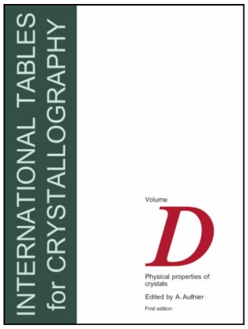

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Calculations with tensors and characters

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1 Introduction

Tensors corresponding to specific physical properties and being invariant under a given point group have been tabulated several times, up to a certain rank. The same holds for the character tables of the crystallographic point groups. Presenting these data in the form of a computer program has, however, several advantages. Access is in general quicker, the flexibility may be greater, the information does not take as much space and there is no *a priori* restriction on rank or dimension. Flexibility includes, for example, the use of several settings of the crystallographic groups. Generality means that character tables can be provided for arbitrary finite point groups.

The theory of invariance of tensors is treated in Chapters 1.1 and 1.2. In Chapter 1.2, the theory of representations of crystallographic groups is also dealt with. For background information the reader is referred to these chapters. In the following, a short introduction is given to the use of the software for calculations of invariant tensors and to character tables as they are given on the accompanying CD-ROM.

2 QuickStart

The program is started by clicking on the icon in the window appearing after opening the CD-ROM. The program allows the determination of the general form of tensors and pseudotensors of arbitary rank, invariant under a chosen two- or three-dimensional crystallographic point group, and under given permutations of the indices. In the second part, calculations can be made with characters of arbitrary finite three- and two-dimensional point groups.

The user is guided through the program with windows in which buttons can be clicked on to select pregiven choices, or with 'fill-in' windows into which information can be typed. The functions of the various buttons are explained in the following section. We start with a guided tour. Clicking on the icon **vol-d.exe** opens a worksheet.

1. Click on the button **Tensor**. An input window opens up.
2. Type **3** in the open fill-in window behind **Dimension**.
3. Type **2** in the open fill-in window **Rank**.
4. Click on **Point Group**. A menu opens. Click on **Orthorhombic**. A new menu opens with the three point groups in the orthorhombic system. Click on **222**. Now this point group is selected. You could also have typed 222 in the fill-in window of **Point Group**.
5. The generators of the point group can be viewed in a separate window after having clicked on **View Point Group**. This can be closed by choosing **Close** under **Window**.
6. Suppose we want to view the metric tensor for the point group 222, which is a second-rank tensor symmetric in both indices. Click on **Perm. Symmetry** and select **(0 1)**. The indices are denoted 0,..., through (rank − 1): here the rank is 2. Notice that 0 1 is written without commas. To indicate that the tensor is symmetric under permutation of both indices, **0 1** is put between parentheses: select **(0 1)**.
7. In the standard setting no basis transformation is needed: click **Basis Transformation** and then select **No transformation**.
8. All information is now available. Click **Tensor** to determine the invariant tensor, which in our example is the metric tensor of a lattice in the orthorhombic system.
9. After a period of time which depends on the dimension, the rank and the symmetry, the results are presented in the main window, the worksheet. For convenience the chosen point group and permutation symmetry are repeated, followed by the number of free parameters in the invariant tensor. The information about the tensor is a block with the following components:
   (a) The dimension: 3.
   (b) The rank: 2.
   (c) The permutation symmetry: (0 1).
   (d) The relations between the tensor elements, and the tensor elements expressed in the free parameters. The information given means: The three diagonal elements are nonzero and generally different, all the off-diagonal elements are zero.

Thus in the window one finds:

$$xx = c, \;\; yy = b, \;\; zz = c$$
$$xy = xz = yx = yz = zx = zy = 0$$

This means:
T$_{xx} = c$, T$_{yy} = b$, T$_{zz} = a$
T$_{xy}$=T$_{yx}$=0, T$_{xz}$=T$_{zx}$=0, T$_{yz}$=T$_{zy}$=0
The invariant tensor then is written as

$$c * xx \;+\; b * yy \;+\; a * zz$$

as a quadratic form, or as

$$\begin{matrix} c & 0 & 0 \\ 0 & b & 0 \\ 0 & 0 & a \end{matrix}$$

in matrix form.
The complete expression is

$$\mathrm{T}_{xx}xx + \mathrm{T}_{yy}yy + \mathrm{T}_{zz}zz + 2\mathrm{T}_{xy}xy + 2\mathrm{T}_{xz}xz + 2\mathrm{T}_{yz}yz$$
$$= (x\; y\; z\,)\,\mathrm{T}\begin{pmatrix} x \\ y \\ z \end{pmatrix}.$$

When there are too many free parameters (more than five) they are denoted as $a_1, a_2, \ldots$.

