double group. If there are extra representations, these are irreducible representations of the double group: see Table 1.2.6.7.

Table 1.2.6.9. For the 32 three-dimensional crystallographic point groups, the character of the vector representation Γ and the number of times the identity representation occurs in a number of tensor products of this vector representation are given. This is identical to the number of free parameters in a tensor of the corresponding type. For the direct products $K \times C_2$, the character is equal to that of K on the rotation subgroup, and its opposite $[\chi(-R) = -\chi(R)]$ for the coset $-K$.

Table 1.2.6.10. The irreducible projective representations of the 32 three-dimensional crystallographic point groups that have a factor system that is not associated to a trivial one. In three (and two) dimensions all factor systems are of order two.

Table 1.2.6.11. The special points in the Brillouin zones. Strata of irreducible representations of the space groups are characterized by the wavevector **k** of such a point and a (possibly projective) irreducible representation of the point group $K_{\mathbf{k}}$. The latter is the intersection of the symmetry group of **k** (the group of **k** for the holohedral point group) and the point group of the space group. For each Bravais class the special points for the holohedry are given. These are given by their coordinates with respect to a basis of the reciprocal lattice of the conventional cell. These points correspond to Wyckoff positions in the corresponding dual lattice. The symbols for these Wyckoff positions and their site symmetry are given. A well known notation for the special points is that of Kovalev, as used in his book on representations of space groups. Correspondence with the notation in Kovalev (1987) is given.

Table 1.2.6.12. The three-dimensional crystallographic magnetic and nonmagnetic point groups of type I (trivial magnetic, no antichronous elements), type II (nonmagnetic, containing time reversal as an element) and type III (nontrivial magnetic, without time reversal itself, but with antichronous elements).

1.2.7. Introduction to the accompanying software *Tenχar*

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1.2.7.1. *Overview*

The determination of tensors with specified properties often requires long calculations. In principle the algorithms are simple, but in complicated cases errors can be made. This is therefore a situation in which it is best to rely on computer calculations. For this reason, this volume is accompanied by two software packages. Here we shall give a short introduction to the *Tenχar* package that deals with tensors with specific symmetry properties in the first module, and with characters of representations of point groups in the second module. The latter play a role when determining the number of independent elements of a tensor invariant under a given point group, but they are much more widely applicable.

The software package has a graphical interface with windows and buttons. When the program is started, a window opens up in which a choice may be made between the tensor part or the character part of the program.

Within each of the two sections of the program, the results of the calculations are given in numbered windows. It is possible to browse through the various pages. Each page may be sent to a separate window (by the command 'to window'), or to a file (by the command 'to file'). Opened windows may be closed again using a 'close' button.

Special features of the package are that it is dimension- and rank-independent, and that it performs the calculations in an exact way. The number of dimensions and the rank are only limited by the computer memory and by the time the program needs for higher dimensions and ranks. The calculations are exact in the sense of the computer algebra software. Here this is achieved by performing the calculations with integers and

Table 1.2.6.9. *Number of free parameters of some tensors*

Group	Isomorphism class	Character of the vector representation	Multiplicity identity representation in				
			$\Gamma^{\otimes 2}$	$\Gamma_s^{\otimes 2}$	$\Gamma^{\otimes 3}$	$\Gamma \otimes \Gamma_s^{\otimes 2}$	$(\Gamma_s^{\otimes 2})_s^{\otimes 2}$
$\underline{1}$	C_1	3	9	6	27	18	21
$\bar{1}$	C_2	3, −3	9	6	0	0	21
2	C_2	3, −1	5	4	13	8	13
m	C_2	3, 1	5	4	14	10	13
$2/m$	$C_2 \times C_2$		5	4	0	0	13
222	D_2	3, −1, −1, −1	3	3	6	3	9
$2mm$	D_2	3, 1, 1, −1	3	3	7	5	9
mmm	$D_2 \times C_2$		3	3	0	0	9
$\underline{3}$	C_3	3, 0, 0	3	2	9	6	9
$\bar{3}$	$C_3 \times C_2$		3	2	0	0	9
32	D_3	3, 0, −1	2	2	4	2	6
$\underline{3}m$	D_3	3, 0, 1	2	2	5	4	6
$\bar{3}m$	$D_3 \times C_2$		2	2	0	0	6
$\underline{6}$	C_6	3, 2, 0, −1, 0, 2	3	2	7	4	5
$\bar{6}$	C_6	3, 2, 0, 1, 0, −2	3	2	2	2	5
$6/m$	$C_6 \times C_2$		3	2	0	0	5
622	D_6	3, 2, 0, −1, −1, −1	2	2	3	1	5
$6mm$	D_6	3, 2, 0, −1, 1, 1	2	2	4	3	5
$\bar{6}2m$	D_6	3, −2, 0, 1, −1, 1	2	2	1	1	5
$6/mmm$	$D_6 \times C_2$		2	2	0	0	5
$\underline{4}$	C_4	3, 1, −1, 1	3	2	7	4	7
$\bar{4}$	C_4	3, −1, −1, −1	3	2	6	4	7
$4/m$	$C_4 \times C_2$		3	2	0	0	7
422	D_4	3, 1, −1, −1, −1	2	2	3	1	6
$4mm$	D_4	3, 1, −1, 1, 1	2	2	4	3	6
$\bar{4}2m$	D_4	3, −1, −1, −1, 1	2	2	3	2	6
$4/mmm$	$D_4 \times C_2$		2	2	0	0	6
23	T	3, 0, 0, −1	1	1	2	1	3
$m3$	$T \times C_2$		1	1	0	0	3
432	O	3, 0, −1, 1, −1	1	1	1	0	3
$\bar{4}3m$	O	3, 0, −1, −1, 1	1	1	1	1	3
$m3m$	$O \times C_2$		1	1	0	0	3

