Table 1.2.6.11 (*cont.*)

(*k*) Hexagonal *P*

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*

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*

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*

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

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 $\exp(2\pi i n/m)$. 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 4*mm* 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.

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

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

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 $i_1, \ldots, i_p$, 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: