

1.2. REPRESENTATIONS OF CRYSTALLOGRAPHIC GROUPS

However, many entries for the three-dimensional point groups are simply integers.

The program provides the following information as rows above the characters of the irreducible representation:

- (1) Representative elements of the conjugacy classes expressed in terms of the generators a, b, \dots
- (2) The number of elements of each class.
- (3) The order of the elements of the classes: the lowest positive power of an element that equals the identity.

Below the character table, the following information is displayed:

(1) In the m th row after the square character table, the class to which the $(m + 1)$ th powers of the elements from this column belong is given. If a conjugacy class has elements of order p , then only the $p - 1$ first entries are given, because in the column there exists p periodicity.

(2) The determinant of the three-dimensional matrix for the element of the point group (or the elements of the conjugacy class). This is the character of an irreducible representation.

(3) Finally, the character of the vector representation is given.

As an example, the generalized character table for the three-dimensional point group $4mm$ is given in Table 1.2.7.1.

The data connected with a character table can be seen by choosing ‘view character table’. The characters of the irreducible representations, the determinant representation and the vector representation are shown in the main window after selection of ‘accept character table’. From the character of these representations, characters of other representations may be calculated. The results are added as rows to the table, which is shown after each calculation.

Calculations using rows from the table may have one or more arguments. Operations with one argument will produce, for example, the decomposition into irreducible components, the character of the p th power, the symmetrized or antisymmetrized square, or the character of the corresponding physical (real) representation. Operations with two or more arguments yield products and sums of characters. The arguments of a unitary, binary or multiple operation are selected by clicking on the button in front of the corresponding characters. If the result is a new character (e.g. the product of two characters), it is added as a row to the list of characters. If the result is not a character (e.g. the decomposition into irreducible components), the result is given on the worksheet.

Suppose one wants to determine the number of elastic constants for a material with cubic 432 symmetry. After selecting the character table for the group 432, one clicks on the button in front of ‘vector representation’ in the character table. This yields the character of the three-dimensional vector representation of the group. The character of the symmetrized square is obtained by selecting ‘symmetrized square’. This gives the character of a six-dimensional representation. Determining the number of times the trivial representation occurs by selecting ‘decompose’ gives the number of free parameters in the metric tensor, i.e. 1. Clicking on ‘symmetrized square’ for the character of the six-dimensional representation gives the character of a

21-dimensional representation. Decomposition yields the multiplicity 3 for the trivial representation, which means that there are three independent tensor elements for a tensor of symmetry type $((01)(23))$, which in turn means that there are three elastic constants for the group 432 (see Table 1.2.6.9). For the explicit determination of the independent tensor elements, the tensor module of the program should be used.

Of course, many kinds of calculations unrelated to tensors can be carried out using the character module. Examples include the calculation of selection rules in spectroscopy or the splitting of energy levels under a symmetry-breaking perturbation.

1.2.7.4. Algorithms

1.2.7.4.1. Construction of a basis

As a basis for a tensor space without permutation symmetry, one may choose one consisting of non-commutative monomials. It has d^r elements, where d is the dimension and r is the rank. In two dimensions, these are x, y for $r = 1$, xx, xy, yx, yy for $r = 2$ and $xxx, xxy, xyx, xyy, yxx, yxy, yyx, yyy$ for $r = 3$. Note that $xy \neq yx$.

If there is permutation symmetry among the indices i_1, \dots, i_p , only polynomials $x_{i_1}x_{i_2} \dots x_{i_p}$ occur in the basis for which $i_1 \leq i_2 \leq \dots \leq i_p$. Then $x_{i_1}x_{i_2} = x_{i_2}x_{i_1}$. If there is antisymmetry among these indices, one has the condition $i_1 < i_2 < \dots < i_p$ and $x_{i_1}x_{i_2} = -x_{i_2}x_{i_1}$. Therefore, in two dimensions, the basis for tensors of type (1 3)2 is $xxx, xxy, xyx, xyy, yxy, yyy$ and for those of type [1 3]2 it is xxy, xyy . These bases can be obtained from the general basis by elimination.

1.2.7.4.2. Action of the generators of the point group G on the basis

The transformation of the monomial $x_i x_j \dots$ under the matrix $g \in G$ is given by the polynomial

$$\left[\sum_{m=1}^d g_{im} x_m \right] \times \left[\sum_{n=1}^d g_{jn} x_n \right] \dots,$$

which is in principle non-commutative. This polynomial can be written as a sum of the monomials in the basis taking into account the eventual (anti)symmetry of xy and yx . In this way, basis element (a monomial) e_i is transformed to

$$g e_i = \sum_{j=1}^d M(g)_{ji} e_j.$$

To each generator of G corresponds such an action matrix M .

The action matrix changes if one considers pseudotensors. In the case of pseudotensors, the previous equation changes to

$$g e_i = \text{Det}(g) \sum_{j=1}^d M(g)_{ji} e_j.$$

The function $\text{Det}(g)$ is just a one-dimensional representation of the group G . The determinant is either +1 or -1.

1.2.7.4.3. Diagonalization of the action matrix and determination of the invariant tensor

An invariant element of the tensor space under the group G is a vector v that is left invariant under each generator:

$$\begin{pmatrix} M_1 - E \\ M_2 - E \\ \vdots \\ M_s - E \end{pmatrix} v = \Omega v = 0.$$

If the number of generators is one, $\Omega = M - E$. This equation is solved by diagonalization:

Table 1.2.7.1. Data connected with the character table for point group $4mm$

e	a	a^2	b	ab
1	2	1	2	2
1	4	2	2	2
1	1	1	1	1
1	1	1	-1	-1
1	-1	1	1	-1
1	-1	1	-1	1
2	0	-2	0	0
1	3	1	1	1
	2			
	1			
1	1	1	-1	-1
3	1	-1	1	1

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$$P\Omega QQ^{-1}v = DQ^{-1}v = 0,$$

where $D_{ij} = d_i\delta_{ij}$. The dimension of the solution space is the number of elements d_i that are equal to zero. The corresponding rows of Q form a basis for the solution space. (See example further on.)

1.2.7.4.4. Determination of the vector representation

For a point group G , its isomorphism class and its character table are known. For each conjugacy class, a representative element is given as word $A_1A_2 \dots$ where the A_i 's correspond to generators. Replacing the letters by the generating matrices, one obtains as product a matrix for which the trace is the character of the vector representation in the conjugacy class. The characters of all conjugacy classes being known, the representation can be decomposed into irreducible components by means of

$$m_\alpha = (1/|G|) \sum_i n_i \chi_\alpha^*(i) \chi(i),$$

where α labels the irreducible representations (the row number in the character table), m_α the number of times the representation α occurs, $|G|$ the order of the group G , n_i the number of elements in the i th conjugacy class (given as the second row in the character table), $\chi_\alpha(i)$ the cyclotomic in the i th row and α th column of the character table, and $\chi(i)$ the calculated character in the i th conjugacy class.

1.2.7.4.5. Determination of tensor products and their decomposition

Given a character (for an irreducible representation from the character table, or for the vector representation, for example), the character of the standard rank n tensor is the n th power of the character and can be decomposed with the multiplicity formula for m_α given above.

