Z. Kristallogr. **226** (2011) 32–39 / **DOI** 10.1524/zkri.2011.1260

Crystallographic point groups in five dimensions

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Received March 3, 2010; accepted September 13, 2010

Five dimensional / Point groups / Laue sets / Group generators / Penta-inversion

Abstract. This paper describes an approach to the deduction and labeling of crystallographic point groups in n-dimensional spaces where n is an odd number. It shows that point groups in such spaces may be formed from the generators of rotational groups and a single inversion operation characteristic of the odd dimension. Results are given for 188 of the 955 crystallographic point groups in a five dimensional space and the extension to the remainder of the groups is made clear. Since 3 is an odd number, the 32 classical point groups are used to illustrate the use of generators for this purpose. Further extensions to seven dimensions and to even dimensions are then discussed.

Introduction

W. Plesken [1] showed that there are 955 Q classes of crystallographic point groups distributed among 32 families in a five dimensional space. J. Opgenorth, W. Plesken and T. Schulz [2] later explained in detail a computer package (CARAT) capable of enumerating Q, Z and affine classes to 6 dimensions. A summary of the results is contained in W. Plesken and T. Schulz [3]. R. Veysseyre, D. Weigel, Th. Phan and H. Vesseyre [4] provided an alternative geometrical derivation and an extended form of the Hermann-Mauguin notation to label 5D groups. This work was further developed in R. Veysseyre, D. Weigel and Th. Phan [5] and in D. Weigel, Th. Phan and R. Vesseyre [6] so that it covers most 5D point groups. D. Weigel, Th. Phan and R. Vesseyre [7] had previously produced geometric symbols for 4D point groups following earlier work defining those groups by H. Brown, R. Bülow, J. Neubüser, H. Wondratsheck and H. Zassenhaus [8]. The variety of extended Hermann-Mauguin notations prompted an attempt to standardize such notations in T. Janssen, J. L. Birman, V. A. Koptsik, M. Senechal, D. Weigel, A. Yamamoto, S. C. Abrahams and T. Hahn [9] and the work of Weigel, Phan and Vesseyre, called WPV notation, largely complies with these standards.

The treatment below describes a quite different approach to finding and denoting point groups in nD spaces where n is an odd number, exploiting a particular property of such spaces. Given the rotational groups in a suitable notation, all non-rotational groups may be derived by a systematic search for index-2 subgroups. Computer programs to extract such subgroups are easily written and may be of help for larger groups but most of the examples below are obvious from manual inspection. The familiar three dimensional groups are used to illustrate the method and then the technique is applied to deduce and denote 188 crystallographic point groups in the two lowest partitions of 5D space. Point groups in even-dimensional spaces may be labeled as polar groups of the next highest odd dimensional space.

Each transformation generator or point group in an n-dimensional space belongs to a partition derived from its standard reduction in representation theory. Distinct partitions are denoted by square bracketed combinations of ordinals with a sum of n, producing the result shown Table 1.

It is convenient to describe partitions as lower or higher according to the numbers they contain, so that [n] is always the highest partition in an n dimensional space and [1, 1, 1] is the lowest. They may then be arranged in a hierarchy such that point groups in one partition can only have subgroups in the same or lower partitions. For example, point groups in [2, 1, 1, 1] might have subgroups in that partition or in the [1, 1, 1, 1, 1] partition, but in no other.

Generators

Geometrical point groups may be constructed from a limited number of transformation generators that arise with increasing dimensional spaces. These generators are described as positive or negative according to the signs of their determinants and groups containing only positive transformations are called positive or rotational groups.

Table 1. Allowed partitions in increasing dimensions.

Dimension	Partitions
1	[1]
2	[1, 1], [2]
3	[1, 1, 1], [2, 1], [3]
4	[1, 1, 1, 1], [2, 1, 1], [2, 2], [3, 1], [4]
5	[1, 1, 1, 1, 1], [2, 1, 1, 1], [2, 2, 1], [3, 1, 1], [3, 2], [4, 1], [5]

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A one dimensional space permits only one partition [1] that allows only one positive transformation, the identity operation and one other operation of order 2 that inverts points on the single axis. This is the familiar mirror inversion operation usually labeled m and is the only non-trivial generator in one-dimensional space. Four new rotational generators arise on moving to two dimensions, these being transformation 2 in the [1, 1] partition and transformations 3, 4 and 6 in the [2] partition. Each of these transformations is described by the following generic 2×2 matrix

$$\begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix}.$$

No further rotational generators arise on moving from 2 to 3 dimensions so rotations in this space are summarized by the following 3×3 matrix

$$\begin{pmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

One new generator does arise in three dimensions: the negative parity inversion operation usually labeled i. Each of the five generators inherited from two dimensions may be multiplied by parity inversion to produce a set of 10 generators. The resulting operations are used to construct the familiar 32 crystallographic point groups.

Four dimensional space permits two rotations in a single transformation. One rotation may be imagined to take place in the *xy* plane while the other occurs simultaneously in the *zt* plane, assuming that axes in higher spaces are labeled *x*, *y*, *z*, *t*, u etc. Such transformations are denoted by the generator symbol nm and extend over the 19 generators shown in Table 2. This table includes four generators {n} that generate cyclic groups of order 5, 8, 10 and 12 and are of interest only in point groups of the [4] partition. Each generator shown in Table 2 is capable of producing all of the elements of a cyclic group of order equal to the lowest common multiple of the two rotations.

No new rotational transformations arise on passing from four to five dimensions and the generators of Table 2 apply equally in 5D. Double rotations in 5D may be described by a 5×5 matrix as follows

$$\begin{pmatrix} \cos\theta & -\sin\theta & 0 & 0 & 0 \\ \sin\theta & \cos\theta & 0 & 0 & 0 \\ 0 & 0 & \cos\varphi & -\sin\varphi & 0 \\ 0 & 0 & \sin\varphi & \cos\varphi & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

The only new generator that does arise in 5D is a negative inversion operation which, in the following text, is called the penta-inversion and given the symbol j. Each of the 19

Table 2. Rotational generators in four and five dimensions.

1					
2	22				{5}
3	32	33			{8}
4	42	43	44		{10}
6	62	63	64	66	{12}

positive generators may be combined with this operation to provide a total of 38 generators in five dimensions. Negative generator operations are represented by an overbar symbol above the positive generator in all odd dimensional spaces. Distinct and different symbols could be used, but in this article the meaning is obvious from the context. Generators in the first two columns of Table 2, belonging to the [1, 1, 1, 1, 1] and [2, 1, 1, 1] partitions, are used in the paper. The six remaining double rotations could not occur in a point group belonging to a partition lower than [2, 2, 1].

An alternating pattern is clear in the above listing of generators. With increasing n an nD space gains new rotations when n increases to an even number and gains a new inversion operator when n increases to an odd number. New inversions are always in the lowest partitions: [1], [1, 1, 1], [1, 1, 1, 1, 1] and so forth. Symbols m and i are widely accepted for inversions in one and three dimensions and may be followed by *j*, *k* and *l* for five, seven and nine dimensions. Higher inversions may be described as penta-inversion, hepta inversion and so forth. Multiplication by an inversion or the inclusion of an inversion in a group does not alter the partition of the generator or group because it is simply a negated identity matrix.

Point groups in n dimensions

Orthogonal groups in n dimensions may be formed from a union of special orthogonal groups as follows

$$O(n) = SO(n) \cup \beta SO(n)\,,$$

in which matrix β has determinant -1 (R. L. E. Schwarzenberger [10]). However, in an n-dimensional space where n is an odd number a more restrictive definition is possible and in this case we may write

$$O(n) = SO(n) \cup \bar{1}SO(n)\,.$$

The symbol $\bar{1}$ in this equation represents an inversion in n axes. Finite groups in such situations are formed in one of two ways. In the first case a non-rotational group G' is related to a rotational group G and its index-2 subgroup H as follows

$$G' = H \cup \bar{1}(G - H)\,.$$

G' thus consists of the set of elements in subgroup H together with those elements of G not contained in H multiplied by the inversion operation. It is a combination of an invariant subgroup of rotations with a coset of negative transformations. The inversion operation itself does not occur in groups of this kind. Groups G and G' are distinct representations of the same abstract group and, since group G may have more than one index-2 subgroup, a rotational group G might have multiple isomorphs of this kind. The inversion operation commutes with all other operations, thus preserving the product structure of the rotational group. An index-2 subgroup implies an invariant subgroup and the existence of an isomorphic non-rotational group.

Non-rotational groups may also be formed as the direct product of a rotational group G and the inversion operation as follows

$$G'' = G \cup \bar{1}G\,.$$

In this case group G is retained as an index-2 subgroup together with all its inversion products including the inversion operation itself. Obviously the order of G'' is twice that of G.

In summary it is clear that every rotational group defines a set of groups that contains
- one rotational group
- zero or more non-rotational groups isomorphic to the rotational group
- one direct product of the rotational group and an inversion

Collections of this kind are called Laue sets in three dimensions but the concept is equally applicable in any n-dimensional space where n is odd and is applied to the five dimension case below.

Point groups in 3 dimensions

A suitable choice of basis functions may be used to transform an individual matrix into a partition but it does not follow that the same functions transform every element of a point group into that partition. Although generators in three dimensions belong only to the [1, 1, 1] and [2, 1] partitions they generate cubic groups in three dimensions belonging to the [3] partition. For cyclic groups, the partition of the point group is that of its generating transformation but other situations are more complex. The three partitions of three dimensions are subdivided into six families but it is convenient to further divide the crystallographic hexagonal family into separate threefold and sixfold systems. Individual positive groups then define Laue sets at the finest level of definition. The five rotational generators of 3D together with parity inversion are capable of generating all 3D groups and their matrices may be summarized as follows

$$n = \begin{pmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix} \qquad i = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}.$$

A partition defines a block structure for each group it contains. Partition [3] is defined by 3×3 matrices that cannot be reduced by changing basis functions. Two, three and fourfold rotational generators combine to form the cubic groups. All of the generators of these groups operate within the block and are therefore labeled by numbers, 232 and 432. Rotations within a block are always labeled with Arabic numerals. On the other hand, groups belonging to partitions [1, 1, 1] and [2, 1] may be represented by matrices partitioned into a 2×2 and single element blocks, even though groups of the lower partition could be further reduced. It is convenient to introduce the following "join" matrix u to describe the one allowed interaction between the blocks

$$u = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}.$$

Rotational point groups in these partitions are either cyclic or dihedral groups shown as, for example, 4 and 4u. An Arabic numeral is used for the rotation within the block while a letter is used for the join between blocks. It is worth noting that transformations shown as 2 and u both correspond to the 2 fold generator, the former being used within a block the latter between blocks.

Table 3. Crystallographic point groups in three dimensions.

Partition	System	G	$H \cup \mathrm{i}(G-H)$		$G \times \mathrm{i}$
[1, 1, 1]	Triclinic	1			i
	Monoclinic	2	$\bar{2}$		2i
	Orthorhombic	2u		$2\bar{\mathrm{u}}$	2ui
[2, 1]	Trigonal	3			3i
		3u		$3\bar{\mathrm{u}}$	3ui
	Tetragonal	4	$\bar{4}$		4i
		4u	$\bar{4}$u	$4\bar{\mathrm{u}}$	4ui
	Hexagonal	6	$\bar{6}$		6i
		6u	$\bar{6}$u	$6\bar{\mathrm{u}}$	6ui
[3]	Cubic	232			232i
		432	$\bar{4}32$		432i

Table 3 shows the 32 crystallographic point groups in rows of Laue sets and the column of rotation groups labeled in this way. The final column of direct product groups is equally simple, consisting of the products of rotational groups and parity inversion.

Non-rotational isomorphic groups are formed when the generator of a rotation group is replaced by the product of that generator and parity inversion. In a sense the generator is negated and this is indicated by an overbar. Cyclic groups (n) of even order form isomorphic groups ($\bar{\mathrm{n}}$) in this way. Dihedral groups (nu) have two generators and two distinct isomorphic groups ($\bar{\mathrm{n}}$u and n$\bar{\mathrm{u}}$) may appear in these cases. Cubic groups are more restricted and only one octahedral isomorph is possible in three dimensions.