10. The results can be shown in a separate window: click on **To window** at the left. The window that appears can be closed by the button in the left upper corner.

11. The results can be kept in a file by clicking on **To file** and giving a file name, for example C:/temp/sample1.

12. Repeat the sequence with the elasticity tensor. The dimension remains three. Click in the window behind **Rank**: 4.

13. Select a point group. Click **Point Group**, click on **Cubic**, click on **432**.

14. Select the permutation symmetry, click on **Perm. Symmetry**, click on **((0 1)(2 3))**.

15. Select **No basis transformation**.

16. Click on **Tensor**. The results appear on the worksheet, page 1. The tensor invariant under 432 and of type ((0 1)(2 3)) has three free parameters. The relations between the tensor elements are given, as well as their expression in terms of the free parameters.

17. One can switch between the pages of the worksheet by means of the buttons **Next** and **Previous**.

18. Close the input window by clicking **Close**.

19. Click the button **Character** to use the second part. A new window (Character window) opens up.

20. Select a point group, *e.g.* the point group 432.

21. The character table for this point group can be viewed using **View character table**. In a separate window this character table is presented as follows. The first row gives representatives of the conjugation classes expressed in generators. For 432 there are five classes (e, b, a^2, a, ab). The second row gives the number of elements in each of the (five) classes. The third row gives the orders of the elements, e.g. $b^3 = e$. Then follows a square matrix with the characters arranged in columns for the classes and rows for the irreducible representations. The next block contains the numbers of the conjugation classes to which the pth power of an element of the class belongs. In a column the numbers have as repetition rate the order of the elements in the class. For example, b belongs to class 2, b^2 belongs to class 2 as well, b^1 belongs to class 1, $b^4 = b$ belongs to class 2 *etc*. The last row gives the character of the three-dimensional vector representation, the representation with which a vector transforms under the action of the chosen point group. Close the window.

22. Now click on **Accept character table**. This displays the characters of the irreducible representations and that of the vector representation in the character window.

23. Operations on the characters can be performed. For a unary operation select one character in the character window, and click a button on the right-hand side (power, symmetric square, antisymmetric square). For a power the exponent is specified in the fill-in window **n=**. For a binary operation (add, product) select two characters by clicking the corresponding buttons at the left-hand side. These operations provide a new character that in the character window is added to the existing list. Clicking on **Decompose** yields the multiplicities of the irreducible characters in a selected character. Click on the button in front of irrep 3, fill in n=2 and click on **Power**. The square of the third character appears as the last line in the character window. Clicking the button in front and selecting Decompose yields the multiplicities (1 1 1 0 0) of the irreps on the worksheet. Selection of characters can be cancelled by clicking again, or clicking **Reset character list**.

24. Selected characters in the character window can be transferred to the worksheet by means of **Copy**. There they can again be viewed using **To window**, or sent to a file using **To file**.

25. The session can be closed by clicking **Quit** in the top line of the screen.

3 The Buttons

3.1 The top line buttons

Quit: Quit the program. Unsaved results from the worksheet will be lost.
Tensor: Starts the part of the program for determining invariant tensors.
Character Table: Starts the part of the program for calculations with characters of finite two-dimensional and three-dimensional point groups.

3.2 Next

The results of the calculation are kept on consecutively numbered pages of the worksheet. This button goes to the next page, if it exists. The pages are numbered 0,1,. . ..

3.3 Previous

The results of the calculation are kept on consecutively numbered pages of the worksheet. This button goes to the previous page, if it exists.

3.4 To window

The contents of the present page of the worksheet are copied to a separate window. This can be moved and scrolled.

