 2_{xy}$ (D_{4z})	A0	1. $C_2 \Downarrow C_1$
	$4_z m_x m_{xy}$ (C_{4vz})	A0	1. $C_2 \Downarrow C_1$
	$\overline{4}_z 2_x m_{xy}$ (D_{2dz})	A0	1. $C_2 \Downarrow C_1$
	$\overline{4}_z m_x 2_{xy}$ $(\widehat{D}_{2dz})$	A0	1. $C_2 \Downarrow C_1$
	$2_z/m_z$ (C_{2hz})	A2	5. $D_2 \Downarrow C_1$
	4_z (C_{4z})	A2	5. $D_2 \Downarrow C_1$
	$2_x 2_y 2_z$ (D_2)	A2	5. $D_2 \Downarrow C_1$
	$2_{x\overline{y}} 2_{xy} 2_z$ $(\widehat{D}_{2z})$	A2	5. $D_2 \Downarrow C_1$
	$\overline{4}_z$ (S_{4z})	A2	5. $D_2 \Downarrow C_1$
	$m_x m_y 2_z$ (C_{2vz})	A2	5. $D_2 \Downarrow C_1$
	$m_{x\overline{y}} m_{xy} 2_z$ $(\widehat{C}_{2vz})$	A2	5. $D_2 \Downarrow C_1$
	2_z (C_{2z})	A2	11. $D_{2h} \Downarrow C_1$
	$2_x/m_x, 2_y/m_y$ (C_{2hx}, C_{2hy})	B1b	7b. $D_4 \Downarrow C_{2i}$
	$2_{xy}/m_{xy}, 2_{x\overline{y}}/m_{x\overline{y}}$ $(C_{2hxy}, C_{2hx\overline{y}})$	B1b	7b. $D_4 \Downarrow C_{2i}$
	$\overline{1}$ (C_i)	A1b	7a. $D_4 \Downarrow C_1$
	$2_x m_y m_z, m_x 2_y m_z$ (C_{2vx}, C_{2vy})	B1b	7b. $D_4 \Downarrow C_{2i}$
	$m_{x\overline{y}} 2_{xy} m_z, 2_{x\overline{y}} m_{xy} m_z$ $(C_{2vxy}, C_{2vx\overline{y}})$	B1b	7b. $D_4 \Downarrow C_{2i}$
	m_z (C_{sz})	A1b	7a. $D_4 \Downarrow C_1$
	$2_x, 2_y$ (C_{2x}, C_{2y})	B2	14b. $D_{4h} \Downarrow C_{2i}$
	$2_{xy}, 2_{x\overline{y}}$ $(C_{2xy}, C_{2x\overline{y}})$	B2	14b. $D_{4h} \Downarrow C_{2i}$
	m_x, m_y (C_{sx}, C_{sy})	B2	14b. $D_{4h} \Downarrow C_{2i}$
	$m_{xy}, m_{x\overline{y}}$ $(C_{sxy}, C_{sx\overline{y}})$	B2	14b. $D_{4h} \Downarrow C_{2i}$
	1 (C_1)	A2	14a. $D_{4h} \Downarrow C_1$

