

1. TENSORIAL ASPECTS OF PHYSICAL PROPERTIES

$$D(a^{-2}ha^2) = U^{*-1}U^{-1}D(h)UU^*$$

$$D(a^{-2}ha^2) = D(a^2)^{-1}D(h)D(a^2).$$

(Notice that $a^2 \in H$.) Because $D(H)$ is irreducible, it follows that $UU^*D(a^{-2})$ is a multiple of the identity: $UU^* = \chi D(a^2)$. The factor χ is real because

$$D(a^2)^* = U^{-1}D(a^2)U = U^{-1}UU^*U/\chi$$

and

$$D(a^2)^* = U^*U/\chi^*.$$

Hence $\chi = \chi^* = \pm 1$.

The conditions for the transformed matrix $M(ah)$ to be block diagonal then read

$$\pm|\mu|^2D(a^2)D(a^{-1}ha) = |\sigma|^2D(aha), \quad (1.2.5.16)$$

with the corresponding expressions for λ and ρ . If χ is equal to -1 , these equations do not have a solution. However, when $\chi = +1$ there is a solution, which means that the co-representation is reducible, contrary to the assumption. Therefore, this situation can not occur.

One can summarize these considerations in the following theorem.

Theorem 1. If the restriction of an irreducible co-representation to the orthochronous subgroup is reducible, then either the (two) irreducible components are non-equivalent, or they are equivalent and connected by a basis transformation U for which $UU^* = -D(a^2)$. If the restriction $M(H)$ is irreducible, it is equivalent to $M(a^{-1}Ha)^*$.

In the former case, the dimension of the co-representation is twice that of the restriction, in the latter case they are equal. Therefore, one has the following corollary.

Corollary. A d -dimensional irreducible representation of the orthochronous subgroup H can occur as irreducible component of the restriction of an irreducible co-representation of G with dimension m with

$$\begin{aligned} m &= 2d \text{ if } D(H) \text{ nonequivalent to } D(a^{-1}Ha)^* \\ m &= 2d \text{ if } D(H) \text{ equivalent to } D(a^{-1}Ha)^* \text{ and } UU^* = -D(a^2) \\ m &= d \text{ if } D(H) \text{ equivalent to } D(a^{-1}Ha)^* \text{ and } UU^* = +D(a^2). \end{aligned}$$

The three cases from theorem (1) can be distinguished by the following theorem:

Theorem 2. The irreducible representation $D(H)$ with character $\chi(H)$ belongs to the respective cases of theorem (1) if

$$\sum_{h \in H} \chi(ahah) = \begin{cases} 0 & \text{for the first case} \\ -N & \text{for the second case} \\ N & \text{for the third case.} \end{cases} \quad (1.2.5.17)$$

The proof of theorem (2) goes as follows. We have

$$\begin{aligned} \sum_{h \in H} \chi(ahah) &= \sum_{h \in H} \sum_{i=1}^d D(ahah)_{ii} \\ &= \sum_{i,k,l} D(a^2)_{ik} \sum_{h \in H} D(a^{-1}ha)_{kl} D(h)_{li}, \end{aligned} \quad (1.2.5.18)$$

and this gives zero if $D(H)$ and $D(a^{-1}Ha)^*$ are non-equivalent, because of the orthogonality relations. If the two representations are equivalent, we take for convenience unitary representations. Then there is a unitary matrix U with

$$D(a^{-1}ha)^* = U^{-1}D(h)U.$$

Then we have

$$\begin{aligned} \sum_{h \in H} \chi(ahah) &= \sum_{iklmn} D(a^2)_{ik}(U^{*-1})_{km} \sum_{h \in H} D(h)_{mn}^* U_{nl} D(h)_{li} \\ &= (N/d) \sum_{i,k,\ell} D(a^2)_{ik}(U^{*-1})_{k\ell} U_{i\ell}^* \\ &= (N/d) \sum_{i,k} D(a^2)_{ik}(U^*U)_{ik} \\ &= \pm(N/d) \sum_{i,k} D(a^2)_{ik} D(a^{-2})_{ki} = \pm N. \end{aligned}$$

This proves theorem (2).