3.5 To file

The contents of the present page of the worksheet are copied to a file. The file name must be given in a separately opened window. On a machine running Windows95 the name should start with C://

3.6 Delete

The contents of the present page of the worksheet are removed.

3.7 Tensor

Starts the part of the program for determining invariant tensors.

3.7.1 Dimension

Type the number of dimensions in the open fill-in window.

3.7.2 Rank

Type the rank of the tensor in the open fill-in window.

3.7.3 Point Group

The name of the point group with which one wants to work can be given in the open fill-in window, or selected from a list. Clicking on the button **Point Group** opens a list of the seven systems in three dimensions or of the four systems in two dimensions. Clicking on one of the selection buttons opens a window with the symbols of the point groups in the selected system. The difference from the international notation is a - symbol in front of a digit, instead of a bar above it. By clicking on a button in the window a point group is selected.

3.7.4 View

A separate window is opened in which the generating matrices for the point group are shown as an object:
group(generator no. matrix<int>(matrix elements)
generator no. ...
).

3.7.5 Permutation Symmetry

The intrinsic or permutation symmetry can be typed into the open window or can be selected from a list for the lower dimensions (up to four).

The format is as follows: the indices of the tensor are numbered from 0 to rank $-$ 1. They should be typed with a space between the numbers. The order of the numbers is free. A change in the order corresponds to a change in setting.

Indices that are symmetric in the tensor are surrounded by (round) parentheses, antisymmetric indices by square brackets.

0 1 2 or 2 0 1 or 2 1 0 denote an arbitary rank-three tensor without permutation symmetry of the indices.

(0 1) 2 is a rank-three tensor symmetric in the first two indices (T_{ijk}=T_{jik}), (2 0) 1 a rank-three tensor symmetric under exchange of the first and third index (T_{ijk}=T_{kji}), and [2 1] 0 a rank-three tensor antisymmetric in the last two indices (T_{ijk}= -T_{ikj}).

Multiple symmetrizations are allowed: ((0 1)(2 3)) is a tensor of rank four invariant under permutation of first and second, third and fourth, and first and second pair of indices (T_{ijkm}=T_{jikm}=T_{ijmk}=T_{kmij}).

For low-rank tensors a list of preselected symmetries appears in a window opened by clicking on **Perm. Symmetry**, from which a specific choice can be made by clicking on one of the buttons.

3.7.6 Basis Transformation

The invariant tensors are calculated on the standard basis for the point group. For a different setting a basis transformation is applied by clicking on **Basis Transformation** and selecting a transformation. Even for the case of the standard setting one has to make a choice: **No Transformation**.

3.7.7 Tensor

Starts the calculation of the tensor of the given rank, invariant under the chosen point group and under the chosen permutations of the indices. The result appears in the worksheet.

3.7.8 Pseudo tensor

Starts the calculation of the pseudotensor of the given rank, invariant under the rotations of the chosen point group and under the chosen permutations of the indices, and obtaining an additional minus sign for the elements with determinant -1 in the point group. The result appears in the worksheet.

3.7.9 Close

Closes the window **Tensor**. This can be reopened by clicking on the top line button **Tensor**.

3.8 Character

Starts the part of the program for calculations with characters of finite three-dimensional point groups.

3.8.1 Point Group

Click on the button to open a menu for selecting a point group.

3.8.2 View Character Table

Opens a separate window with the character table of the selected point group. Each column corresponds to a conjugation class.

1. Conjugation classes represented by elements expressed in terms of generators $a, b, \ldots$.
2. The number of elements in each conjugation class.
3. The order of the elements in the class.
4. The characters of the irreducible representations.
5. The classes to which the pth power of an element of this class belongs. These numbers are periodic with as period the order of the elements of the class. The pth power corresponds to the pth row.
6. The three-dimensional vector representation. Tensors can be obtained by taking (symmetrized or antisymmetrized) powers of the vector representation.

3.8.3 Accept character table

Presents in the character window the characters for the irreducible representations and the vector representation. They form the first lines in the list of characters.

3.8.4 Power n=

The exponent needed for the specification of a power of a character.

3.8.5 Add

Add two characters selected in the character window by clicking the buttons at the beginning of the line. The result is added as a new line in the character window.