Point groups in 5 dimensions

The 19 rotational generators of 5D listed in Table 2 act in x, y, z, t and u axes Only the [1, 1, 1, 1, 1] and [2, 1, 1, 1] partitions are described below and so only the subset of 9 rotational generators shown in Table 4 is required. Combinations of these operations with the penta-inversion generator (j) are sufficient to generate the 32 and 156 groups in these two partitions.

All of the rotational generators nm are expressed in the general matrix form below and substitutions for this matrix together with the penta-inversion (j) are capable of generating all 5D point groups based on double rotations.

$$nm = \begin{pmatrix} \cos\theta & -\sin\theta & 0 & 0 & 0 \\ \sin\theta & \cos\theta & 0 & 0 & 0 \\ 0 & 0 & \cos\varphi & -\sin\varphi & 0 \\ 0 & 0 & \sin\varphi & \cos\varphi & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}.$$

Table 4. Positive generators in five dimensions.

Partition	generators	
[1, 1, 1, 1, 1]	1	
	2	22
[2, 1, 1, 1]	3	32
	4	42
	6	62

Rotations θ and φ occur in the xy and zt planes and it is convenient to treat both the [1, 1, 1, 1, 1] and [2, 1, 1, 1] partitions as if they were [2, 2, 1]. As a result the block structure for all of these groups consists of two 2×2 blocks and a single element. A group may be formed from two separate rotational generators, one operating only in the xy plane, the other only in the zt plane. The resulting group, labeled n.m is a direct product of two groups operating in disjoint spaces. In effect the dot between the two numbers is an instruction to drop down along the diagonal of a matrix by one block. A matrix product then represents the two operations

$$\mathrm{n.m} = \begin{pmatrix} \cos\theta & -\sin\theta & 0 & 0 & 0 \\ \sin\theta & \cos\theta & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix} \times \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & \cos\varphi & -\sin\varphi & 0 \\ 0 & 0 & \sin\varphi & \cos\varphi & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}.$$

Operation nm has an order equal to the lowest common multiple of n and m. In some cases groups nm are equivalent to groups n.m, for example, 32 and 3.2 are both of order 6 and represent the same group.

Only one join is required between the two blocks of the [2, 1] partition in 3D but three are required in the [2, 2, 1] partition of 5D. Transformation u is a two-fold rotation in the y and z axes similar to that described for 3 dimensions. Operation v is a similar transformation in the t and u axes, joining the two lower blocks. Finally, b is a double two fold rotation involving y, z, t and u axes equivalent to the simultaneous operation of both u and v.

$$u = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix},$$

$$v = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & -1 \end{pmatrix},$$

$$b = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & -1 \end{pmatrix}.$$

Obviously, these operations are just special cases of transformations 2 and 22. As in three dimensions, numbers are used when the transformations occur within blocks and letters when they are between blocks. Only order 2 operations occur between blocks.

Nineteen non-rotational cyclic group generators may be formed simply by multiplying each of the positive generators by the penta-inversion (j).

$$j = \begin{pmatrix} -1 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & -1 \end{pmatrix}.$$

Not all of these are of interest here for two reasons. Firstly, generators in the [1, 1, 1, 1, 1] and [2, 1, 1, 1] partitions are restricted to negations of positive generators in Table 4. Additionally, negations of three fold rotations do not occur because the order of these generators is increased and the resulting group is changed. As a result the non-rotational generators of use in the first two partitions are those shown in Table 5. Just as with the rotational generators, negated joins are special cases of negated two fold rotations.

There are 32 crystallographic families in five dimensional space and these are easily derived from the families of lower dimensional spaces. Such derivations are particularly easy in nD spaces where n is an odd number while they are a more difficult when n is even because new families arise as a result of new rotational generators. Combinations of cells from lower dimensions are used to define new families and to produce a holohedry group representative for the family. In an odd n dimensional space these groups must contain n-fold inversion which can be extracted to leave a representative rotational group for the family. Subgroups of this group then define Laue sets for the family.

Point groups in the [1, 1, 1, 1, 1] partition

Given families in lower dimensions, the process of finding crystallographic families in an odd dimensional space is a straightforward exercise. As in other dimensions, the lowest partition contains an unusually large number of families and these are listed in Table 6.