In the special case of a group G in which the time reversal $1'$ occurs as element, one may choose $a = 1'$. In this case, a^2 is the identity and the expressions simplify. Theorem (1) now states that an irreducible d -dimensional representation $D(H)$ of an orthochronous group can occur as irreducible component in the restriction of an irreducible m -dimensional co-representation of $H \times \{E, 1'\}$, with

$$\begin{aligned} m &= 2d \text{ if } D(H) \text{ nonequivalent to } D(H)^* \\ m &= 2d \text{ if } D(H) = UD(H)^*U^{-1} \text{ and } UU^* = -E \\ m &= d \text{ if } D(H) = UD(H)^*U^{-1} \text{ and } UU^* = +E, \end{aligned}$$

which correspond to, respectively, [cf. theorem (2)]

$$\sum_{h \in H} \chi(h^2) = \begin{cases} 0 \\ -N \\ +N \end{cases} \quad (1.2.5.19)$$

For a spinless particle, the time-reversal operator is the complex conjugation θ . This generates a co-representation of the group \mathbb{Z}_2 . The symmetry group is the direct product of the point group H and \mathbb{Z}_2 . Compared to the degeneracy d of a state characterized by the irreducible representation $D(H)$, the degeneracy is double ($m = 2d$) for the first two cases and the same for the third case. When it is a particle with spin $\frac{1}{2}$, the time-reversal operator is $\sigma_2\theta$, which is of order 4. If one takes for the coset representative a the time reversal, one has $D(a^2) = -E$. Therefore, the degeneracy is now doubled in the first and third case, and the same for the second. This is Kramer's degeneracy.

1.2.6. Tables

In the following, a short description of the tables is given in order to facilitate consultation without reading the introductory theoretical Sections 1.2.2 to 1.2.5.

Table 1.2.6.1. Finite point groups in three dimensions. The point groups are grouped by isomorphism class. There are four infinite families and six other isomorphism classes. (Notation: C_n for the cyclic group of order n , D_n for the dihedral group of order $2n$, T , O and I the tetrahedral, octahedral and icosahedral groups, respectively). Point groups of the first class are subgroups of $SO(3)$, those of the second class contain $-E$, and those of the third class are not subgroups of $SO(3)$, but do not contain $-E$ either. The families C_n and D_n are also isomorphism classes of two-dimensional finite point groups.

Table 1.2.6.2. Among the infinite number of finite three-dimensional point groups, 32 are crystallographic.

Table 1.2.6.3. Character table for the cyclic groups C_n . The generator is denoted by α . The number of elements in the conjugacy classes (n_i) is one for each class. The order is the smallest nonnegative power p for which $A^p = E$. The n irreducible representations are denoted by Γ_i .

Table 1.2.6.4. Character tables for the dihedral groups D_n of order $2n$. n_i is the number of elements in the conjugacy class C_i . The irreducible representations are denoted by Γ_i .

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Table 1.2.6.1. Finite point groups in three dimensions

Isomorphism class	First class with determinants > 0	Second class with $-E$	Third class without $-E$	Order
C_n	n		\bar{n} (n even, > 2) m ($n = 2$)	n
D_n	$n22$ (n even) $n2$ (n odd, > 1)		mmm (n even) $\bar{n}2m$ (n even) nm (n odd)	$2n$
$C_n \times C_2$		\bar{n} (n odd) n/m (n even)		$2n$
$D_n \times C_2$		n/mmm (n even, ≥ 4) mmm ($n = 2$) $\bar{n}m$ (n odd, > 0)		$4n$
T	23			12
O	432		$\bar{4}3m$	24
I	532			60
$T \times C_2$		$m\bar{3}$		24
$O \times C_2$		$m\bar{3}m$		48
$I \times C_2$		$\bar{5}3m$		120

Table 1.2.6.5. The character tables for the 32 three-dimensional crystallographic point groups. The groups are grouped by isomorphism class (there are 18 isomorphism classes).

For each isomorphism class, the character table is given, including the symbol for the isomorphism class, the number n of elements per conjugacy class and the order of the elements in each such class. The conjugation classes are specified by representative elements expressed in terms of the generators α, β, \dots . The irreps are denoted by Γ_i , where i takes as many values as there are conjugation classes. In each isomorphism class for each point group, given by its international symbol and its Schoenflies symbol, identification is made between the generators of the abstract group (α, β) and the generating orthogonal transformations. Notation: C_{nx} is a rotation of $2\pi/n$ along the x axis, σ_x is a reflection from a plane perpendicular to the x axis, S_{nz} is a rotation over $2\pi/n$ along the z axis multiplied by $-E$ and σ_v is a reflection from a plane through the unique axis.

The notation for the irreducible representations can be given as Γ_i , but other systems have been used as well. Indicated below are the relations between Γ_i and a system that uses a characterization according to the dimension of the representation and (for

groups of the second kind) the sign of the representative of $-E$. This nomenclature is often used by spectroscopists.

A, A_1, A_2, A', A''	one-dimensional
B, B_1, B_2, B_3	one-dimensional
E	two-dimensional
T, T_1, T_2	three-dimensional
A_g, B_g etc.	gerade
A_u, B_u etc.	ungerade

The other notation for which the relation with the present notation is indicated is that of Kopský, and is used in the accompanying software.