Parent symmetry	Ferroic symmetry	Type of descent	Exomorphic type
	Trigonal parent group		
$3_z\ (C_3) \Downarrow$	$1\ (C_1)$	A1a	2. $C_3 \Downarrow C_1$
$\overline{3}_z\ (C_3) \Downarrow$	$3_z\ (C_3)$	A0	1. $C_2 \Downarrow C_1$
	$\overline{1}\ (C_i)$	A1a	2. $C_3 \Downarrow C_1$
	$1\ (C_1)$	A1b	4. $C_6 \Downarrow C_1$
$3_z2_x\ (D_{3x}) \Downarrow$	$3_z\ (C_3)$	A0	1. $C_2 \Downarrow C_1$
	$2_x, 2_{x'}, 2_{x''}\ (C_{2x}, C_{2x'}, C_{2x''})$	B1a	6b. $D_3 \Downarrow C_{2j}$
	$1\ (C_1)$	A1b	6a. $D_3 \Downarrow C_1$
$3_zm_x\ (C_{3vx}) \Downarrow$	$3_z\ (C_3)$	A0	1. $C_2 \Downarrow C_1$
	$m_x, m_{x'}, m_{x''}\ (C_{sx}, C_{sx'}, C_{sx''})$	B1a	6b. $D_3 \Downarrow C_{2j}$
	$1\ (C_1)$	A1b	6a. $D_3 \Downarrow C_1$
$\overline{3}_zm_x\ (D_{3dx}) \Downarrow$	$\overline{3}_z\ (C_{3i})$	A0	1. $C_2 \Downarrow C_1$
	$3_z2_x\ (D_{3x})$	A0	1. $C_2 \Downarrow C_1$
	$3_zm_x\ (C_{3vx})$	A0	1. $C_2 \Downarrow C_1$
	$3_z\ (C_3)$	A2	5. $D_2 \Downarrow C_1$
	$2_x/m_x, 2_{x'}/m_{x'}, 2_{x''}/m_{x''}\ (C_{2hx}, C_{2hx'}, C_{2hx''})$	B1a	6b. $D_3 \Downarrow C_{2j}$
	$\overline{1}\ (C_i)$	A1b	6a. $D_3 \Downarrow C_1$
	$2_x, 2_{x'}, 2_{x''}\ (C_{2x}, C_{2x'}, C_{2x''})$	B1b	8b. $D_6 \Downarrow C_{2j}$
	$m_x, m_{x'}, m_{x''}\ (C_{sx}, C_{sx'}, C_{sx''})$	B1b	8b. $D_6 \Downarrow C_{2j}$
	$1\ (C_1)$	A1b	8a. $D_6 \Downarrow C_1$
$3_z2_y\ (D_{3y}) \Downarrow$	$3_z\ (C_3)$	A0	1. $C_2 \Downarrow C_1$
	$2_y, 2_{y'}, 2_{y''}\ (C_{2y}, C_{2y'}, C_{2y''})$	B1a	6b. $D_3 \Downarrow C_{2j}$
	$1\ (C_1)$	A1b	6a. $D_3 \Downarrow C_1$
$3_zm_y\ (C_{3vy}) \Downarrow$	$3_z\ (C_3)$	A0	1. $C_2 \Downarrow C_1$
	$m_y, m_{y'}, m_{y''}\ (C_{sy}, C_{sy'}, C_{sy''})$	B1a	6b. $D_3 \Downarrow C_{2j}$
	$1\ (C_1)$	A1b	6a. $D_3 \Downarrow C_1$
$\overline{3}_zm_x\ (D_{3dx}) \Downarrow$	$\overline{3}_z\ (C_{3i})$	A0	1. $C_2 \Downarrow C_1$
	$3_z2_y\ (D_{3y})$	A0	1. $C_2 \Downarrow C_1$
	$3_zm_y\ (C_{3vy})$	A0	1. $C_2 \Downarrow C_1$
	$3_z\ (C_3)$	A2	5. $D_2 \Downarrow C_1$
	$2_y/m_y, 2_{y'}/m_{y'}, 2_{y''}/m_{y''}\ (C_{2hy}, C_{2hy'}, C_{2hy''})$	B1a	6b. $D_3 \Downarrow C_{2j}$
	$\overline{1}\ (C_i)$	A1b	6a. $D_3 \Downarrow C_1$
	$2_y, 2_{y'}, 2_{y''}\ (C_{2y}, C_{2y'}, C_{2y''})$	B1b	8b. $D_6 \Downarrow C_{2j}$
	$m_y, m_{y'}, m_{y''}\ (C_{sy}, C_{sy'}, C_{sy''})$	B1b	8b. $D_6 \Downarrow C_{2j}$
	$1\ (C_1)$	A1b	8a. $D_6 \Downarrow C_1$

Parent symmetry	Ferroic symmetry	Type of descent	Exomorphic type
	Hexagonal parent group		
$6_z\ (C_6) \Downarrow$	$3_z\ (C_3)$	A0	1. $C_2 \Downarrow C_1$
	$2_z\ (C_{2z})$	A1a	2. $C_3 \Downarrow C_1$
	$1\ (C_1)$	A1b	4. $C_6 \Downarrow C_1$
$\overline{6}_z\ (C_{3h}) \Downarrow$	$3_z\ (C_3)$	A0	1. $C_2 \Downarrow C_1$
	$m_z\ (C_{sz})$	A1a	2. $C_3 \Downarrow C_1$
	$1\ (C_1)$	A1b	4. $C_6 \Downarrow C_1$
$6_z/m_z\ (C_{6h}) \Downarrow$	$\overline{3}_z\ (C_{3i})$	A0	1. $C_2 \Downarrow C_1$
	$6_z\ (C_6)$	A0	1. $C_2 \Downarrow C_1$
	$\overline{6}_z\ (C_{3h})$	A0	1. $C_2 \Downarrow C_1$
	$3_z\ (C_3)$	A2	5. $D_2 \Downarrow C_1$
	$2_z/m_z\ (C_{2hz})$	A1a	2. $C_3 \Downarrow C_1$
	$\overline{1}\ (C_i)$	A1b	4. $C_6 \Downarrow C_1$
	$2_z\ (C_{2z})$	A1b	4. $C_6 \Downarrow C_1$
	$m_z\ (C_{sz})$	A1b	4. $C_6 \Downarrow C_1$
	$1\ (C_1)$	A2	13. $C_{6h} \Downarrow C_1$
$6_z2_x2_y\ (D_6) \Downarrow$	$6_z\ (C_6)$	A0	1. $C_2 \Downarrow C_1$
	$3_z2_x\ (D_{3x})$	A0	1. $C_2 \Downarrow C_1$
	$3_z2_y\ (D_{3y})$	A0	1. $C_2 \Downarrow C_1$
	$3_z\ (C_3)$	A2	5. $D_2 \Downarrow C_1$
	$2_x2_y2_z, 2_{x'}2_{y'}2_z, 2_{x''}2_{y''}2_z\ (D_2, D_{2'}, D_{2''})$	B1a	6b. $D_3 \Downarrow C_{2j}$
	$2_z\ (C_{2z})$	A1b	6a. $D_3 \Downarrow C_1$
	$2_x, 2_{x'}, 2_{x''}\ (C_{2x}, C_{2x'}, C_{2x''})$	B1b	8b. $D_6 \Downarrow C_{2j}$
	$2_y, 2_{y'}, 2_{y''}\ (C_{2y}, C_{2y'}, C_{2y''})$	B1b	8b. $D_6 \Downarrow C_{2j}$
	$1\ (C_1)$	A1b	8a. $D_6 \Downarrow C_1$
$6_zm_xm_y\ (C_{6v}) \Downarrow$	$6_z\ (C_6)$	A0	1. $C_2 \Downarrow C_1$
	$3_zm_x\ (C_{3vx})$	A0	1. $C_2 \Downarrow C_1$
	$3_zm_y\ (C_{3vy})$	A0	1. $C_2 \Downarrow C_1$
	$3_z\ (C_3)$	A2	5. $D_2 \Downarrow C_1$
	$m_xm_y2_z, m_{x'}m_{y'}2_z, m_{x''}m_{y''}2_z\ (C_{2vz}, C_{2vz'}, C_{2vz''})$	B1a	6b. $D_3 \Downarrow C_{2j}$
	$2_z\ (C_{2z})$	A1b	6a. $D_3 \Downarrow C_1$
	$m_x, m_{x'}, m_{x''}\ (C_{sx}, C_{sx'}, C_{sx''})$	B1b	8b. $D_6 \Downarrow C_{2j}$
	$m_y, m_{y'}, m_{y''}\ (C_{sy}, C_{sy'}, C_{sy''})$	B1b	8b. $D_6 \Downarrow C_{2j}$
	$1\ (C_1)$	A1b	8a. $D_6 \Downarrow C_1$
$\overline{6}_z2_xm_y\ (D_{3h}) \Downarrow$	$\overline{6}_z\ (C_{3h})$	A0	1. $C_2 \Downarrow C_1$
	$3_z2_x\ (D_{3x})$	A0	1. $C_2 \Downarrow C_1$
	$3_zm_y\ (C_{3vy})$	A0	1. $C_2 \Downarrow C_1$
	$3_z\ (C_3)$	A2	5. $D_2 \Downarrow C_1$
	$2_xm_ym_z, 2_{x'}m_{y'}m_z, 2_{x''}m_{y''}m_z\ (C_{2vx}, C_{2vx'}, C_{2vx''})$	B1a	6b. $D_3 \Downarrow C_{2j}$
	$m_z\ (C_{sz})$	A1b	6a. $D_3 \Downarrow C_1$
	$2_x, 2_{x'}, 2_{x''}\ (C_{2x}, C_{2x'}, C_{2x''})$	B1b	8b. $D_6 \Downarrow C_{2j}$
	$m_y, m_{y'}, m_{y''}\ (C_{sy}, C_{sy'}, C_{sy''})$	B1b	8b. $D_6 \Downarrow C_{2j}$
	$1\ (C_1)$	A1b	8a. $D_6 \Downarrow C_1$