Table 1.2.6.10. *Irreducible projective representations of the 32 crystallographic point groups*

(*a*) D_2

$A^2 = B^2 = E, (AB)^2 = -E$				
Elements	E	A	B	AB
Γ'_5	2	0	0	0

(*b*) D_4

$A^4 = -E, B^2 = (AB)^2 = E$								
Elements	E	A^2	A	A^3	B	A^2B	AB	A^3B
Γ'_6	2	0	$i\sqrt{2}$	$i\sqrt{2}$	0	0	0	0
Γ'_7	2	0	$-i\sqrt{2}$	$-i\sqrt{2}$	0	0	0	0

(*c*) D_6

$A^6 = B^2 = E, (AB)^2 = -E$												
Elements	E	A^2	A^4	B	A^2B	A^4B	A^3	A	A^5	AB	A^3B	A^5B
Γ'_7	2	2	2	0	0	0	0	0	0	0	0	0
Γ'_8	2	−1	−1	0	0	0	0	$i\sqrt{3}$	$-i\sqrt{3}$	0	0	0
Γ'_9	2	−1	−1	0	0	0	0	$-i\sqrt{3}$	$i\sqrt{3}$	0	0	0

(*d*) T [$\omega = \exp(2\pi i/3)$].

$A^3 = E, B^2 = (AB)^3 = -E$						
Elements	E	A	BAB	BA	AB	A^2
Γ'_5	2	−1	1	1	1	−1
Γ'_6	2	ω^5	ω^2	ω^2	ω^2	ω^5
Γ'_7	2	ω	ω^4	ω^4	ω^4	ω
Elements	ABA	A^2B	BA^2	B	ABA^2	A^2BA
Γ'_5	−1	−1	−1	0	0	0
Γ'_6	ω^5	ω^5	ω^5	0	0	0
Γ'_7	ω	ω	ω	0	0	0

(*e*) O

$A^4 = -E, B^3 = (AB)^2 = E$						
Elements	E	B	AB^2A	A^2B	BA^2	B^2
Γ'_6	2	−1	1	−1	−1	−1
Γ'_7	2	−1	1	−1	−1	−1
Γ'_8	4	1	−1	1	1	1
Elements	BA^2B	ABA^3	A^2B^2	A^2	BA^2B^2	B^2A^2B
Γ'_6	1	1	1	0	0	0
Γ'_7	1	1	1	0	0	0
Γ'_8	−1	−1	−1	0	0	0
Elements	A	A^3	A^3B	BA^3	B^2A	AB^2
Γ'_6	$i\sqrt{2}$	$i\sqrt{2}$	$-i\sqrt{2}$	$-i\sqrt{2}$	$-i\sqrt{2}$	$-i\sqrt{2}$
Γ'_7	$-i\sqrt{2}$	$-i\sqrt{2}$	$i\sqrt{2}$	$i\sqrt{2}$	$i\sqrt{2}$	$i\sqrt{2}$
Γ'_8	0	0	0	0	0	0
Elements	A^2B^2A	BA	AB	AB^2A^2	AB^2A^2B	B^2AB^2
Γ'_6	0	0	0	0	0	0
Γ'_7	0	0	0	0	0	0
Γ'_8	0	0	0	0	0	0

(*f*) $C_4 \times C_2$

$A^4 = B^2 = E, AB = -BA$								
Elements	E	A	A^2	A^3	B	AB	A^2B	A^3B
Γ'_9	2	0	2	0	0	0	0	0
Γ'_{10}	2	0	−2	0	0	0	0	0

(*g*) $C_6 \times C_2$

$A^6 = B^2 = E, AB = -BA$												
Elements	E	A	A^2	A^3	A^4	A^5	B	AB	A^2B	A^3B	A^4B	A^5B
Γ'_{13}	2	0	2	0	2	0	0	0	0	0	0	0
Γ'_{14}	2	0	$2\omega^2$	0	$2\omega^4$	0	0	0	0	0	0	0
Γ'_{15}	2	0	$2\omega^4$	0	$2\omega^4$	0	0	0	0	0	0	0

Table 1.2.6.10 (*cont.*)