Fully symmetrized or antisymmetrized tensor products have characters given by

$$\begin{aligned} n = 2 : \chi^\pm(R) &= \frac{1}{2!} (\chi(R)^2 \pm \chi(R^2)) \\ n = 3 : \chi^\pm(R) &= \frac{1}{3!} (\chi(R)^3 \pm 3\chi(R^2)\chi(R) + 2\chi(R^3)) \\ n = 4 : \chi^\pm(R) &= \frac{1}{4!} (\chi(R)^4 \pm 6\chi(R^2)\chi(R)^2 + 3\chi(R^2)^2 \\ &\quad + 8\chi(R^3)\chi(R) \pm 6\chi(R^4)) \\ n = 5 : \chi^\pm(R) &= \frac{1}{5!} (\chi(R)^5 \pm 10\chi(R^2)\chi(R)^3 + 15\chi(R^2)^2\chi(R) \\ &\quad + 20\chi(R^3)\chi(R)^2 \pm 20\chi(R^3)\chi(R^2) \\ &\quad \pm 30\chi(R^4)\chi(R) + 24\chi(R^5)) \\ n = 6 : \chi^\pm(R) &= \frac{1}{6!} (\chi(R)^6 \pm 15\chi(R^2)\chi(R)^4 + 45\chi(R^2)^2\chi(R)^2 \\ &\quad + 40\chi(R^3)^2 \pm 15\chi(R^2)^3 + 40\chi(R^3)\chi(R)^3 \\ &\quad \pm 120\chi(R^3)\chi(R^2)\chi(R) \pm 90\chi(R^4)\chi(R)^2 \\ &\quad + 90\chi(R^4)\chi(R^2) + 144\chi(R^5)\chi(R) \\ &\quad \pm 120\chi(R^6)). \end{aligned}$$

From this follows immediately the dimension of the subspaces of symmetric and antisymmetric tensors:

$$\begin{aligned} n = 2 : & \frac{1}{2}(d^2 \pm d) \\ n = 3 : & \frac{1}{6}(d^3 \pm 3d^2 + 2d) \\ n = 4 : & \frac{1}{24}(d^4 \pm 6d^3 + 11d^2 \pm 6d) \\ n = 5 : & \frac{1}{120}(d^5 \pm 10d^4 + 35d^3 \pm 50d^2 + 24d) \\ n = 6 : & \frac{1}{720}(d^6 \pm 15d^5 + 85d^4 \pm 225d^3 + 274d^2 \pm 120d). \end{aligned}$$

The general expression for arbitrary rank can be determined as follows. (See also Section 1.2.2.7)

(1) If n is the rank, the first step is to determine all possible decompositions

$$n = \sum_{i=1}^n f_i$$

with non-negative integers f_i satisfying $f_i \leq f_{i-1}$.

(2) For each such decomposition $m = 1, \dots, n_{\text{tot}}$ there is a term

$$P_m = \prod_{i=1}^p \binom{N_i}{f_i} (f_i - 1)!,$$

where $N_1 = n$, $N_i = N_{i-1} - f_{i-1}$ ($i > 1$) and p is the number of nonzero integers f_i .

(3) If there are equal values of f_i in the m th decomposition, P_m should be divided by $t!$ for each t -tuple of equal values ($f_{k+1} = \dots = f_{k+t}$).

(4) The sign of the term P_m is $+1$ for a symmetrized power and

$$\prod_{i=1}^p (-1)^{(f_i-1)}$$

for an antisymmetrized power.

(5) The expression for the character of the (anti)symmetrized power then is

$$\chi^\pm(R) = (1/M!) \sum_{m=1}^{n_{\text{tot}}} \text{sign}_m P_m \prod_{i=1}^p \chi(R^{f_i}).$$

1.2.7.4.6. Invariant tensors

Once one has the character of the properly symmetrized tensor, the number of invariants is just m_1 , the number of times the trivial representation occurs in the decomposition.

Example (1). Dimension 3, rank 3, symmetry type (123), group 3. Basis: $xxx, xxy, xxz, xyy, xyz, xzz, yyy, yyz, yzz, zzz$. Under

$$\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}$$

the basis elements go to $yyy, yyz, yyx, yzz, yzx, yxx, zzz, zzx, zxx, xxx$, respectively, and these are equivalent to $yyy, yyz, xyy, yzz, xyz, xxy, zzz, xzz, xxz, xxx$, respectively. This gives the ten-dimensional matrix