International Tables for Crystallography (2013). Vol. D, Section 1.2.7, pp. 62–70.

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*

By M. Ephraïm, T. Janssen, A. Janner and A. Thiers

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				
			$\Gamma^{\otimes 2}$	$\Gamma_s^{\otimes 2}$	$\Gamma^{\otimes 3}$	$\Gamma \otimes \Gamma_s^{\otimes 2}$	$(\Gamma_s^{\otimes 2})_s^{\otimes 2}$
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
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
$3m$	D_3	3, 0, 1	2	2	5	4	6
$\bar{3}m$	$D_3 \times C_2$		2	2	0	0	6
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
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 *Tenχar* 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

Table 1.2.6.11. *Special points in the Brillouin zones in three dimensions*

(*a*) Triclinic

k		$K_{\mathbf{k}}$	Kovalev
a	000	$\bar{1}$	k_8
b	$00\frac{1}{2}$	$\bar{1}$	k_7
c	$0\frac{1}{2}0$	$\bar{1}$	k_6
d	$\frac{1}{2}00$	$\bar{1}$	k_5
e	$\frac{1}{2}\frac{1}{2}0$	$\bar{1}$	k_4
f	$\frac{1}{2}0\frac{1}{2}$	$\bar{1}$	k_3
g	$0\frac{1}{2}\frac{1}{2}$	$\bar{1}$	k_2
h	$\frac{1}{2}\frac{1}{2}\frac{1}{2}$	$\bar{1}$	k_1

(*b*) Monoclinic *P*

k		$K_{\mathbf{k}}$	Kovalev
a	000	$2/m$	k_7
b	$00\frac{1}{2}$	$2/m$	k_{11}
c	$\frac{1}{2}00$	$2/m$	k_{12}
d	$0\frac{1}{2}0$	$2/m$	k_{13}
e	$0\frac{1}{2}\frac{1}{2}$	$2/m$	k_9
f	$\frac{1}{2}0\frac{1}{2}$	$2/m$	k_8
g	$\frac{1}{2}\frac{1}{2}0$	$2/m$	k_{14}
h	$\frac{1}{2}\frac{1}{2}\frac{1}{2}$	$2/m$	k_{10}
i	00γ	2	k_3
j	$0\frac{1}{2}\gamma$	2	k_5
k	$\frac{1}{2}0\gamma$	2	k_4
l	$\frac{1}{2}\frac{1}{2}\gamma$	2	k_6
m	$\alpha\beta0$	m	k_1
n	$\alpha\beta\frac{1}{2}$	m	k_2

(*c*) Monoclinic *A*

k		$K_{\mathbf{k}}$	Kovalev
a	000	$2/m$	k_6
b	010	$2/m$	k_8
c	$\frac{1}{2}00$	$2/m$	k_7
d	$\frac{1}{2}10$	$2/m$	k_9
e	$0\frac{1}{2}\frac{1}{2}$	$\bar{1}$	k_4
f	$\frac{1}{2}\frac{1}{2}\frac{1}{2}$	$\bar{1}$	k_5
g	00γ	2	k_2
h	$\frac{1}{2}0\gamma$	2	k_3
i	$\alpha\beta0$	m	k_1