The three functions x, y and z transform according to the vector representation of the point group, which is generally reducible. The reduction into irreducible components of this three-dimensional vector representation is indicated.

The six bilinear functions $x^2, xy, xz, y^2, yz, z^2$ transform according to the symmetrized product of the vector representation. The basis functions of the irreducible components are indicated. Because the basis functions are real, one should consider the physically irreducible representations.

Table 1.2.6.6. The point groups of the second class containing $-E$ are obtained from those of the first class by taking the direct product with the group generated by $\bar{1}$. From the point groups, one obtains nonmagnetic point groups by the direct product with the group generated by the time reversal $1'$. The relation between the characters of a point group and its direct products with

Table 1.2.6.2. Crystallographic point groups in three dimensions

Isomorphism class	First class	Second class with $-E$	Third class without $-E$	Order
C_1	1			1
C_2	2	$\bar{1}$	m	2
C_3	3			3
C_4	4		$\bar{4}$	4
D_2	222	$2/m$	$2mm$	4
C_6	6	$\bar{3}$	$\bar{6}$	6
D_3	32		$3m$	6
$C_4 \times C_2$		$4/m$		8
D_4	422		$4mm, \bar{4}2m$	8
$D_2 \times C_2$		mmm		8
D_6	622	$\bar{3}m$	$6mm, \bar{6}2m$	12
T	23			12
$C_6 \times C_2$		$6/m$		12
$D_4 \times C_2$		$4/mmm$		16
O	432		$\bar{4}3m$	24
$D_6 \times C_2$		$6/mmm$		24
$T \times C_2$		$m\bar{3}$		24
$O \times C_2$		$m\bar{3}m$		48

Table 1.2.6.3. Irreducible representations for cyclic groups C_n

$\omega = \exp(2\pi i/n)$, l.c.d. = largest common divisor.

n_i	ε	α	α^2	α^3	...	α^{n-1}
Order	1	n	$n/\text{l.c.d.}(n, 2)$	$n/\text{l.c.d.}(n, 3)$...	n
Γ_1	1	1	1	1	...	1
Γ_2	1	ω	ω^2	ω^3	...	ω^{-1}
\vdots	\vdots	\vdots	\vdots	\vdots	\ddots	\vdots
Γ_n	1	ω^{-1}	ω^{-2}	ω^{-3}	...	ω

Table 1.2.6.4. Irreducible representations for dihedral groups D_n

(a) n odd. $m = 1, \dots, (n-1)/2$; $j = 1, \dots, (n-1)/2$, l.c.d. = largest common divisor.

n_i	ε	α^j	...	β
Order	1	$n/\text{l.c.d.}(n, j)$...	n
Γ_1	1	1	...	1
Γ_2	1	1	...	-1
Γ_{2+m}	2	$2\cos(2\pi mj/n)$...	0

(b) n even. $m = 1, \dots, (n/2 - 1)$; $j = 1, \dots, (n/2 - 1)$, l.c.d. = largest common divisor.

n_i	ε	$\alpha^{n/2}$	α^j	...	β	$\alpha\beta$
Order	1	2	$n/\text{l.c.d.}(n, j)$...	$n/2$	$n/2$
Γ_1	1	1	1	...	1	1
Γ_2	1	1	1	...	-1	-1
Γ_3	1	$(-1)^{n/2}$	$(-1)^j$...	1	-1
Γ_4	1	$(-1)^{n/2}$	$(-1)^j$...	-1	1
Γ_{4+m}	2	$(-1)^{m/2}$	$2\cos(2\pi mj/n)$...	0	0

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Table 1.2.6.5. Irreducible representations and character tables for the 32 crystallographic point groups in three dimensions

(a) C_1

C_1	ε
n	1
Order	1
Γ_1	1

$$1 \quad \Gamma_1 : A = \chi_1 \quad x, y, z \quad x^2, y^2, z^2, yz, xz, xy$$

(e) C_6 [$\omega = \exp(\pi i/3)$].

C_6	ε	α	α^2	α^3	α^4	α^5
n	1	1	1	1	1	1
Order	1	6	3	2	3	6
Γ_1	1	1	1	1	1	1
Γ_2	1	ω	ω^2	-1	- ω	- ω^2
Γ_3	1	ω^2	- ω	1	ω^2	- ω
Γ_4	1	-1	1	-1	1	-1
Γ_5	1	- ω	ω^2	1	- ω	ω^2
Γ_6	1	- ω^2	- ω	-1	ω^2	ω

(b) C_2

C_2	ε	α
n	1	1
Order	1	2
Γ_1	1	1
Γ_2	1	-1

$$2 \quad \alpha = C_{2z} \quad \Gamma_1 : A = \chi_1 \quad z \quad x^2, y^2, z^2, xy$$

$$C_2 \quad \Gamma_2 : B = \chi_3 \quad x, y \quad yz, xz$$

$$m \quad \alpha = \sigma_z \quad \Gamma_1 : A' = \chi_1 \quad x, y \quad x^2, y^2, z^2, xy$$

$$C_s \quad \Gamma_2 : A'' = \chi_3 \quad z \quad yz, xz$$

$$\bar{1} \quad \alpha = I \quad \Gamma_1 : A_g = \chi_1^+ \quad x^2, y^2, z^2, yz, xz, xy$$

$$C_i \quad \Gamma_2 : A_u = \chi_1^- \quad x, y, z$$

Matrices of the real representations:

	$\Gamma_2 \oplus \Gamma_6$	$\Gamma_3 \oplus \Gamma_5$
ε	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$
α	$\begin{pmatrix} 1 & -1 \\ 1 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & -1 \\ 1 & -1 \end{pmatrix}$
α^2	$\begin{pmatrix} 0 & -1 \\ 1 & -1 \end{pmatrix}$	$\begin{pmatrix} -1 & 1 \\ -1 & 0 \end{pmatrix}$
α^3	$\begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$
α^4	$\begin{pmatrix} -1 & 1 \\ -1 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & -1 \\ 1 & -1 \end{pmatrix}$
α^5	$\begin{pmatrix} 0 & 1 \\ -1 & 1 \end{pmatrix}$	$\begin{pmatrix} -1 & 1 \\ -1 & 0 \end{pmatrix}$

(c) C_3 [$\omega = \exp(2\pi i/3)$].

C_3	ε	α	α^2
n	1	1	1
Order	1	3	3
Γ_1	1	1	1
Γ_2	1	ω	ω^2
Γ_3	1	ω^2	ω

Matrices of the real two-dimensional representation:

	ε	α	α^2
$\Gamma_2 \oplus \Gamma_3$	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 0 & -1 \\ 1 & -1 \end{pmatrix}$	$\begin{pmatrix} -1 & 1 \\ -1 & 0 \end{pmatrix}$

$$3 \quad \alpha = C_{3z} \quad \Gamma_1 : A = \chi_1 \quad z \quad x^2 + y^2, z^2$$

$$C_3 \quad \Gamma_2 \oplus \Gamma_3 : E = \chi_{1c} + \chi_{1c}^* \quad x, y \quad x^2 - y^2, xz, yz, xy$$

$$6 \quad \alpha = C_{6z} \quad \Gamma_1 : A = \chi_1 \quad z \quad x^2 + y^2, z^2$$

$$C_6 \quad \Gamma_4 : B = \chi_3 \quad x, y \quad xz, yz$$

$$\Gamma_2 \oplus \Gamma_6 : E_1 = \chi_{1c} + \chi_{1c}^* \quad x, y \quad x^2 - y^2, xy$$

$$\Gamma_3 \oplus \Gamma_5 : E_2 = \chi_{2c} + \chi_{2c}^* \quad x, y \quad x^2 - y^2, xy$$

$$\bar{3} \quad \alpha = S_{3z} \quad \Gamma_1 : A_g = \chi_1^+ \quad x^2 + y^2, z^2$$

$$S_6 \quad \Gamma_4 : A_u = \chi_1^- \quad z$$

$$\Gamma_2 \oplus \Gamma_6 : E_u = \chi_{1c}^- + \chi_{1c}^{*-} \quad x, y$$

$$\Gamma_3 \oplus \Gamma_5 : E_g = \chi_{1c}^+ + \chi_{1c}^{*+} \quad x^2 - y^2, xy, xz, yz$$

$$\bar{6} \quad \alpha = S_{6z} \quad \Gamma_1 : A' = \chi_1 \quad x^2 + y^2, z^2$$

$$C_{3h} \quad \Gamma_4 : A'' = \chi_3 \quad z$$

$$\Gamma_2 \oplus \Gamma_6 : E' = \chi_{2c} + \chi_{2c}^* \quad xz, yz$$

$$\Gamma_3 \oplus \Gamma_5 : E'' = \chi_{1c} + \chi_{1c}^* \quad x, y \quad x^2 - y^2, xy$$

(d) C_4

C_4	ε	α	α^2	α^3
n	1	1	1	1
Order	1	4	2	4
Γ_1	1	1	1	1
Γ_2	1	i	-1	- i
Γ_3	1	-1	1	-1
Γ_4	1	- i	-1	i

Matrices of the real two-dimensional representation:

	ε	α	α^2	α^3
$\Gamma_2 \oplus \Gamma_4$	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$	$\begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$

$$4 \quad \alpha = C_{4z} \quad \Gamma_1 : A = \chi_1 \quad z \quad x^2 + y^2, z^2$$

$$C_4 \quad \Gamma_3 : B = \chi_3 \quad x^2 - y^2, xy$$

$$\Gamma_2 \oplus \Gamma_4 : E = \chi_{1c} + \chi_{1c}^* \quad x, y \quad yz, xz$$

$$\bar{4} \quad \alpha = S_4 \quad \Gamma_1 : A = \chi_1 \quad x^2 + y^2, z^2$$

$$S_4 \quad \Gamma_3 : B = \chi_3 \quad z \quad x^2 - y^2, xy$$

$$\Gamma_2 \oplus \Gamma_4 : E = \chi_{1c} + \chi_{1c}^* \quad x, y \quad yz, xz$$

(f) D_2

D_2	ε	α	β	$\alpha\beta$
n	1	1	1	1
Order	1	2	2	2
Γ_1	1	1	1	1
Γ_2	1	1	-1	-1
Γ_3	1	-1	1	-1
Γ_4	1	-1	-1	1

$$222 \quad \alpha = C_{2x} \quad \Gamma_1 : A_1 = \chi_1 \quad x^2, y^2, z^2$$

$$D_2 \quad \beta = C_{2y} \quad \Gamma_2 : B_3 = \chi_3 \quad x \quad yz$$

$$\alpha\beta = C_{2z} \quad \Gamma_3 : B_2 = \chi_4 \quad y \quad xz$$

$$\Gamma_4 : B_1 = \chi_2 \quad z \quad xz$$

$$mm2 \quad \alpha = C_{2z} \quad \Gamma_1 : A_1 = \chi_1 \quad z \quad x^2, y^2, z^2$$

$$C_{2v} \quad \beta = \sigma_x \quad \Gamma_2 : A_2 = \chi_2 \quad xy$$

$$\alpha\beta = \sigma_y \quad \Gamma_3 : B_2 = \chi_3 \quad y \quad yz$$

$$\Gamma_4 : B_1 = \chi_4 \quad x \quad xz$$

$$2/m \quad \alpha = C_{2z} \quad \Gamma_1 : A_g = \chi_1^+ \quad x^2, y^2, z^2, xy$$

$$C_{2h} \quad \beta = \sigma_z \quad \Gamma_2 : A_u = \chi_1^- \quad z \quad z$$

$$\alpha\beta = I \quad \Gamma_3 : B_u = \chi_3^- \quad x, y$$

$$\Gamma_4 : B_g = \chi_3^+ \quad x, y$$

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Table 1.2.6.5 (cont.)

(g) D_3

D_3	ε	α	β
n	1	2	3
Order	1	3	2
Γ_1	1	1	1
Γ_2	1	1	-1
Γ_3	2	-1	0

Matrices of the two-dimensional representation:

	ε	α	β
Γ_3	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 0 & -1 \\ 1 & -1 \end{pmatrix}$	$\begin{pmatrix} -1 & 1 \\ 0 & 1 \end{pmatrix}$

32	$\alpha = C_{3z}$	$\Gamma_1 : A_1 = \chi_1$	z	$x^2 + y^2, z^2$
D_3	$\beta = C_{2x}$	$\Gamma_2 : A_2 = \chi_2$	x, y	$xz, yz, xy, x^2 - y^2$
		$\Gamma_3 : E = \chi_1$		
3m	$\alpha = C_{3z}$	$\Gamma_1 : A_1 = \chi_1$	z	$x^2 + y^2, z^2$
C_{3v}	$\beta = \sigma_v$	$\Gamma_2 : A_2 = \chi_2$	x, y	$xz, yz, xy, x^2 - y^2$
		$\Gamma_3 : E = \chi_1$		

(h) D_4

D_4	ε	α	α^2	β	$\alpha\beta$
n	1	2	1	2	2
Order	1	4	2	2	2
Γ_1	1	1	1	1	1
Γ_2	1	1	1	-1	-1
Γ_3	1	-1	1	1	-1
Γ_4	1	-1	1	-1	1
Γ_5	2	0	-2	0	0

Matrices of the two-dimensional representation:

	Γ_5
ε	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$
α	$\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$
α^2	$\begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}$
β	$\begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$
$\alpha\beta$	$\begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix}$

422	$\alpha = C_{4z}$	$\Gamma_1 : A_1 = \chi_1$	z	$x^2 + y^2, z^2$
D_4	$\beta = C_{2x}$	$\Gamma_2 : A_2 = \chi_2$	x, y	$x^2 - y^2, xy, xz, yz$
		$\Gamma_3 : B_1 = \chi_3$		
		$\Gamma_4 : B_2 = \chi_4$		
		$\Gamma_5 : E = \chi_1$		
4mm	$\alpha = C_{4z}$	$\Gamma_1 : A_1 = \chi_1$	z	$x^2 + y^2, z^2$
C_{4v}	$\beta = \sigma_v$	$\Gamma_2 : A_2 = \chi_2$	x, y	$x^2 - y^2, xy, xz, yz$
		$\Gamma_3 : B_1 = \chi_3$		
		$\Gamma_4 : B_2 = \chi_4$		
		$\Gamma_5 : E = \chi_1$		
$\bar{4}2m$	$\alpha = S_{4z}$	$\Gamma_1 : A_1 = \chi_1$	x, y	$x^2 + y^2, z^2$
D_{2d}	$\beta = C_{2v}$	$\Gamma_2 : A_2 = \chi_2$	z	$x^2 - y^2, xy, xz, yz$
	$\alpha\beta = \sigma_d$	$\Gamma_3 : B_1 = \chi_3$		
		$\Gamma_4 : B_2 = \chi_4$		
		$\Gamma_5 : E = \chi_1$		

(i) D_6

D_6	ε	α	α^2	α^3	β	$\alpha\beta$
n	1	2	2	1	3	3
Order	1	6	3	2	2	2
Γ_1	1	1	1	1	1	1
Γ_2	1	1	1	1	-1	-1
Γ_3	1	-1	1	-1	1	-1
Γ_4	1	-1	1	-1	-1	1
Γ_5	2	1	-1	-2	0	0
Γ_6	2	-1	-1	2	0	0

Matrices of the two-dimensional representations:

	Γ_5	Γ_6
ε	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$
α	$\begin{pmatrix} 1 & -1 \\ 1 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & -1 \\ 1 & -1 \end{pmatrix}$
α^2	$\begin{pmatrix} 0 & -1 \\ 1 & -1 \end{pmatrix}$	$\begin{pmatrix} -1 & 1 \\ -1 & 0 \end{pmatrix}$
α^3	$\begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$
β	$\begin{pmatrix} -1 & 1 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} -1 & 1 \\ 0 & 1 \end{pmatrix}$
$\alpha\beta$	$\begin{pmatrix} -1 & 0 \\ -1 & 1 \end{pmatrix}$	$\begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix}$

622	$\alpha = C_{6z}$	$\Gamma_1 : A_1 = \chi_1$	z	$x^2 + y^2, z^2$
D_6	$\beta = C_{2x}$	$\Gamma_2 : A_2 = \chi_2$	x, y	$x^2 - y^2, xy, xz, yz$
		$\Gamma_3 : B_1 = \chi_3$		
		$\Gamma_4 : B_2 = \chi_4$		
		$\Gamma_5 : E_1 = \chi_1$		
		$\Gamma_6 : E_2 = \chi_2$		
6mm	$\alpha = C_{6z}$	$\Gamma_1 : A_1 = \chi_1$	z	$x^2 + y^2, z^2$
C_{6v}	$\beta = \sigma_v$	$\Gamma_2 : A_2 = \chi_2$	x, y	$x^2 - y^2, xy, xz, yz$
		$\Gamma_3 : B_1 = \chi_3$		
		$\Gamma_4 : B_2 = \chi_4$		
		$\Gamma_5 : E_1 = \chi_1$		
		$\Gamma_6 : E_2 = \chi_2$		
$\bar{6}2m$	$\alpha = S_{6z}$	$\Gamma_1 : A'_1 = \chi_1$	x, y	$x^2 + y^2, z^2$
D_{3h}	$\beta = C_{2v}$	$\Gamma_2 : A'_2 = \chi_2$	z	$x^2 - y^2, xy, xz, yz$
	$\alpha\beta = \sigma_d$	$\Gamma_3 : A''_1 = \chi_3$		
		$\Gamma_4 : A''_2 = \chi_4$		
		$\Gamma_5 : E' = \chi_2$		
		$\Gamma_6 : E'' = \chi_1$		
$\bar{3}m$	$\alpha = S_{3z}$	$\Gamma_1 : A_{1g} = \chi_{1g}^+$	x, y	$x^2 + y^2, z^2$
D_{3d}	$\beta = \sigma_d$	$\Gamma_2 : A_{2g} = \chi_{2g}^+$	z	$x^2 - y^2, xy, xz, yz$
		$\Gamma_3 : A_{1u} = \chi_{1u}^-$		
		$\Gamma_4 : A_{2u} = \chi_{2u}^-$		
		$\Gamma_5 : E_u = \chi_{1u}^-$		
		$\Gamma_6 : E_g = \chi_{1g}^+$		

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

T	ε	α	α^2	β
n	1	4	4	3
Order	1	3	3	2
Γ_1	1	1	1	1
Γ_2	1	ω	ω^2	1
Γ_3	1	ω^2	ω	1
Γ_4	3	0	0	-1

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Table 1.2.6.5 (cont.)

Real representations of dimension $d > 1$:

	$\Gamma_2 \oplus \Gamma_3$	Γ_4
ε	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$
α	$\begin{pmatrix} 1 & -1 \\ 0 & -1 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}$
α^2	$\begin{pmatrix} 1 & -1 \\ 0 & -1 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$
β	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$

23 $\alpha = C_{3d}$ $\Gamma_1 : A = \chi_1$ $x^2 + y^2 + z^2$
 T $\beta = C_{2z}$ $\Gamma_2 \oplus \Gamma_3 : E = \chi_{3c} + \chi_{3c}^*$ $x^2 - y^2, x^2 - z^2$
 $\Gamma_4 : T = \chi_1$ x, y, z xy, xz, yz

(k) O

O	ε	β	α^2	α	$\alpha\beta$
n	1	8	3	6	6
Order	1	3	2	4	2
Γ_1	1	1	1	1	1
Γ_2	1	1	1	-1	-1
Γ_3	2	-1	2	0	0
Γ_4	3	0	-1	1	-1
Γ_5	3	0	-1	-1	1

Higher-dimensional representations:

	Γ_3	Γ_4	Γ_5
ε	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$
β	$\begin{pmatrix} 0 & -1 \\ 1 & -1 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$
α^2	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$
α	$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$
$\alpha\beta$	$\begin{pmatrix} -1 & 0 \\ -1 & 1 \end{pmatrix}$	$\begin{pmatrix} -1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & -1 & 0 \end{pmatrix}$

432 $\alpha = C_{4z}$ $\Gamma_1 : A_1 = \chi_1$ $x^2 + y^2 + z^2$
 O $\beta = C_{3d}$ $\Gamma_2 : A_2 = \chi_2$
 $\alpha\beta = C_2$ $\Gamma_3 : E = \chi_3$ $x^2 - y^2, y^2 - z^2$
 $\Gamma_4 : T_1 = \chi_1$ x, y, z
 $\Gamma_5 : T_2 = \chi_2$ xy, xz, yz

$\bar{4}3m$ $\alpha = S_{4z}$ $\Gamma_1 : A_1 = \chi_1$ $x^2 + y^2 + z^2$
 T_d $\beta = C_{3d}$ $\Gamma_2 : A_2 = \chi_2$
 $\alpha\beta = \sigma_d$ $\Gamma_3 : E = \chi_3$ $x^2 - y^2, y^2 - z^2$
 $\Gamma_4 : T_1 = \chi_1$ x, y, z
 $\Gamma_5 : T_2 = \chi_2$ xy, yz, xz

Other point groups which are of second class and contain $-E$. See Table 1.2.6.6(a).

Group	Isomorphism class	Rotation subgroup
$4/m$	$C_4 \times \mathbb{Z}_2$	4
$6/m$	$C_6 \times \mathbb{Z}_2$	6
mmm	$D_2 \times \mathbb{Z}_2$	222
$4/mmm$	$D_4 \times \mathbb{Z}_2$	422
$6/mmm$	$D_6 \times \mathbb{Z}_2$	622
$m\bar{3}$	$T \times \mathbb{Z}_2$	23
$m\bar{3}m$	$O \times \mathbb{Z}_2$	432

Table 1.2.6.6. Direct products with $\{E, \bar{1}\}$ and $\{E, 1'\}$

(a) With $\{E, \bar{1}\}$.

$K \times \mathbb{Z}_2$	$R \in K$	\bar{R}
Γ_g	$\chi(R)$	$\chi(R)$
Γ_u	$\chi(R)$	$-\chi(R)$

$4/m$ $C_4 \times \mathbb{Z}_2$ cf. 4
 $6/m$ $C_6 \times \mathbb{Z}_2$ cf. 6
 mmm $D_2 \times \mathbb{Z}_2$ cf. 222
 $4/mmm$ $D_4 \times \mathbb{Z}_2$ cf. 422
 $6/mmm$ $D_6 \times \mathbb{Z}_2$ cf. 622
 $m\bar{3}$ $T \times \mathbb{Z}_2$ cf. 23
 $m\bar{3}m$ $O \times \mathbb{Z}_2$ cf. 432

(b) With $\{E, 1'\}$.