3.8.6 Product

Provides the product of two selected characters as a new line in the character list.

3.8.7 Power

Provides the nth power of one character selected in the character window. n is specified in the fill-in window.

3.8.8 Symmetrized Square

Calculates the character of the representation which is the symmetrized second power of a selected representation by means of:

$$\chi(g)^2_{\mathrm{s}} \;=\; \frac{1}{2}\left(\chi(g)^2 + \chi(g^2)\right).$$

3.8.9 Antisymmetrized Square

Calculates the character of the representation which is the antisymmetrized second power of a selected representation by means of:

$$\chi(g)^2_{\mathrm{a}} \;=\; \frac{1}{2}\left(\chi(g)^2 - \chi(g^2)\right).$$

3.8.10 Physical character

For an irreducible representation it is checked whether it is also a physically irreducible representation. The expression

$$\sum_{g \in G} \chi(g^2)/|G| \ = \ P,$$

where $|G|$ is the order of the group G, yields either 1, 0 or -1. If $P = 0$ the representation does not have a real character. The corresponding physical representation is the sum of the representation and its complex conjugate. The character is the sum of the selected character and its complex conjugate. If $P = 1$ the representation is equivalent to a real representation. If $P = -1$ the character is real, but not the representation matrices. The character is the double of the selected character.

3.8.11 Decompose

Gives the multiplicities of the irreducible representations in the decomposition of the selected character.

3.8.12 Copy

Copy the content of the character window to the worksheet, where it can be handled further.

3.8.13 Reset character list

The selection buttons in front of the characters in the list in the character window are made inactive.

3.8.14 Close

Close the character window and return to the worksheet.

4 Examples

4.1 Invariant tensors

4.1.1 Invariant magnetic field

A magnetic field transforms as a pseudotensor of rank one. For the point group *m* one has:

Dimension	3
Rank	1
Point group	*m* (unique axis *y*)
Permutation symmetry	0
Basis transformation	Identity
Type	Pseudotensor

The result: One free parameter, $\mathrm{T}_y = a$, T_x=T_z=0.

4.1.2 Metric tensor

A metric tensor is a symmetric tensor of rank two. In two dimensions one has for the point group 3:

Dimension	2
Rank	2
Point group	3
Permutation symmetry	(0 1)
Basis transformation	Identity
Type	Tensor

The group is generated by a threefold rotation which is represented on a lattice basis by the matrix

$$\begin{array}{cc} 0 & -1 \\ 1 & -1 \end{array}$$

The invariant tensor is:

$$xx = yy = a, \quad xy = yx = -a.$$

This stands for the expression $a * (xx + yy - xy)$.

4.1.3 Metric tensor in three dimensions

The metric tensor invariant under the tetragonal group 4 follows from:

Dimension	3
Rank	2
Point group	4
Permutation symmetry	(0 1)
Basis transformation	Identity
Type	Tensor

There are two free parameters:

$$xx = yy = a, \ zz = b, \ xy = xz = yz = yx = zx = zy = 0.$$

4.1.4 Elastic tensor

The elastic tensor is a rank-four tensor symmetric in the first two, the second two and exchange of first and second pair of indices.

Dimension	3
Rank	4
Point group	4
Permutation symmetry	((0 1)(2 3))
Basis transformation	Identity
Type	Tensor

Result:

$$a * xxxx + b * xxxy + c * xxyy + d * xxzz + e * xyxy + f * xzxz + g * zzzz.$$

There are seven free parameters. For the standard notation where 1=xx, 2=yy, 3=zz, 4=yz, 5=xz, 6=xy the elastic tensor becomes the 6×6 matrix

$$\begin{pmatrix} \alpha_1 & \alpha_3 & \alpha_6 & 0 & 0 & \alpha_2 \\ \alpha_3 & \alpha_1 & \alpha_6 & 0 & 0 & -\alpha_2 \\ \alpha_6 & \alpha_6 & \alpha_5 & 0 & 0 & 0 \\ 0 & 0 & 0 & \alpha_7 & 0 & 0 \\ 0 & 0 & 0 & 0 & \alpha_7 & 0 \\ \alpha_2 & -\alpha_2 & 0 & 0 & 0 & \alpha_4 \end{pmatrix}.$$

$$\alpha_1 = a, \ \alpha_2 = b/4, \ \alpha_3 = c/2, \ \alpha_4 = e/4, \ \alpha_5 = g, \alpha_6 = d/2, \ \alpha_7 = f/4.$$