Parent symmetry	Ferroic symmetry	Type of descent	Exomorphic type
Hexagonal parent group			
$\overline{6}_z m_x 2_y$ $(\widehat{D}_{3h}) \Downarrow$	$\overline{6}_z$ (C_{3h})	A0	1. $C_2 \Downarrow C_1$
	$3_z m_x$ (C_{3vx})	A0	1. $C_2 \Downarrow C_1$
	$3_z 2_y$ (D_{3y})	A0	1. $C_2 \Downarrow C_1$
	3_z (C_3)	A2	5. $D_2 \Downarrow C_1$
	$m_x 2_y m_z, m_{x'} 2_{y'} m_z, m_{x''} 2_{y''} m_z$ $(C_{2vy}, C_{2vy'}, C_{2vy''})$	B1a	6b. $D_3 \Downarrow C_{2j}$
	m_z (C_{sz})	A1b	6a. $D_3 \Downarrow C_1$
	$m_x, m_{x'}, m_{x''}$ $(C_{sx}, C_{sx'}, C_{sx''})$	B1b	8b. $D_6 \Downarrow C_{2j}$
	$2_y, 2_{y'}, 2_{y''}$ $(C_{2y}, C_{2y'}, C_{2y''})$	B1b	8b. $D_6 \Downarrow C_{2j}$
	1 (C_1)	A1b	8a. $D_6 \Downarrow C_1$
$6_z/m_z m_x m_y$ $(D_{6h}) \Downarrow$			
	$6_z/m_z$ (C_{6h})	A0	1. $C_2 \Downarrow C_1$
	$\overline{3}_z m_x$ (D_{3dx})	A0	1. $C_2 \Downarrow C_1$
	$\overline{3}_z 2_y$ (D_{3dy})	A0	1. $C_2 \Downarrow C_1$
	$6_z 2_x 2_y$ (D_6)	A0	1. $C_2 \Downarrow C_1$
	$6_z m_x m_y$ (C_{6v})	A0	1. $C_2 \Downarrow C_1$
	$\overline{6}_z 2_x m_y$ (D_{3h})	A0	1. $C_2 \Downarrow C_1$
	$\overline{6}_z m_x 2_y$ $(\widehat{D}_{3h})$	A0	1. $C_2 \Downarrow C_1$
	$\overline{3}_z$ (C_{3i})	A2	5. $D_2 \Downarrow C_1$
	6_z (C_6)	A2	5. $D_2 \Downarrow C_1$
	$3_z 2_x$ (D_{3x})	A2	5. $D_2 \Downarrow C_1$
	$3_z 2_y$ (D_{3y})	A2	5. $D_2 \Downarrow C_1$
	$\overline{6}_z$ (C_{3h})	A2	5. $D_2 \Downarrow C_1$
	$3_z m_x$ (C_{3vx})	A2	5. $D_2 \Downarrow C_1$
	$3_z m_y$ (C_{3vy})	A2	5. $D_2 \Downarrow C_1$
	3_z (C_3)	A2	11. $D_{2h} \Downarrow C_1$
	$m_x m_y m_z, m_{x'} m_{y'} m_z, m_{x''} m_{y''} m_z$ $(D_{2h}, D_{2h'}, D_{2h''})$	B1a	6b. $D_3 \Downarrow C_{2j}$
	$2_z/m_z$ (C_{2hz})	A1b	6a. $D_3 \Downarrow C_1$
	$2_x/m_x, 2_{x'}/m_{x'}, 2_{x''}/m_{x''}$ $(C_{2hx}, C_{2hx'}, C_{2hx''})$	B1b	8b. $D_6 \Downarrow C_{2j}$
	$2_y/m_y, 2_{y'}/m_{y'}, 2_{y''}/m_{y''}$ $(C_{2hy}, C_{2hy'}, C_{2hy''})$	B1b	8b. $D_6 \Downarrow C_{2j}$
	$\overline{1}$ (C_i)	A1b	8a. $D_6 \Downarrow C_1$
	$2_x 2_y 2_z, 2_{x'} 2_{y'} 2_z, 2_{x''} 2_{y''} 2_z$ $(D_2, D_{2'}, D_{2''})$	B1b	8b. $D_6 \Downarrow C_{2j}$
	$m_x m_y 2_z, m_{x'} m_{y'} 2_z, m_{x''} m_{y''} 2_z$ $(C_{2vz}, C_{2vz'}, C_{2vz''})$	B1b	8b. $D_6 \Downarrow C_{2j}$
	2_z (C_{2z})	A1b	8a. $D_6 \Downarrow C_1$
	$2_x m_y m_z, 2_{x'} m_{y'} m_z, 2_{x''} m_{y''} m_z$ $(C_{2vx}, C_{2vx'}, C_{2vx''})$	B1b	8b. $D_6 \Downarrow C_{2j}$
	$m_x 2_y m_z, m_{x'} 2_{y'} m_z, m_{x''} 2_{y''} m_z$ $(C_{2vy}, C_{2vy'}, C_{2vy''})$	B1b	8b. $D_6 \Downarrow C_{2j}$
	m_z (C_{sz})	A1b	8a. $D_6 \Downarrow C_1$
	$2_x, 2_{x'}, 2_{x''}$ $(C_{2x}, C_{2x'}, C_{2x''})$	B2	15b. $D_{6h} \Downarrow C_{2j}$
	$2_y, 2_{y'}, 2_{y''}$ $(C_{2y}, C_{2y'}, C_{2y''})$	B2	15b. $D_{6h} \Downarrow C_{2j}$
	$m_x, m_{x'}, m_{x''}$ $(C_{sx}, C_{sx'}, C_{sx''})$	B2	15b. $D_{6h} \Downarrow C_{2j}$
	$m_y, m_{y'}, m_{y''}$ $(C_{sy}, C_{sy'}, C_{sy''})$	B2	15b. $D_{6h} \Downarrow C_{2j}$
	1 (C_1)	A2	15a. $D_{6h} \Downarrow C_1$

Parent symmetry	Ferroic symmetry	Type of descent	Exomorphic type
	Cubic parent group		
23 $(T)\Downarrow$			
	$2_x2_y2_z$ (D_2)	A1a	2. $C_3 \Downarrow C_1$
	$2_z, 2_x, 2_y$ (C_{2z}, C_{2x}, C_{2y})	B1b	9c. $T \Downarrow C_{2i}$
	$3_p, 3_q, 3_r, 3_s$ $(C_{3p}, C_{3q}, C_{3r}, C_{3s})$	B1a	9b. $T \Downarrow C_{3j}$
	1 (C_1)	A1b	9a. $T \Downarrow C_1$
$m\overline{3}$ $(T_h)\Downarrow$			
	23 (T)	A0	1. $C_2 \Downarrow C_1$
	$m_xm_ym_z$ (D_{2h})	A1a	2. $C_3 \Downarrow C_1$
	$2_x2_y2_z$ (D_2)	A1b	4. $C_6 \Downarrow C_1$
	$2_z/m_z, 2_x/m_x, 2_y/m_y$ $(C_{2hz}, C_{2hx}, C_{2hy})$	B1b	9c. $T \Downarrow C_{2i}$
	$\overline{3}_p, \overline{3}_q, \overline{3}_r, \overline{3}_s$ $(C_{3ip}, C_{3iq}, C_{3ir}, C_{3is})$	B1a	9b. $T \Downarrow C_{3j}$
	$\overline{1}$ $(C_i))$	A1b	9a. $T \Downarrow C_1$
	$m_xm_y2_z, 2_xm_ym_z, m_x2_ym_z$ $(C_{2vz}, C_{2vx}, C_{2vy})$	B1b	16c. $T_h \Downarrow C_{2vi}$
	$2_z, 2_x, 2_y$ (C_{2z}, C_{2x}, C_{2y})	B2	16d. $T_h \Downarrow C_{2i}$
	m_z, m_x, m_y (C_{sz}, C_{sx}, C_{sy})	B1b	16e. $T_h \Downarrow C_{si}$
	$3_p, 3_q, 3_r, 3_s$ $(C_{3p}, C_{3q}, C_{3r}, C_{3s})$	B1b	16b. $T_h \Downarrow C_{3j}$
	1 (C_1)	A1b	16a. $T_h \Downarrow C_1$
432 $(O)\Downarrow$			
	23 (T)	A0	1. $C_2 \Downarrow C_1$
	$4_z2_x2_{xy}, 4_x2_y2_{yz}, 4_y2_z2_{zx}$ (D_{4z}, D_{4x}, D_{4y})	B1a	6b. $D_3 \Downarrow C_{2j}$
	$2_x2_y2_z$ (D_2)	A1b	6a. $D_3 \Downarrow C_1$
	$4_z, 4_x, 4_y$ (C_{4z}, C_{4x}, C_{4y})	B1b	10b. $O \Downarrow C_{4i}$
	$2_{x\overline{y}}2_{xy}2_z, 2_{y\overline{z}}2_{yz}2_x, 2_{z\overline{x}}2_{zx}2_y$ $(\widehat{D}_{2z}, \widehat{D}_{2x}, \widehat{D}_{2y})$	B1b	10c. $O \Downarrow \widehat{D}_{2i}$
	$2_z, 2_x, 2_y$ (C_{2z}, C_{2x}, C_{2y})	B2	10f. $O \Downarrow C_{2i}$
	$\begin{cases} 2_{xy}, 2_{yz}, 2_{zx} & (C_{2xy}, C_{2yz}, C_{2zx}) \\ 2_{x\overline{y}}, 2_{y\overline{z}}, 2_{z\overline{x}} & (C_{2x\overline{y}}, C_{2y\overline{z}}, C_{2z\overline{x}}) \end{cases}$	B1c	10g. $O \Downarrow C_{2ij}$
	$3_p2_{x\overline{y}}, 3_q2_{x\overline{y}}, 3_r2_{xy}, 3_s2_{xy}$ $(D_{3p}, D_{3q}, D_{3r}, D_{3s})$	B1a	10d. $O \Downarrow D_{3j}$
	$3_p, 3_q, 3_r, 3_s$ $(C_{3p}, C_{3q}, C_{3r}, C_{3s})$	B1b	10e. $O \Downarrow C_{3j}$
	1 (C_1)	A1c	10a. $O \Downarrow C_1$
$\overline{4}3m$ $(T_d)\Downarrow$			
	23 (T)	A0	1. $C_2 \Downarrow C_1$
	$\overline{4}_z2_xm_{xy}, \overline{4}_x2_ym_{yz}, \overline{4}_y2_zm_{zx}$ $(D_{2dz}, D_{2dx}, D_{2dy})$	B1a	6b. $D_3 \Downarrow C_{2j}$
	$2_x2_y2_z$ (D_2)	A1b	6a. $D_3 \Downarrow C_1$
	$\overline{4}_z, \overline{4}_x, \overline{4}_y$ (S_{4z}, S_{4x}, S_{4y})	B1b	10b. $O \Downarrow C_{4i}$
	$m_{x\overline{y}}m_{xy}2_z, m_{y\overline{z}}m_{yz}2_x, m_{z\overline{x}}m_{zx}2_y$ $(\widehat{C}_{2vz}, \widehat{C}_{2vx}, \widehat{C}_{2vy})$	B1b	10c. $O \Downarrow \widehat{D}_{2i}$
	$2_z, 2_x, 2_y$ (C_{2z}, C_{2x}, C_{2y})	B2	10f. $O \Downarrow C_{2i}$
	$\begin{cases} m_{xy}, m_{yz}, m_{zx} & (C_{sxy}, C_{syz}, C_{szx}) \\ m_{x\overline{y}}, m_{y\overline{z}}, m_{z\overline{x}} & (C_{sx\overline{y}}, C_{sy\overline{z}}, C_{sz\overline{x}}) \end{cases}$	B1c	10g. $O \Downarrow C_{2ij}$
	$3_pm_{x\overline{y}}, 3_qm_{x\overline{y}}, 3_rm_{xy}, 3_sm_{xy}$ $(C_{3vp}, C_{3vq}, C_{3vr}, C_{3vs})$	B1a	10d. $O \Downarrow D_{3j}$
	$3_p, 3_q, 3_r, 3_s$ $(C_{3p}, C_{3q}, C_{3r}, C_{3s})$	B1b	10e. $O \Downarrow C_{3j}$
	1 (C_1)	A1c	10a. $O \Downarrow C_1$