(*d*) Orthorhombic *P*

k		$K_{\mathbf{k}}$	Kovalev
a	000	mmm	k_{19}
b	$\frac{1}{2}00$	mmm	k_{20}
c	$00\frac{1}{2}$	mmm	k_{22}
d	$\frac{1}{2}0\frac{1}{2}$	mmm	k_{24}
e	$0\frac{1}{2}0$	mmm	k_{21}
f	$\frac{1}{2}\frac{1}{2}0$	mmm	k_{25}
g	$0\frac{1}{2}\frac{1}{2}$	mmm	k_{23}
h	$\frac{1}{2}\frac{1}{2}\frac{1}{2}$	mmm	k_{26}
i	$\alpha00$	$2mm$	k_7
j	$\alpha0\frac{1}{2}$	$2mm$	k_{12}
k	$\alpha\frac{1}{2}0$	$2mm$	k_{10}
l	$\alpha\frac{1}{2}\frac{1}{2}$	$2mm$	k_{11}
m	$0\beta0$	$m2m$	k_8
n	$0\beta\frac{1}{2}$	$m2m$	k_{15}
o	$\frac{1}{2}\beta0$	$m2m$	k_{13}
p	$\frac{1}{2}\beta\frac{1}{2}$	$m2m$	k_{14}
q	00γ	$mm2$	k_9
r	$0\frac{1}{2}\gamma$	$mm2$	k_{18}
s	$\frac{1}{2}0\gamma$	$mm2$	k_{16}
t	$\frac{1}{2}\frac{1}{2}\gamma$	$mm2$	k_{17}
u	$0\beta\gamma$	m	k_1
v	$\frac{1}{2}\beta\gamma$	$m11$	k_2
w	$\alpha0\gamma$	$1m1$	k_3
x	$\alpha\frac{1}{2}\gamma$	$1m1$	k_4
y	$\alpha\beta0$	$11m$	k_5
z	$\alpha\beta\frac{1}{2}$	$11m$	k_6

(*e*) Orthorhombic *C*

k		$K_{\mathbf{k}}$	Kovalev
a	000	mmm	k_{14}
b	010	mmm	k_{15}
c	$01\frac{1}{2}$	mmm	k_{17}
d	$00\frac{1}{2}$	mmm	k_{16}
e	$\frac{1}{2}\frac{1}{2}0$	$2/m$	k_{12}
f	$\frac{1}{2}\frac{1}{2}\frac{1}{2}$	$2/m$	k_{13}
g	$\alpha00$	$2mm$	k_8
h	$\alpha0\frac{1}{2}$	$2mm$	k_9
i	$0\beta0$	$m2m$	k_{10}
j	$0\beta\frac{1}{2}$	$m2m$	k_{11}
k	00γ	$mm2$	k_6
l	01γ	$mm2$	k_7
m	$\frac{1}{2}\frac{1}{2}\gamma$	112	k_5
n	$0\beta\gamma$	$m11$	k_1
o	$\alpha0\gamma$	$1m1$	k_2
p	$\alpha\beta0$	$11m$	k_3
q	$\alpha\beta\frac{1}{2}$	$11m$	k_4

(*f*) Orthorhombic *I*

k		$K_{\mathbf{k}}$	Kovalev
a	000	mmm	k_{17}
b	001	mmm	k_{18}
c	$0\frac{1}{2}\frac{1}{2}$	$2/m11$	k_{13}
	$1\frac{1}{2}\frac{1}{2}$	$2/m11$	k_{10}
d	$\frac{1}{2}0\frac{1}{2}$	$12/m1$	k_{14}
	$\frac{1}{2}1\frac{1}{2}$	$12/m1$	k_{11}
e	$\frac{1}{2}\frac{1}{2}0$	$112/m$	k_{15}
	$\frac{1}{2}\frac{1}{2}1$	$112/m$	k_{12}
f	$\frac{1}{2}\frac{1}{2}\frac{1}{2}$	222	k_{16}
g	$\alpha00$	$2mm$	k_7
h	$0\beta0$	$m2m$	k_8
i	00γ	$mm2$	k_9
j	$\frac{1}{2}\frac{1}{2}\gamma$	112	k_6
k	$\frac{1}{2}\beta\frac{1}{2}$	121	k_5
l	$\alpha\frac{1}{2}\frac{1}{2}$	211	k_4
m	$0\beta\gamma$	$m11$	k_1
n	$\alpha0\gamma$	$1m1$	k_2
o	$\alpha\beta0$	$11m$	k_3