Table 6 uses Plesken's labeling of 5D families together with WPV names and includes the family holohedry group. Each of the names shows how that family is constructed from cells of lower dimensions, except decaclinic which only arises in 5D. Extensions of 4D cells to five dimensions are shown by the -al extension and orthotopic is the extension of orthorhombic to five dimensions, otherwise the compound cell is obvious from the name [4].

Table 5. Negative generators in 5D.

Partition	Generators	
[1, 1, 1, 1, 1]	j	
[2, 1, 1, 1]	$\bar{2}$, $\bar{u}$, $\bar{v}$	$\overline{22}$, $\bar{b}$
	$\bar{4}$	$\overline{42}$
	$\bar{6}$	$\overline{62}$

Table 6. Families in the [1, 1, 1, 1, 1] partition of 5D.

Family	Name	Cells	Holohedry
I	Decaclinic	j	j
II	Hexaclinic-al	22.m	22j
III	Triclinic Oblique	2.i	2j
IV	Triclinic rectangle	2m.i	22v
V	(Di obliques)-al	2.2.m	2.2j
VIII	Oblique orthorhombic	2.2m.m	2.2vj
IX	Orthotopic	2m.2m.m	2.2uvj

Cells are shown in 1, 2 and 3D generator notation (except for Decaclinic) so a rectangle is shown as 2m rather than 2mm and orthorhombic is shown as 2m.m rather than as a three dimensional cell. Holohedry groups are often constructed in much the same way as the name so, for example, triclinic oblique may be described by the following matrices

$$2 = \begin{pmatrix} -1 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix},$$

$$i = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & -1 \end{pmatrix}.$$

When n is an odd number all nD holohedry groups are direct products of a rotation group and the inversion operation for that dimension so that the triclinic oblique holohedry might equally well be described by transformations 2 and j. In this way an index-2 rotational group is extracted from every holohedry group. Since holohedry groups contain all other family point groups as subgroups their rotational groups must contain the corresponding rotational subgroups. This partition is unusual in that only two rotational subgroups in families VIII and IX arise in this way and these two are included in Table 7. Each one defines a Laue set containing non-rotational isomorphic groups and direct product group with the penta-inversion. Given the rotational groups one can very quickly work out the non-rotational isomorphs for each Laue set in this partition. A list of the index-2 subgroups of each rotational group identifies all such groups. In most cases the resulting group may be labeled by negating a single generator, shown by an overbar. In other cases it is necessary to extend the bar over two generators, for example where 2.2 has index-2 subgroup 22. Direct product groups simply add a j to the rotational group symbol.

Table 7. Point groups in the [1, 1, 1, 1, 1] partition.

Family	G	Non-rotational isomorphs			$G \times j$
I	1				j
III	2	$\bar{2}$			2j
II	22	$\overline{22}$			22j
IV	22v	$\overline{22}$v	$22\bar{v}$		22vj
V	2.2	$\bar{2}.2$	$\bar{2}.\bar{2}$		2.2j
VIII	2u	$2\bar{u}$			2uj
	2.2v	$\bar{2}.2v$	$\bar{2}.\bar{2}v$	$2.2\bar{v}$	2.2vj
IX	2.2u	$\bar{2}.2u$	$2.2\bar{u}$		2.2uj
	2.2uv	$2.2u\bar{v}$	$2.2\bar{u}v$		2.2uvj

Table 8. Hexagonal families in the [2, 1, 1, 1] partition.

Family	Name	Cells	Holohedry
VII	Triclinic hexagon	6m.i	6bj
XI	(Hexagon oblique)-al	6m.2.m	6uvj
XV	Hexagon orthorhombic	6m.2m.m	6.2uvj

Hexagonal groups in the [2, 1, 1, 1] partition

Three hexagonal families in [2, 1, 1, 1] may be constructed from cells of lower dimension and are listed in Table 8 with equivalent holohedry groups in generator notation.

Removal of the penta-inversion reveals rotational groups 6b, 6uv and 6.2uv that have to be searched for subgroups. As in the three dimensional case it is convenient to separate groups based on 6 fold rotations from their index-2 subgroups 3b, 3uv and 3.2uv based on 3 fold rotations. Starting with these three trigonal rotational groups, a search for rotational subgroups proceeds quickly because a three-fold rotation must remain in any such subgroup and the process reduces to finding subgroups of the two-fold rotations. Having found the rotational groups shown in Table 9, most of the information necessary to construct the non-rotational isomorphic groups has already been found. For example, 3uv has index-2 subgroups 3.2, 3u and 3b and therefore three isomorphic groups. Notice that the index-2 subgroup does not have to be in the same family or even in the same partition. Direct product groups with penta-inversion just take an additional j generator.

Groups 6b, 6uv and 6.2uv produce a larger number of rotational subgroups because the main rotor itself has an index-2 subgroup. Even so, the procedure remains unchanged and produces the 13 groups shown in Table 10. A systematic search for the index-2 subgroups of each of the 13 rotational groups then reveals the non-rotational isomorphs also shown in Table 10. Most of these can be

Table 9. Trigonal point groups in the [2, 1, 1, 1] partition.

Family	G	Non-rotational isomorphs			$G \times j$
VII	3				3j
	3b	$3\bar{b}$			3bj
XI	3u	$3\bar{u}$			3uj
	3.2	$3.\bar{2}$			3.2j
	3uv	$3\bar{u}v$	$3u\bar{v}$	$3\overline{uv}$	3uvj
XV	3.2u	$3.\bar{2}u$	$3.2\bar{u}$		3.2uj
	3.2v	$3.2\bar{v}$			3.2vj
	3.2uv	$3.\bar{2}uv$	$3.2\bar{u}v$	$3.2u\bar{v}$	3.2uvj

Table 10. Hexagonal point groups in the [2, 1, 1, 1] partition.

Family	G	Non-rotational isomorphs			$G \times$ j
VII	6	$\bar{6}$			6j
	6b	$\bar{6}$b	6$\bar{\mathrm{b}}$		6bj
XI	62	$\overline{62}$			62j
	62b	$\overline{62}$b	62$\bar{\mathrm{b}}$	$\overline{62}\bar{\mathrm{b}}$	62bj
	6u	$\bar{6}$u	6$\bar{\mathrm{u}}$		6uj
	6.2	$\bar{6}$.2	6.$\bar{2}$	$\bar{6}$.$\bar{2}$	6.2j
	6uv	$\bar{6}$uv	6$\bar{\mathrm{u}}$v	6u$\bar{\mathrm{v}}$	6uvj
		6$\overline{\mathrm{uv}}$	$\bar{6}$u$\bar{\mathrm{v}}$		
XV	62u	$\overline{62}$u	62$\bar{\mathrm{u}}$		62uj
	62v	$\overline{62}$v	62$\bar{\mathrm{v}}$		62vj
	62uv	$\overline{62}$uv	62$\bar{\mathrm{u}}$v	62u$\bar{\mathrm{v}}$	62uvj
		62$\bar{\mathrm{u}}\bar{\mathrm{v}}$	$\overline{62}$u$\bar{\mathrm{v}}$		
	6.2u	$\bar{6}$.2u	6.$\bar{2}$u	$\bar{6}$.$\bar{2}$u	6.2uj
		6.2$\bar{\mathrm{u}}$			
	6.2v	$\bar{6}$.2v	6.2$\bar{\mathrm{v}}$	$\bar{6}$.$\bar{2}$v	6.2vj
	6.2uv	$\bar{6}$.2uv	6.$\bar{2}$uv	$\bar{6}$.$\bar{2}$uv	6.2uvj
		6.2$\bar{\mathrm{u}}$v	6.2u$\bar{\mathrm{v}}$		

shown by negating one generator of the positive group symbols but again, in a few cases, two generators are negated to indicate a subgroup. Fortunately, a computer program to detect index-2 subgroups is easily produced and each possibility corresponds to a distinct isomorphic group. Direct products are again formed from rotation groups and the penta-inversion.

Trigonal point groups have the form shown in Table 9 because the main rotor is an odd number that cannot itself have an index-2 sub-rotation. Other odd numbered rotors produce similar tables, allowing the production of (non-crystallographic) pentagonal and heptagonal tables from the trigonal one. For similar reasons even numbered rotors have tables similar to Table 10 and so the tetragonal groups described below follow a pattern set by the hexagonal groups already described.

Tetragonal groups in the [2, 1, 1, 1] partition

There are three tetragonal families with names and holohedries similar to those of the hexagonal family and these are shown in Table 11.