Parent symmetry	Ferroic symmetry	Type of descent	Exomorphic type
	Cubic parent group		
$m\overline{3}m$ $(O_h)\Downarrow$			
	$m\overline{3}$ (T_h)	A0	1. $C_2 \Downarrow C_1$
	432 (O)	A0	1. $C_2 \Downarrow C_1$
	$\overline{4}3m$ (T_d)	A0	1. $C_2 \Downarrow C_1$
	23 (T)	A2	5. $D_2 \Downarrow C_1$
	$4_z/m_z m_x m_{xy}, 4_x/m_x m_y m_{yz}, 4_y/m_y m_z m_{zx}$ $(D_{4hz}, D_{4hx}, D_{4hy})$	B1a	6b. $D_3 \Downarrow C_{2j}$
	$m_x m_y m_z$ (D_{2h})	A1b	6a. $D_3 \Downarrow C_1$
	$4_z/m_z, 4_x/m_x, 4_y/m_y$ $(C_{4hz}, C_{4hx}, C_{4hy})$	B1b	10b. $O \Downarrow C_{4i}$
	$m_{x\overline{y}} m_{xy} m_z, m_{y\overline{z}} m_{yz} m_x, m_{z\overline{x}} m_{zx} m_y$ $(\widehat{D}_{2hz}, \widehat{D}_{2hx}, \widehat{D}_{2hy})$	B1b	10c. $O \Downarrow \widehat{D}_{2i}$
	$2_z/m_z, 2_x/m_x, 2_y/m_y$ $(C_{2hz}, C_{2hx}, C_{2hy})$	B2	10f. $O \Downarrow C_{2i}$
	$\left\{\begin{array}{l} 2_{xy}/m_{xy}, 2_{yz}/m_{yz}, 2_{zx}/m_{zx} \quad (C_{2hxy}, C_{2hyz}, C_{2hzx}) \\ 2_{x\overline{y}}/m_{x\overline{y}}, 2_{y\overline{z}}/m_{y\overline{z}}, 2_{z\overline{x}}/m_{z\overline{x}} \quad (C_{2hx\overline{y}}, C_{2hy\overline{z}}, C_{2hz\overline{x}}) \end{array}\right.$	B1c	10g. $O \Downarrow C_{2ij}$
	$\overline{3}_p m_{x\overline{y}}, \overline{3}_q m_{x\overline{y}}, \overline{3}_r m_{xy}, \overline{3}_s m_{xy}$ $(D_{3dp}, D_{3dq}, D_{3dr}, D_{3ds})$	B1a	10d. $O \Downarrow D_{3j}$
	$\overline{3}_p, \overline{3}_q, \overline{3}_r, \overline{3}_s$ $(C_{3ip}, C_{3iq}, C_{3ir}, C_{3is})$	B1b	10e. $O \Downarrow C_{3j}$
	$\overline{1}$ (C_i)	A1c	10a. $O \Downarrow C_1$
	$4_z 2_x 2_{xy}, 4_x 2_y 2_{yz}, 4_y 2_z 2_{zx}$ (D_{4z}, D_{4x}, D_{4y})	B1b	8b. $D_6 \Downarrow C_{2i}$
	$\overline{4}_z 2_x m_{xy}, \overline{4}_x 2_y m_{yz}, \overline{4}_y 2_z m_{zx}$ $(D_{2dz}, D_{2dx}, D_{2dy})$	B1b	8b. $D_6 \Downarrow C_{2i}$
	$2_x 2_y 2_z$ (D_2)	A1b	8a. $D_6 \Downarrow C_1$
	$4_z m_x m_{xy}, 4_x m_y m_{yz}, 4_y m_z m_{zx}$ $(C_{4vz}, C_{4vx}, C_{4vy})$	B1b	17b. $O_h \Downarrow C_{4vi}$
	$\overline{4}_z m_x 2_{xy}, \overline{4}_x m_y 2_{yz}, \overline{4}_y m_z 2_{zx}$ $(\widehat{D}_{2dz}, \widehat{D}_{2dx}, \widehat{D}_{2dy})$	B1b	17b. $O_h \Downarrow C_{4vi}$
	$4_z, 4_x, 4_y$ (C_{4z}, C_{4x}, C_{4y})	B2	17e. $O_h \Downarrow C_{4i}$
	$2_{x\overline{y}} 2_{xy} 2_z, 2_{y\overline{z}} 2_{yz} 2_x, 2_{z\overline{x}} 2_{zx} 2_y$ $(\widehat{D}_{2z}, \widehat{D}_{2x}, \widehat{D}_{2y})$	B2	17f. $O_h \Downarrow \widehat{C}_{2vi}$
	$\overline{4}_z, \overline{4}_x, \overline{4}_y$ (S_{4z}, S_{4x}, S_{4y})	B2	17e. $O_h \Downarrow C_{4i}$
	$m_{x\overline{y}} m_{xy} 2_z, m_{y\overline{z}} m_{yz} 2_x, m_{z\overline{x}} m_{zx} 2_y$ $(\widehat{C}_{2vz}, \widehat{C}_{2vx}, \widehat{C}_{2vy})$	B2	17f. $O_h \Downarrow \widehat{C}_{2vi}$
	$m_x m_y 2_z, 2_x m_y m_z, m_x 2_y m_z$ $(C_{2vz}, C_{2vx}, C_{2vy})$	B2	17g. $O_h \Downarrow C_{2vi}$
	$2_z, 2_x, 2_y$ (C_{2z}, C_{2x}, C_{2y})	B2	17k. $O_h \Downarrow C_{2i}$
	m_z, m_x, m_y (C_{sz}, C_{sx}, C_{sy})	B1c	17j. $O_h \Downarrow C_{si}$
	$\left\{\begin{array}{l} m_{x\overline{y}} 2_{xy} m_z, m_{y\overline{z}} 2_{yz} m_x, m_{z\overline{x}} 2_{zx} m_y \quad (\widehat{C}_{2vxy}, \widehat{C}_{2vyz}, \widehat{C}_{2vzx}) \\ 2_{x\overline{y}} m_{xy} m_z, 2_{y\overline{z}} m_{yz} m_x, 2_{z\overline{x}} m_{zx} m_y \quad (\widehat{C}_{2vx\overline{y}}, \widehat{C}_{2vy\overline{z}}, \widehat{C}_{2vz\overline{x}}) \end{array}\right.$	B1c	17h. $O_h \Downarrow \widehat{C}_{2vij}$
	$\left\{\begin{array}{l} 2_{xy}, 2_{yz}, 2_{zx} \quad (C_{2xy}, C_{2yz}, C_{2zx}) \\ 2_{x\overline{y}}, 2_{y\overline{z}}, 2_{z\overline{x}} \quad (C_{2x\overline{y}}, C_{2y\overline{z}}, C_{2z\overline{x}}) \end{array}\right.$	B1b	17l. $O_h \Downarrow C_{2ij}$
	$\left\{\begin{array}{l} m_{xy}, m_{yz}, m_{zx} \quad (C_{sxy}, C_{syz}, C_{szx}) \\ m_{x\overline{y}}, m_{y\overline{z}}, m_{z\overline{x}} \quad (C_{sx\overline{y}}, C_{sy\overline{z}}, C_{sz\overline{x}}) \end{array}\right.$	B1b	17l. $O_h \Downarrow C_{2ij}$
	$3_p 2_{x\overline{y}}, 3_q 2_{x\overline{y}}, 3_r 2_{xy}, 3_s 2_{xy}$ $(D_{3p}, D_{3q}, D_{3r}, D_{3s})$	B1b	17c. $O_h \Downarrow D_{3j}$
	$3_p m_{x\overline{y}}, 3_q m_{x\overline{y}}, 3_r m_{xy}, 3_s m_{xy}$ $(C_{3vp}, C_{3vq}, C_{3vr}, C_{3vs})$	B1b	17c. $O_h \Downarrow D_{3j}$
	$3_p, 3_q, 3_r, 3_s$ $(C_{3p}, C_{3q}, C_{3r}, C_{3s})$	B2	17d. $O_h \Downarrow C_{3j}$
	1 (C_1)	A1c	17a. $O_h \Downarrow C_1$