(*g*) Orthorhombic *F*

k		$K_{\mathbf{k}}$	Kovalev
a	000	mmm	k_{14}
b	100	mmm	k_{15}
c	010	mmm	k_{16}
d	001	mmm	k_{17}
e	$\alpha00$	$2mm$	k_4
f	$\alpha10$	$2mm$	k_5
g	$0\beta0$	$m2m$	k_6
h	$1\beta0$	$m2m$	k_7
i	00γ	$mm2$	k_8
j	01γ	$mm2$	k_9
k	$\frac{1}{2}\frac{1}{2}\frac{1}{2}$	$\bar{1}$	k_{10}
	$-\frac{1}{2}\frac{1}{2}\frac{1}{2}$	$\bar{1}$	k_{11}
	$\frac{1}{2}-\frac{1}{2}\frac{1}{2}$	$\bar{1}$	k_{12}
	$\frac{1}{2}\frac{1}{2}-\frac{1}{2}$	$\bar{1}$	k_{13}
l	$0\beta\gamma$	$m11$	k_1
m	$\alpha0\gamma$	$1m1$	k_2
n	$\alpha\beta0$	$11m$	k_3

(*h*) Tetragonal *P*

k		$K_{\mathbf{k}}$	Kovalev
a	000	$4/mmm$	k_{17}
b	$00\frac{1}{2}$	$4/mmm$	k_{19}
c	$\frac{1}{2}\frac{1}{2}0$	$4/mmm$	k_{18}
d	$\frac{1}{2}\frac{1}{2}\frac{1}{2}$	$4/mmm$	k_{20}
e	$0\frac{1}{2}\frac{1}{2}$	mmm	k_{16}
f	$0\frac{1}{2}0$	mmm	k_{15}
g	00γ	$4mm$	k_{13}
h	$\frac{1}{2}\frac{1}{2}\gamma$	$4mm$	k_{14}
i	$0\frac{1}{2}\gamma$	$mm2$	k_{12}
j	$\alpha\alpha0$	$2mm$	k_{10}
k	$\alpha\alpha\frac{1}{2}$	$2mm$	k_{11}
l	$0\beta0$	$m2m$	k_8
m	$0\beta\frac{1}{2}$	$m2m$	k_9
n	$\alpha\frac{1}{2}0$	$2mm$	k_6
o	$\alpha\frac{1}{2}\frac{1}{2}$	$2mm$	k_7
p	$\alpha\beta0$	$11m$	k_1
q	$\alpha\beta\frac{1}{2}$	$11m$	k_2
r	$\alpha\alpha\gamma$	m	k_5
s	$0\beta\gamma$	$m11$	k_3
t	$\alpha\frac{1}{2}\gamma$	$1m1$	k_4

(*i*) Tetragonal *I*

k		$K_{\mathbf{k}}$	Kovalev
a	000	$4/mmm$	k_{14}
b	001	$4/mmm$	k_{15}
c	$\frac{1}{2}\frac{1}{2}0$	mmm	k_{13}
d	$\frac{1}{2}\frac{1}{2}\frac{1}{2}$	$\bar{4}m2$	k_{12}
e	00γ	$4mm$	k_{10}
f	$\frac{1}{2}0\frac{1}{2}$	$12/m1$	k_{11}
g	$\frac{1}{2}\frac{1}{2}\gamma$	$2mm$	k_9
h	$\alpha\alpha0$	$2mm$	k_7
i	$\alpha00$	$2mm$	k_7
j	$\alpha(1-\alpha)0$	$2mm$	k_8
k	$\frac{1}{2}\beta\frac{1}{2}$	121	k_5
l	$\alpha\beta0$	$11m$	k_2
m	$\alpha\alpha\gamma$	m	k_3
	$\alpha(1-\alpha)\gamma$	m	k_4
n	$\alpha0\gamma$	$1m1$	k_1

(*j*) Trigonal *R* (rhombohedral axes)

k		$K_{\mathbf{k}}$	Kovalev
a	000	$\bar{3}m$	k_7
b	$\frac{1}{2}\frac{1}{2}\frac{1}{2}$	$\bar{3}m$	k_8
c	$\alpha\alpha\alpha$	$3m$	k_6
d	$00\frac{1}{2}$	$2/m$	k_4
e	$\frac{1}{2}\frac{1}{2}0$	$2/m$	k_5
f	$\alpha(-\alpha)0$	2	k_2
g	$\alpha(-\alpha)\frac{1}{2}$	2	k_2
h	$\alpha\beta\beta$	m	k_1