Once again 5D holohedry groups are formed from lower dimensions and converted into inversion forms 4bj, 4uvj and 4.2uvj. Rotational groups 4b, 4uv and 4.2uv are extracted and these groups and in turn searched for subgroups to provide the 13 rotational groups of Table 12. Non-rotational isomorphic groups are derived in the same way as the hexagonal examples described earlier and produce the strikingly similar results shown in Table 12. This table is completed by the direct product groups shown by attaching j to the rotational group.

Table 11. Tetragonal families in the [2, 1, 1, 1] partition.

Family	Name	Cells	Holohedry
VII	Triclinic square	4m.i	4bj
XI	(Square oblique)-al	4m.2.m	4uvj
XV	Square orthorhombic	4m.2m.m	4.2uvj

Table 12. Tetragonal point groups in the [2, 1, 1, 1] partition.

Family	G	Non-rotational isomorphs			$G \times$ j
VI	4	$\bar{4}$			4j
	4b	$\bar{4}$b	4$\bar{\mathrm{b}}$		4bj
X	42	$\overline{42}$			42j
	42b	$\overline{42}$b	42$\bar{\mathrm{b}}$	$\overline{42\mathrm{b}}$	42bj
	4u	$\bar{4}$u	4$\bar{\mathrm{u}}$		4uj
	4.2	$\bar{4}$.2	4.$\bar{2}$	$\bar{4}$.$\bar{2}$	4.2j
	4uv	$\bar{4}$uv	4$\bar{\mathrm{u}}$v	4u$\bar{\mathrm{v}}$	4uvj
		4$\overline{\mathrm{uv}}$	$\bar{4}$u$\bar{\mathrm{v}}$		
XIV	42u	$\overline{42}$u	42$\bar{\mathrm{u}}$		42uj
	42v	$\overline{42}$v	42$\bar{\mathrm{v}}$		42vj
	42uv	$\overline{42}$uv	42$\bar{\mathrm{u}}$v	42u$\bar{\mathrm{v}}$	42uvj
		42$\bar{\mathrm{u}}\bar{\mathrm{v}}$	$\overline{42}$u$\bar{\mathrm{v}}$		
	4.2u	$\bar{4}$.2u	4.$\bar{2}$u	$\bar{4}$.$\bar{2}$u	4.2u$\bar{\mathrm{v}}$j
		4.2$\bar{\mathrm{u}}$			
	4.2v	$\bar{4}$.2v	4.2$\bar{\mathrm{v}}$	$\bar{4}$.$\bar{2}$v	4.2vj
	4.2uv	$\bar{4}$.2uv	4.$\bar{2}$uv	$\bar{4}$.$\bar{2}$uv	4.2uvj
		4.2$\bar{\mathrm{u}}$v	4.2u$\bar{\mathrm{v}}$		

There are 28 trigonal point groups which, together with 64 for each of the hexagonal six-fold and tetragonal families, gives a total of 156 groups for the [2, 1, 1, 1] partition.

Subgroups of the (Hexagon oblique)-al holohedry group 6uvj

Point group 6uvj is the holohedry group of the (hexagon oblique)-al family and so contains every other group in this family as a subgroup. These groups in turn contain further subgroups. One way of following this cascade of subgroups is to first list all the centrosymmetric subgroups of 6uvj. Each centrosymmetric group must, by definition, contain all other members of its Laue set as index-2 subgroups that can be read from Table 10, but only the number of these groups is shown in Table 13. In total 6uvj has 71 subgroups (itself included). Group 6uvj of order 48 has 5 index-2 centrosymmetric subgroups listed below itself in Table 13. Further centrosymmetric subgroups of order 12 and 6 follow in the same column. Point group 6uvj also has an index-3 subgroup 2uvj of order 16 which in turn has further index-2 centrosymmetric groups culminating in the inversion operation itself. The table shows 19 such groups. The number corresponding groups that can be read from Table 10 in this way is shown in the third column of Table 13, producing a total of 52 groups.