Appendix G: Nonstandard lattice letters

Orthorhombic to Monoclinic:

$$\begin{array}{ll} \widehat{P}_c = P[(\mathbf{a}-\mathbf{b})/2, (\mathbf{a}+\mathbf{b})/2, \mathbf{c}] & \widehat{I}_c = I[(\mathbf{a}-\mathbf{b})/2, (\mathbf{a}+\mathbf{b})/2, \mathbf{c}] \\ \widehat{P}_a = P[\mathbf{a}, (\mathbf{b}-\mathbf{c})/2, (\mathbf{b}+\mathbf{c})/2] & \widehat{I}_a = I[\mathbf{a}, (\mathbf{b}-\mathbf{c})/2, (\mathbf{b}+\mathbf{c})/2] \\ \widehat{P}_b = P[(\mathbf{c}+\mathbf{a})/2, \mathbf{b}, (\mathbf{c}-\mathbf{a})/2] & \widehat{I}_b = I[(\mathbf{c}+\mathbf{a})/2, \mathbf{b}, (\mathbf{c}-\mathbf{a})/2] \end{array}$$

Tetragonal to Orthorhombic:

$$\widehat{C} = C[\mathbf{a}-\mathbf{b}, \mathbf{a}+\mathbf{b}, \mathbf{c}] \qquad \widehat{F} = F[\mathbf{a}-\mathbf{b}, \mathbf{a}+\mathbf{b}, \mathbf{c}]$$

Tetragonal to Monoclinic:

$$\widehat{C} = C[\mathbf{a}-\mathbf{b}, \mathbf{a}+\mathbf{b}, \mathbf{c}]$$

$$\begin{array}{c} \widehat{A} = A[(\mathbf{a}-\mathbf{b}+\mathbf{c})/2, \mathbf{a}+\mathbf{b}, \mathbf{c}] \\ \widehat{B} = B[\mathbf{a}-\mathbf{b}, (\mathbf{a}+\mathbf{b}+\mathbf{c})/2, \mathbf{c}] \end{array}$$

Rhombohedral to Monoclinic:

$$\begin{array}{c} I_1 = I(\mathbf{a}, -\mathbf{c}_o, \mathbf{c}) \\ I_2 = I(\mathbf{b}, -\mathbf{a}_o, \mathbf{c}) \\ I_3 = I(-\mathbf{a}-\mathbf{b}, -\mathbf{b}_o, \mathbf{c}) \end{array}$$

Hexagonal to Orthorhombic and Monoclinic:

$$\begin{array}{c} C_1 = C(\mathbf{a}, 2\mathbf{b}+\mathbf{a}, \mathbf{c}) \\ C_2 = C(\mathbf{b}, -2\mathbf{a}-\mathbf{b}, \mathbf{c}) \\ C_3 = C(-\mathbf{a}-\mathbf{b}, \mathbf{a}-\mathbf{b}, \mathbf{c}) \end{array}$$

Cubic to Tetragonal Groups:

$$P_c = P(\mathbf{a}, \mathbf{b}, \mathbf{c}) \quad P_a = P(\mathbf{b}, \mathbf{c}, \mathbf{a}) \quad P_b = P(\mathbf{c}, \mathbf{a}, \mathbf{b})$$

$$I_c = I(\mathbf{a}, \mathbf{b}, \mathbf{c}) \quad I_a = I(\mathbf{b}, \mathbf{c}, \mathbf{a}) \quad I_b = I(\mathbf{c}, \mathbf{a}, \mathbf{b}).$$

$$\overline{I}_c = I[(\mathbf{a}-\mathbf{b})/2, (\mathbf{a}+\mathbf{b})/2, \mathbf{c}]$$

$$\begin{array}{c} \widehat{I}_a = I[(\mathbf{b}-\mathbf{c})/2, (\mathbf{b}+\mathbf{c})/2, \mathbf{a}] \\ \widehat{I}_b = I[(\mathbf{c}-\mathbf{a})/2, (\mathbf{c}+\mathbf{a})/2, \mathbf{b}]. \end{array}$$