Table 1.2.6.11 (*cont.*)

(k) Hexagonal P

$\mathbf{k}$		$K_{\mathbf{k}}$	Kovalev
a	000	$6/mmm$	k_{16}
b	$00\frac{1}{2}$	$6/mmm$	k_{17}
c	$\frac{1}{3}\frac{1}{3}0$	$\bar{6}m2$	k_{13}
d	$\frac{1}{3}\frac{1}{3}\frac{1}{2}$	$\bar{6}m2$	k_{15}
e	00γ	$6mm$	k_{11}
f	$\frac{1}{2}00$	mmm	k_{12}
g	$\frac{1}{2}0\frac{1}{2}$	mmm	k_{14}
h	$\frac{1}{3}\frac{1}{3}\gamma$	$3m$	k_{10}
i	$\frac{1}{2}0\gamma$	$2mm$	k_9
j	$\alpha 00$	$2mm$	k_5
k	$\alpha 0\frac{1}{2}$	$2mm$	k_7
l	$\alpha\alpha 0$	$2mm$	k_6
m	$\alpha\alpha\frac{1}{2}$	$2mm$	k_8
n	$\alpha 0\gamma$	m	k_3
o	$\alpha\alpha\gamma$	m	k_4
p	$\alpha\beta 0$	m	k_1
q	$\alpha\beta\frac{1}{2}$	m	k_2

(l) Cubic P

$\mathbf{k}$		$K_{\mathbf{k}}$	Kovalev
a	000	$m\bar{3}m$	k_{12}
b	$\frac{1}{2}\frac{1}{2}\frac{1}{2}$	$m\bar{3}m$	k_{13}
c	$\frac{1}{2}\frac{1}{2}0$	$4/mmm$	k_{11}
d	$00\frac{1}{2}$	$4/mmm$	k_{10}
e	00γ	$4mm$	k_8
f	$\frac{1}{2}\frac{1}{2}\gamma$	$4mm$	k_7
g	$\alpha\alpha\alpha$	$3m$	k_9
h	$\frac{1}{2}0\gamma$	$mm2$	k_6
i	$\alpha\alpha 0$	$2mm$	k_4
j	$\alpha\alpha\frac{1}{2}$	$2mm$	k_5
k	$\alpha\beta 0$	$11m$	k_1
l	$\alpha\beta\frac{1}{2}$	$11m$	k_2
m	$\alpha\alpha\gamma$	m	k_3

(m) Cubic F

$\mathbf{k}$		$K_{\mathbf{k}}$	Kovalev
a	000	$m\bar{3}m$	k_{11}
b	001	$4/mmm$	k_{10}
c	$\frac{1}{2}\frac{1}{2}\frac{1}{2}$	$\bar{3}m$	k_9
d	$10\frac{1}{2}$	$\bar{4}m2$	k_8
e	$\alpha 00$	$4mm$	k_6
f	$\alpha\alpha\alpha$	$3m$	k_5
g	$\alpha 01$	$2mm$	k_7
h	$\alpha\alpha 0$	$2mm$	k_4
i	$\alpha(1-\alpha)\frac{1}{2}$	2	k_3
j	$\alpha\beta$	$11m$	k_1
k	$\alpha\alpha\gamma$	m	k_2