(*h*) $D_2 \times C_2$

$A^2 = -E, B^2 = C^2 = (AB)^2 = E, AC = CA, BC = CB$								
Elements	E	A	B	AB	C	AC	BC	ABC
Γ'_9	2	0	0	0	2	0	0	0
Γ'_{10}	2	0	0	0	−2	0	0	0
$A^2 = E, B^2 = C^2 = (AB)^2 = E, AC = -CA, BC = CB$								
Elements	E	A	B	AB	C	AC	BC	ABC
Γ'_{11}	2	0	2	0	0	0	0	0
Γ'_{12}	2	0	−2	0	0	0	0	0
$A^2 = E, B^2 = C^2 = (AB)^2 = E, AC = CA, BC = -CB$								
Elements	E	A	B	AB	C	AC	BC	ABC
Γ'_{13}	2	$2i$	0	0	0	0	0	0
Γ'_{14}	2	$-2i$	0	0	0	0	0	0
$A^2 = -E, B^2 = C^2 = (AB)^2 = E, AC = -CA, BC = CB$								
Elements	E	A	B	AB	C	AC	BC	ABC
Γ'_{15}	2	0	0	0	0	0	2	0
Γ'_{16}	2	0	0	0	0	0	−2	0
$A^2 = -E, B^2 = C^2 = (AB)^2 = E, AC = CA, BC = -CB$								
Elements	E	A	B	AB	C	AC	BC	ABC
Γ'_{17}	2	0	0	0	0	$2i$	0	0
Γ'_{18}	2	0	0	0	0	$-2i$	0	0
$A^2 = E, B^2 = C^2 = (AB)^2 = E, AC = -CA, BC = -CB$								
Elements	E	A	B	AB	C	AC	BC	ABC
Γ'_{19}	2	0	0	$2i$	0	0	0	0
Γ'_{20}	2	0	0	$-2i$	0	0	0	0
$A^2 = -E, B^2 = C^2 = (AB)^2 = E, AC = -CA, BC = -CB$								
Elements	E	A	B	AB	C	AC	BC	ABC
Γ'_{21}	2	0	0	0	0	0	0	$2i$
Γ'_{22}	2	0	0	0	0	0	0	$-2i$

cyclotomics. Use of arbitrary real numbers would imply a finite precision.

Detailed instructions for the use of the program, together with a guided tour (*QuickStart*), can be found in the manual for the program.

1.2.7.2. *Tensors*

The tensor module of *Ten*χ*ar* determines the number of independent elements and the relations between the elements of tensors and pseudotensors invariant under a chosen point group and with specified permutation symmetry of the indices. Although the list of point groups provided in a database is limited to dimensions two and three, the program runs for arbitrary dimensions. Similarly, the choice of index permutation symmetry is limited to rank smaller than or equal to four. This is also not a restriction of the program, which works for arbitrary rank. For higher dimensions and higher ranks, the user needs to provide additional information. The limiting factors are in fact the speed, which becomes low for higher dimensions and/or higher rank, and the available memory, which must be sufficient to store the tensor elements.

When the program is started and the tensor part is chosen *via* a button, a selection box opens. The user can specify dimension and rank in open fields. A field without a coloured border has a formally correct content, but the user should check whether the pregiven numbers correspond to his wishes. In open fields with a coloured border, additional information must be given. Clicking on the button 'point group' results in the opening of a new selection window. A specific two- or three-dimensional point group may be chosen *via* geometric crystal classes. This point group may be viewed if wished. The chosen point group is given by generating matrices and is the one under which the (pseudo)tensor is invariant.

The second symmetry is the index permutation symmetry. For tensors and pseudotensors up to rank four, all possible symmetries are tabulated after clicking 'permutation symmetry'. The indices are numbered from 0 to $r - 1$, where r is the rank. The symbol for a tensor symmetric in the indices 2 and 3 is (2 3), and it is [2 3] if the tensor gets a minus sign under permutation. Arbitrary combinations of symmetric and antisymmetric series can be made. For example, (0 1) 2 [3 4] is a rank-five tensor which is symmetric in the first two indices and antisymmetric in the last two indices. The symbol (0 1 2) characterizes a rank-three tensor that is fully symmetric in all indices. For (pseudo)tensors of rank five and higher, the user needs to specify the permutation symmetry using parentheses in this way. Symmetrization of other pairs is similar. For example, if the rank-three tensor T is symmetric in the first and last indices, the symbol for its permutation character is (0 2) 1. Then $T_{xyz} = T_{zyx}$.

Different settings of the point group may be specified. The standard setting of a point group as given in *International Tables for Crystallography* Volume A may be different from the one to be specified. In this case, the user may perform a basis transformation which transforms the standard setting to the desired setting. This is done *via* the button 'basis transformation'. The standard setting is chosen with 'no transformation'. The transformation from a hexagonal to an orthogonal (Cartesian) basis is performed by selecting 'hC transformation'.

Finally, the tensor or pseudotensor with the specified point group and permutation symmetry is calculated and displayed in a (numbered) window. The command for this is given by clicking on the button 'tensor' or 'pseudotensor', respectively. In the window appear the input data, such as the point group, the