Cubic to Orthorhombic and Monoclinic Groups:

$$\widehat{C}_c = C[\mathbf{a}-\mathbf{b}, \mathbf{a}+\mathbf{b}, \mathbf{c}]$$
$$\widehat{C}_a = C[\mathbf{b}-\mathbf{c}, \mathbf{b}+\mathbf{c}, \mathbf{a}]$$
$$\widehat{C}_b = C[\mathbf{c}-\mathbf{a}, \mathbf{c}+\mathbf{a}, \mathbf{b}].$$

$$\overline{I}_c = I[(\mathbf{a}-\mathbf{b})/2, (\mathbf{a}+\mathbf{b})/2, \mathbf{c}]$$
$$\widehat{I}_a = I[(\mathbf{b}-\mathbf{c})/2, (\mathbf{b}+\mathbf{c})/2, \mathbf{a}]$$
$$\widehat{I}_b = I[(\mathbf{c}-\mathbf{a})/2, (\mathbf{c}+\mathbf{a})/2, \mathbf{b}].$$

$$\widehat{F}_c = F[\mathbf{a}-\mathbf{b}, \mathbf{a}+\mathbf{b}, \mathbf{c}]$$
$$\widehat{F}_a = F[\mathbf{b}-\mathbf{c}, \mathbf{b}+\mathbf{c}, \mathbf{a}]$$
$$\widehat{F}_b = F[\mathbf{c}-\mathbf{a}, \mathbf{c}+\mathbf{a}, \mathbf{b}].$$

$$\widehat{A}_c = A[(\mathbf{a}-\mathbf{b}+\mathbf{c})/2, \mathbf{a}+\mathbf{b}, \mathbf{c}]$$
$$\widehat{B}_c = B[\mathbf{a}-\mathbf{b}, (\mathbf{a}+\mathbf{b}+\mathbf{c})/2, \mathbf{c}]$$

$$\widehat{A}_a = A[(\mathbf{b}-\mathbf{c}+\mathbf{a})/2, \mathbf{b}+\mathbf{c}, \mathbf{a}]$$
$$\widehat{B}_a = B[\mathbf{b}-\mathbf{c}, (\mathbf{b}+\mathbf{c}+\mathbf{a})/2, \mathbf{a}]$$

$$\widehat{A}_b = A[(\mathbf{c}-\mathbf{a}+\mathbf{b})/2, \mathbf{c}+\mathbf{a}, \mathbf{b}]$$
$$\widehat{B}_b = B[\mathbf{c}-\mathbf{a}, (\mathbf{c}+\mathbf{a}+\mathbf{b})/2, \mathbf{b}]$$

Cubic to Trigonal Groups:

$$\begin{aligned} P \Longrightarrow \quad & R_{P,p} = T(\mathbf{a}, \mathbf{b}, \mathbf{c}) \\ & R_{P,q} = T(-\mathbf{a}, -\mathbf{b}, \mathbf{c}) \\ & R_{P,r} = T(\mathbf{a}, -\mathbf{b}, -\mathbf{c}) \\ & R_{P,s} = T(-\mathbf{a}, \mathbf{b}, -\mathbf{c}) \end{aligned}$$

$$\begin{aligned} I \Longrightarrow \quad & R_{I,p} = T[(\mathbf{a}+\mathbf{b}-\mathbf{c})/2, (\mathbf{b}+\mathbf{c}-\mathbf{a})/2, (\mathbf{c}+\mathbf{a}-\mathbf{b})/2] \\ & R_{I,q} = T[(-\mathbf{a}-\mathbf{b}-\mathbf{c})/2, (-\mathbf{b}+\mathbf{c}+\mathbf{a})/2, (\mathbf{c}-\mathbf{a}+\mathbf{b})/2] \\ & R_{I,r} = T[(\mathbf{a}-\mathbf{b}+\mathbf{c})/2, (-\mathbf{b}-\mathbf{c}-\mathbf{a})/2, (-\mathbf{c}+\mathbf{a}+\mathbf{b})/2] \\ & R_{I,s} = T[(-\mathbf{a}+\mathbf{b}+\mathbf{c})/2, (\mathbf{b}-\mathbf{c}+\mathbf{a})/2, (-\mathbf{c}-\mathbf{a}-\mathbf{b})/2] \end{aligned}$$

$$\begin{aligned} F \Longrightarrow \quad & R_{F,p} = T[(\mathbf{a}+\mathbf{b})/2, (\mathbf{b}+\mathbf{c})/2, (\mathbf{c}+\mathbf{a})/2] \\ & R_{F,q} = T[(-\mathbf{a}-\mathbf{b})/2, (-\mathbf{b}+\mathbf{c})/2, (\mathbf{c}-\mathbf{a})/2] \\ & R_{F,r} = T[(\mathbf{a}-\mathbf{b})/2, (-\mathbf{b}-\mathbf{c})/2, (-\mathbf{c}+\mathbf{a})/2] \\ & R_{F,s} = T[(-\mathbf{a}+\mathbf{b})/2, (\mathbf{b}-\mathbf{c})/2, (-\mathbf{c}-\mathbf{a})/2] \end{aligned}$$