(n) Cubic I

$\mathbf{k}$		$K_{\mathbf{k}}$	Kovalev
a	000	$m\bar{3}m$	k_{11}
b	001	$m\bar{3}m$	k_{10}
c	$\frac{1}{2}\frac{1}{2}\frac{1}{2}$	$\bar{4}3m$	k_{10}
d	$\frac{1}{2}\frac{1}{2}0$	mmm	k_9
e	$\alpha 00$	$4mm$	k_8
f	$\alpha\alpha\alpha$	$3m$	k_7
g	$\alpha\frac{1}{2}\frac{1}{2}$	$2mm$	k_6
h	$\alpha\alpha 0$	$2mm$	k_4
i	$\alpha(1-\alpha)0$	$2mm$	k_9
j	$\alpha\beta$	$11m$	k_1
k	$\alpha\alpha\gamma$	m	k_2
	$\alpha(1-\alpha)\gamma$	m	k_3

Table 1.2.6.12. *Magnetic point groups*

Type I	Type II	Type III
1	$1'$	
$\bar{1}$	$\bar{1}1'$	$\bar{1}'$
2	$21'$	$2'$
m	$m1'$	m'
$2/m$	$21'/m$	$2'/m$, $2/m'$, $2'/m'$,
222	$2221'$	$2'2'$
$2mm$	$2mm1'$	$2'mm'$, $2m'm'$
mmm	$mmm1'$	$m'mm$, $m'm'm$, $m'm'm'$
4	$41'$	$4'$
$\bar{4}$	$\bar{4}1'$	$\bar{4}'$
$4/m$	$41'/m$	$4'/m$, $4/m'$, $4'/m'$
422	$4221'$	$4'22'$, $42'2'$
$4mm$	$4mm1'$	$4'mm'$, $4m'm'$
$\bar{4}2m$	$\bar{4}2m1'$	$\bar{4}'2'm$, $\bar{4}'2m'$, $\bar{4}2'm'$
$4/mmm$	$4/mmm1'$	$4/m'mm$, $4'/mm'm$, $4'/m'm'm$, $4/mm'm'$, $4/m'm'm'$
3	$31'$	
$\bar{3}$	$\bar{3}1'$	$\bar{3}'$
32	$321'$	$32'$
$3m$	$3m1'$	$3m'$
$\bar{3}m$	$\bar{3}m1'$	$\bar{3}'m$, $\bar{3}'m'$, $\bar{3}m'$
6	$61'$	$6'$
$\bar{6}$	$\bar{6}1'$	$\bar{6}'$
$6/m$	$61'/m$	$6'/m$, $6/m'$, $6'/m'$
622	$6221'$	$6'22'$, $62'2'$
$6mm$	$6mm1'$	$6'mm'$, $6m'm'$
$\bar{6}2m$	$\bar{6}2m1'$	$\bar{6}'2'm$, $\bar{6}'2m'$, $\bar{6}2'm'$
$6/mmm$	$6/mmm1'$	$6/m'mm$, $6'/mm'm$, $6'/m'm'm$, $6/mm'm'$, $6/m'm'm'$
23	$231'$	
$m\bar{3}$	$m\bar{3}1'$	$m'\bar{3}$
432	$4321'$	$4'32'$
$\bar{4}3m$	$\bar{4}3m1'$	$\bar{4}'3m'$
$m\bar{3}m$	$m\bar{3}m1'$	$m'\bar{3}m$, $m\bar{3}m'$, $m'\bar{3}m'$

dimension, the rank, the permutation symmetry and the setting basis transformation, and the calculated data: the number of independent elements (f) and the relations of these elements. They are either zero or expressed in terms of the free parameters $a_0, \ldots, a_{f-1}$. The tensor elements are given by sequences $x, y, z, \ldots$. The four elements of a general rank-two tensor in two dimensions are xx, xy, yx, yy, corresponding to T_{11}, T_{12}, T_{21} and T_{22}, respectively.

1.2.7.3. *Characters*

Calculations with characters of representations of point groups can be done in the character module of the program. It is selected in the main window by clicking ‘character’. A selection window opens in which a point group may be selected just as in the tensor module. The point groups are organized according to dimension and geometric crystal class. Selection of a point group leads to the display of the character table if one asks for it by selecting ‘view character table’.