Five dimensional space allows also the partitions [2, 2, 1], [3, 1, 1], [3, 2], [4, 1] and [5] and work on these is progressing in the same order. Partition [2, 2, 1] is treated in much the same way as the partitions described above except that the order in which rotations are labeled becomes important so, for example rotations 6.3 and 3.6 may be used within the context of joins. In fact, the examples above have been treated as though partitioned in [2, 2, 1]. Partitions containing cubic sub-groups occur as

Table 13. Subgroups of *6uvj.*

Order	Laue set	No in set
48	6uvj	6
24	3uvj	4
	6.2j	4
	6uj	3
	6bj	3
	62bj	4
12	62j	2
	3uj	2
	3.2j	2
	6j	2
	3bj	2
6	3j	1
16	2uvj	4
8	2.2j	3
	22vj	3
	2uj	2
4	2j	2
	22j	2
2	j	1
Totals	19	52

$[3, 1, 1]$ and $[3, 2]$ and have to be treated in terms of 3×3 and 2×2 blocks with a join between the z and t axes. Point groups in the $[3, 2]$ partition have a block structure of 3×3 and 2×2 blocks that might contain, for example, 432 and 6 groups together with a join between the blocks. However, the principle of the approach is not altered Again the procedure is to find rotational groups then to use index-2 subgroups to discover isomorphic non-rotational groups. Direct product groups are deduced in the same way. The approach advocated above follows from the algebra of transformations in nD when n is an odd number and obtains in any partition. Clearly, this method applies only to nD when n is odd but all point groups in an even dimensional space are polar in the next highest dimensional space. It follows that they can be generated and labeled in this way and then collapsed into the lower space. Enumerating the 137 crystallographic families of 7D from those of lower dimensions is a straightforward process and produces holohedry groups from which Laue sets can be derived. Subgroups of these then produce other rotational and non-rotational groups. As the number and order of the groups increases there is a corresponding need for efficient computer programs. Fortunately the similarities between abstract algebraic structures (abstract types) and functional programming languages noted in M. Downward [11] allow structures to be modelled in the functional style. This may be done directly in the language or through a computational group theory package such as GAP.

Magnetic point groups

H. Heesch [12] described 122 three dimensional magnetic point groups in terms of 3 spatial axes and a spin axis, producing reducible 4D representations. More recently, B. Souvignier [13] counted 1025 four dimensional magnetic point groups in reducible 5D representations, 4 spatial one 1 spin. Magnetic point groups are subdivided into white, proper magnetic and grey groups in much the same way as the groups described above are divided into rotational, non-rotational isomorphic and centrosymmetric groups. This similarity arises because the spin inversion operation and the spatial inversion operations act in the same way in the defining equations so that in both cases groups are found by searching for index-2 subgroups. White groups G are simply the spatial groups of the appropriate dimension so, for example, there are 227 4D white groups. A proper magnetic group G' is related to a spatial group G and its index-2 subgroup H as follows

$$G' = H \cup m(G - H)$$

Groups G and H may be non-rotational and the inversion operation m is that of spin inversion. Group 42 in 4D has one index-2 subgroup and forms a proper magnetic group of order 4 from the single reducible 5D generator $\bar{4}\bar{2}$ shown below

$$m = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & -1 \end{pmatrix},$$

$$\overline{42} = \begin{pmatrix} 0 & -1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & -1 \end{pmatrix}.$$

Magnetic generators of this kind are simpler than their spatial counterparts. In the above example a spin inversion is added to the 42 matrix while in the spatial case a penta-inversion changes all matrix entries. There are 571 4D proper magnetic groups. Finally. there are 227 grey groups G'' analogous to the centrosymmetric spatial groups

$$G'' = G \cup \mathrm{m}G.$$

Comparisons between the 1025 4D magnetic point groups and the 955 5D spatial point groups are not as simple as the defining formulae might suggest. Index-2 subgroups are required for all 4D groups to form magnetic groups while only those of rotational groups are required to form 5D spatial groups. A spin inversion axis is distinct and rotations into it from spatial axes could not occur while an added spatial axis is indistinguishable and permits such transformations. Magnetic point groups may be formed in any dimension while the spatial groups described earlier are only possible in nD where n is odd.

Acknowledgments. The author is greatly indebted to an anonymous referee for a number of comments and corrections to the original manuscript. Support provided by resources departments in the University of Birmingham, England is also appreciated.

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