4.1.5 Vector product

A vector product in three dimensions is an antisymmetric rank-two tensor. For the point group 4 one has:

Dimension	3
Rank	2
Point group	4
Permutation symmetry	[0 1]
Basis transformation	Identity
Type	Pseudotensor

There is one free parameter:

$xy = -yx = a, \quad xx = xz = yy = yz = zx = zy = zz = 0.$

4.1.6 Magnetoelectric tensor

An electric field E may induce a magnetic field M: $M = \chi^{\mathrm{ME}}E$. It is a second-rank pseudotensor. For the point group *mm*2 one has

Dimension	3
Rank	2
Point group	*mm*2 (unique axis *z*)
Permutation symmetry	0 1
Basis transformation	Identity
Type	Pseudotensor

There are two free parameters, and the elements of the invariant tensor are
$xy = a$, $yx = b$, $xx = yy = zz = xz = yz = zx = zy = 0$.

4.2 Character tables

4.2.1 Invariant magnetic field

Point group	*m*
Vector character	3 1
Determinant character	1 -1
Product(1,2)	3 -1
Decompose(3)	1 2

The multiplicity of the trivial representation in the pseudovector representation which is the product of the vector representation and the determinant representation is one. Therefore, there is one free parameter.

4.2.2 Metric tensor

Point group	3
Vector representation	3 0 0
Symmetrized square	6 0 0
Decompose	2 2 2
Physical representation of irrep 2	2 -1 -1

The metric tensor invariant under the three-dimensional group 3 has two free parameters. The six-dimensional space of symmetric rank-two tensors has a two-dimensional invariant subspace. The remaining four-dimensional space carries the irreducible representations 2 and 3 twice. This space is twice the physically irreducible representation 2+3.

4.2.3 Elastic tensor

Point group	4
Vector representation	3 1 -1 1
Symmetrized square	6 0 2 0
Symmetrized square of the former	21 1 5 1
Decompose	7 4 6 4

The elastic tensor is a rank-four tensor with intrinsic symmetry ((1 2)(3 4)). It can be obtained by taking twice the symmetrized square.

4.2.4 Vector product

Point group	4
Vector representation	3 1 -1 1
Antisymmetrized square	3 1 -1 1
Decompose	1 1 1

The vector product of two vectors corresponds to a rank-two tensor with intrinsic symmetry [1 2]. The number of free parameters if the symmetry group is 4 is equal to 1.

4.2.5 Magnetoelectric tensor

Point group	*mm*2
Vector representation	3 -1 1 1
Determinant representation	1 1 -1 -1
Power $n = 2$ of the vector representation	9 1 1 1
Product(former, determinant rep.)	9 1 -1 -1
Decompose	2 3 2 2

The multiplicity of the trivial representation in the decomposition being 2, the number of free parameters in a pseudotensor of rank two invariant under *mm*2 is 2.

4.2.6 Selection rules

Matrix elements $< k|A|m >$ of an operator A transforming with an irreducible representation β between states $|m >$ and $|k >$ transforming with irreducible representations γ and α, respectively, vanish if α is not a component in the decomposition of the tensor product of β and γ. Take as example the group 432. The tensor products of the irreducible representations are given in the following table.

	1	2	3	4	5	γ
1	1	2	3	4	5	
2	2	1	3	5	4	
3	3	3	1+2+3	4+5	4+5	
4	4	5	4+5	1+3+4+5	2+3+4+5	
5	5	4	4+5	2+3+4+5	1+3+4+5	
β						

If $\alpha = 3$ the selection rules for the matrix element $< k|A|m >$ are given in the following table.

	1	2	3	4	5	γ
1	0	0	*	0	0	
2	0	0	*	0	0	
3	*	*	*	0	0	
4	0	0	0	*	*	
5	0	0	0	*	*	
β						