The character table consists of a square array of (complex) numbers. The number of rows is the number of nonequivalent irreducible representations and is equal to the number of columns, which is the number of conjugacy classes of the group. For crystallographic groups, the complex numbers that form the entries of the character table are cyclotomic numbers. These are linear combinations with fractions as coefficients of complex numbers of the form $\exp(2\pi in/m)$. For example, the square root of -1 (i) can be written as $\exp(2\pi i 1/4)$. A real number like $\sqrt{2}$ can be written as

$$\sqrt{2} = \tfrac{1}{2}\sqrt{2}(1 + i + 1 - i) = \exp(2\pi i \tfrac{1}{8}) + \exp(2\pi i \tfrac{7}{8}).$$

Another example is

$$\sqrt{5} = 1 + 2\exp(2\pi i \tfrac{1}{5}) + 2\exp(2\pi i \tfrac{4}{5}).$$

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 $a, b, \ldots$.

(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 mth 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 pth 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 ((0 1)(2 3)), 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.

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

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 $i_1, \ldots, i_p$, only polynomials $x_{i_1}x_{i_2}\ldots x_r$ occur in the basis for which $i_1 \leq i_2 \leq \ldots \leq i_p$. Then $x_{i_1}x_{i_2} = x_{i_2}x_{i_1}$. If there is antisymmetry among these indices, one has the condition $i_1 < i_2 < \ldots < i_p$ 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 $x_ix_j\ldots$ under the matrix $g \in G$ is given by the polynomial

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

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

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

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

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

The function $\mathrm{Det}(g)$ 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:

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

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 $A_1A_2\ldots$ 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 ith conjugacy class (given as the second row in the character table), $\chi_\alpha(i)$ the cyclotomic in the ith row and αth column of the character table, and $\chi(i)$ the calculated character in the ith 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 nth 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

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

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 $f_i \le f_{i-1}$.

(2) For each such decomposition $m = 1,\ldots n_{\rm tot}$ 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 mth decomposition, P_m should be divided by $t!$ for each t-tuple of equal values $(f_{k+1} = \ldots = f_{k+t})$.

(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

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

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

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

Then $P(M-E)Q = D$, with D diagonal. There are four diagonal elements of D which are zero, and the invariant tensors correspond to the corresponding four columns of the matrix Q. The invariant polynomials are

$$xxx + yyy + zzz, \quad xxy + xzz + yyz, \quad xxz + yzz + xyy, \quad xyz.$$

Example (2). Dimension 2, rank 2, symmetry type (12). Group generated by

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

Basis xx, xy, yy goes to yy, $-xy + yy$, $xx - 2xy + yy$. This gives

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

Because

$$\begin{pmatrix} 1&0&0\\ 2&1&2\\ 1&0&1 \end{pmatrix}(M-E)\begin{pmatrix} 1&-1&1\\ 0&1&0\\ 0&-1&1 \end{pmatrix} = \begin{pmatrix} -1&0&0\\ 0&0&0\\ 0&0&2 \end{pmatrix},$$

the invariant tensor corresponds to the second column of Q, which as a polynomial reads $-xx + xy - yy$. This can be written with the tensor T_{ij} as

$$-xx + xy - yy = -\sum_{i,j} T_{ij} x_i x_j, \quad T_{ij} = \begin{pmatrix} 1 & -\frac{1}{2} \\ -\frac{1}{2} & 1 \end{pmatrix}.$$

This tensor T is invariant under the group.

Example (3). Dimension 3, rank 2, tensor type (12). Group generated by matrix([[0 −1 0][1 0 0][0 0 1]]). The basis xx, xy, xz, yy, yz, zz goes under the generator to yy, $-xy$, $-yz$, xx, xz, zz. The solution of $(M-E)v = 0$ is

$$\alpha_1(xx + yy) + \alpha_2 zz.$$

The matrix D has two zeros on the diagonal.

Example (4). Dimension 3, rank 3, type (123). Same group as in Example (3). Basis xxx, xxy, xxz, xyy, xyz, xzz, yyy, yyz, yzz, zzz. The solution

$$\alpha_1(xxz + yyz) + \alpha_2 zzz$$

corresponds to a tensor with relations $T_{113} = T_{223}$, $T_{111} = T_{112} = T_{122} = T_{123} = T_{133} = T_{222} = T_{233} = 0$.

Example (5). Dimension 3, rank 4, type ((12)(34)). Not only $i_1 \le i_2$ and $i_3 \le i_4$, but also $(i_1 i_2)$, should come lexicographically before $(i_3 i_4)$. Basis $xxxx$, $xxxy$, $xxxz$, $xxyy$, $xxyz$, $xxzz$, $xyxy$, $xyxz$, $xyyy$, $xyyz$, $xyzz$, $xzxz$, $xzyy$, $xzyz$, $xzzz$, $yyyy$, $yyyz$, $yyzz$, $yzyz$, $yzzz$, $zzzz$. Under the same group as in example (3), there are seven invariants. Invariant polynomial:

$$\alpha_1(xxxx + yyyy) + \alpha_2(xxxy - xyyy) + \alpha_3 xxyy + \alpha_4 xyxy + \alpha_5 zzzz + \alpha_6(xxzz + yyzz) + \alpha_7(xzxz + yzyz).$$

Table 1.2.7.2. *Calculation with characters*

Generator	Composite character	Characters				Decomposition
$\begin{pmatrix} 0&1&0\\ 0&0&1\\ 1&0&0 \end{pmatrix}$	R	E	A	AA		
	$\chi(R)$	3	0	0		
	$\chi(R)^3$	27	0	0		
	$\chi(R^2)$	3	0	0		
	$\chi(R^2)\chi(R)$	9	0	0		
	$\chi(R^3)$	3	3	3		
Example (1)	$\frac{1}{6}(\chi(R)^3 + 3\chi(R^2)\chi(R) + 2\chi(R^3))$	10	1	1		$4D_1 + 3D_2 + 3D_3$
$\begin{pmatrix} 0&-1\\ 1&-1 \end{pmatrix}$	R	E	A	AA		
	$\chi(R)$	2	−1	−1		
	$\chi(R)^2$	4	1	1		
	$\chi(R^2)$	2	−1	−1		
Example (2)	$\frac{1}{2}(\chi(R)^2 + \chi(R^2))$	3	0	0		$D_1 + D_2 + D_3$
$\begin{pmatrix} 0&-1&0\\ 1&0&0\\ 0&0&1 \end{pmatrix}$	R	E	A	AA	AAA	
	$\chi(R)$	3	1	−1	1	
	$\chi(R)^2$	9	1	1	1	
	$\chi(R^2)$	3	−1	3	−1	
Example (3)	$\frac{1}{2}(\chi(R)^2 + \chi(R^2))$	6	0	2	0	$2D_1 + D_2 + 2D_3 + D_4$
As above	$\chi(R)$	3	1	−1	1	
Example (4)	$\chi(R)^3$	27	1	−1	1	
	$\chi(R^2)$	3	−1	3	−1	
	$\chi(R^2)\chi(R)$	9	−1	−3	−1	
	$\chi(R^3)$	3	1	−1	1	
	$\frac{1}{6}(\chi(R)^3 + 3\chi(R^2)\chi(R) + 2\chi(R^3))$	10	0	−2	0	$2D_1 + 3D_2 + 2D_3 + 3D_4$
As above	$\chi(R)$	3	1	−1	1	
Example (5)	$\frac{1}{2}(\chi(R)^2 + \chi(R^2)) = \chi_s(R)$	6	0	2	0	
	$\chi_s(R)^2$	36	0	4	0	
	$\chi_s(R^2)$	6	2	6	2	
	((12)(34))	21	1	5	1	$7D_1 + 4D_2 + 6D_3 + 4D_4$
As above, example (6)	$\frac{1}{2}(\chi(R)^2 - \chi(R^2))$	3	1	−1	1	$D_1 + D_2 + D_4$
As above, example (7)	$\frac{1}{6}(\chi(R)^3 - 3\chi(R^2)\chi(R) + 2\chi(R^3))$	1	1	1	1	D_1

This corresponds to the tensor relations

$$\begin{array}{lll} \mathrm{T}_{xxxx} = -\mathrm{T}_{yyyy} & \mathrm{T}_{xxxy} = \mathrm{T}_{xyyy} & \mathrm{T}_{xxxz} = 0 \\ \mathrm{T}_{xxyz} = 0 & \mathrm{T}_{xxzz} = \mathrm{T}_{yyzz} & \mathrm{T}_{xyxz} = 0 \\ \mathrm{T}_{xyyz} = 0 & \mathrm{T}_{xyzz} = 0 & \mathrm{T}_{xzxz} = \mathrm{T}_{yzyz} \\ \mathrm{T}_{xzyy} = 0 & \mathrm{T}_{xzyz} = 0 & \mathrm{T}_{xzzz} = 0 \\ \mathrm{T}_{yyyz} = 0 & \mathrm{T}_{yzzz} = 0 & \end{array}$$

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

The latter form is that of an elastic tensor with the usual convention $1 = xx$, $2 = yy$, $3 = zz$, $4 = yz$, $5 = xz$, $6 = xy$.

Example (6). Dimension 3, rank 2, type [12]. The same group as in example (3). Basis $xy, xz, yz \rightarrow -yx, -yz, xz$, which are equivalent to $xy, -yz, xz$. The transformation in the tensor space is

$$M = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & -1 & 0 \end{pmatrix} \rightarrow \begin{pmatrix} 0 & 0 & 0 \\ 0 & -1 & 1 \\ 0 & -1 & -1 \end{pmatrix} v = 0:$$

$$v = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \sim xy.$$

There is just one invariant antisymmetric polynomial $xy = -yx$ corresponding to the tensor

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

Example (7). Dimension 3, rank 3, type [123]. Basis xyz invariant under the group: $xyz \rightarrow -yxz \sim xyz$. The corresponding tensor is the fully antisymmetric rank 3 tensor: $\mathrm{T}_{ijk} = 1$ if ijk is an even permutation of 123, $= -1$ if ijk is an odd permutation, and $= 0$ if two or three indices are equal (permutation tensor, see Section 1.1.3.7.2).

Example (8). Calculation with characters. See Table 1.2.7.2.

Example (9). The action matrix for a pseudotensor.

Take the group $4/m$ with generators

$$\begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}.$$

Consider the rank 3 pseudotensor (123). The action matrix is determined from the action of the generators A and B on the basis:

	A	B
xxx	$-yyy$	$-xxx$
xxy	xyy	$-xxy$
xxz	yyz	xxz
xyy	$-xxy$	$-xyy$
xyz	$-xyz$	xyz
xzz	$-yzz$	$-xzz$
yyy	xxx	$-yyy$
yyz	xxz	yyz
yzz	xzz	$-yzz$
zzz	zzz	zzz

Therefore, the action matrix becomes

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

After diagonalization, one finds two nonzero elements on the diagonal:

$$zzz = a; \quad xxz = yyz = b;$$
$$xxx = xxy = xyy = xyz = xzz = yyy = yzz = 0.$$

1.2.8. Glossary

$\mathrm{T}_{i_1 \ldots i_n}$	tensor of rank n
$O(n)$	orthogonal group
$\mathbb{Z}$	ring of integers
$\mathbf{e}_i$	basis vectors
g	metric tensor
K	point group
R	orthogonal transformation
C_m	cyclic group of order m
$SO(n)$	special orthogonal group
$\mathbb{Z}^+$	positive integers
D_n	dihedral group of order n
E	unit transformation, matrix or element
I	inversion
$D(K)$	representation of K
$\Gamma(K)$	matrix representation of K
$\lvert K \rvert$	order of K
$\oplus$	sum of spaces or operators
$\otimes$	tensor product
$\in$	element of
$\mathbf{a}_i$	basis of space or lattice