$K \times \mathbb{Z}_2$	$R \in K$	R'
Γ_+	$\chi(R)$	$\chi(R)$
Γ_-	$\chi(R)$	$-\chi(R)$

$1'$ $C_1 \times \mathbb{Z}_2$ cf. 1
 $21'$ $C_2 \times \mathbb{Z}_2$ cf. 2
 $m1'$ $C_2 \times \mathbb{Z}_2$ cf. m
 $2221'$ $D_2 \times \mathbb{Z}_2$ cf. 222
 $2mm1'$ $D_2 \times \mathbb{Z}_2$ cf. $2mm$
 $41'$ $C_4 \times \mathbb{Z}_2$ cf. 4
 $41'$ $C_4 \times \mathbb{Z}_2$ cf. 4
 $4mm1'$ $D_4 \times \mathbb{Z}_2$ cf. $4mm$
 $4221'$ $D_4 \times \mathbb{Z}_2$ cf. 422
 $42m1'$ $D_4 \times \mathbb{Z}_2$ cf. $42m$
 $31'$ $C_3 \times \mathbb{Z}_2$ cf. 3
 $321'$ $D_3 \times \mathbb{Z}_2$ cf. 32
 $31'$ $C_6 \times \mathbb{Z}_2$ cf. 3
 $3m1'$ $D_3 \times \mathbb{Z}_2$ cf. $3m$
 $6mm1'$ $D_6 \times \mathbb{Z}_2$ cf. $6mm$
 $61'$ $C_6 \times \mathbb{Z}_2$ cf. 6
 $61'$ $C_6 \times \mathbb{Z}_2$ cf. 6
 $6221'$ $D_6 \times \mathbb{Z}_2$ cf. 622
 $62m1'$ $D_6 \times \mathbb{Z}_2$ cf. $62m$
 $231'$ $T \times \mathbb{Z}_2$ cf. 23
 $4321'$ $O \times \mathbb{Z}_2$ cf. 432
 $43m1'$ $O \times \mathbb{Z}_2$ cf. $43m$

(c) With $\{E, \bar{1}\}$ and $\{E, 1'\}$.

$K \times \mathbb{Z}_2 \times \mathbb{Z}_2$	$R \in K$	\bar{R}	R'	\bar{R}'
Γ_{g+}	$\chi(R)$	$\chi(R)$	$\chi(R)$	$\chi(R)$
Γ_{u+}	$\chi(R)$	$-\chi(R)$	$\chi(R)$	$-\chi(R)$
Γ_{g-}	$\chi(R)$	$\chi(R)$	$-\chi(R)$	$-\chi(R)$
Γ_{u-}	$\chi(R)$	$-\chi(R)$	$-\chi(R)$	$\chi(R)$

$\bar{1}'$ $C_1 \times \mathbb{Z}_2 \times \mathbb{Z}_2$ cf. 1
 $21'/m$ $C_2 \times \mathbb{Z}_2 \times \mathbb{Z}_2$ cf. 2
 $4/m1'$ $C_4 \times \mathbb{Z}_2 \times \mathbb{Z}_2$ cf. 4
 $6/m1'$ $C_6 \times \mathbb{Z}_2 \times \mathbb{Z}_2$ cf. 6
 $mmm1'$ $D_2 \times \mathbb{Z}_2 \times \mathbb{Z}_2$ cf. 222
 $4/mmm1'$ $D_4 \times \mathbb{Z}_2 \times \mathbb{Z}_2$ cf. 422
 $\bar{3}m1'$ $D_6 \times \mathbb{Z}_2 \times \mathbb{Z}_2$ cf. $3m$
 $6/mmm1'$ $D_6 \times \mathbb{Z}_2 \times \mathbb{Z}_2$ cf. 622
 $m31'$ $T \times \mathbb{Z}_2 \times \mathbb{Z}_2$ cf. 23
 $m(\bar{3})m1'$ $O \times \mathbb{Z}_2 \times \mathbb{Z}_2$ cf. 432

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groups generated by $\bar{1}$, $1'$ and $\{\bar{1}, 1'\}$ are given in Tables 1.2.6.6(a), (b) and (c), respectively.

Table 1.2.6.7. The representations of a point group are also representations of their double groups. In addition, there are extra representations which give projective representations of the point groups. For several cases, these are associated with an ordinary representation. As extra representations, those irreducible representations of the double point groups that give rise to projective representations of the point groups with a factor system that is not associated with the trivial one are given. These do not correspond to ordinary representations of the single group.

Table 1.2.6.8. If one chooses for each element of a point group one of the two corresponding $SU(2)$ elements, the latter form a projective representation of the point group. If one selects for the rotation $R \in K \subset SO(3)$ the element

$$u(R) = E \cos(\varphi/2) + i(\boldsymbol{\sigma} \cdot \mathbf{n}) \sin(\varphi/2),$$

where φ is the rotation angle and \mathbf{n} the rotation axis, and for $R \in K \subset O(3) \setminus SO(3)$ the element

$$u(R) = E \cos(\psi/2) + i(\boldsymbol{\sigma} \cdot \mathbf{n}) \sin(\psi/2),$$

where ψ and \mathbf{n} are the rotation angle and axis of the rotation $-R$, the matrices $u(R)$ form a projective representation:

$$u(R)u(R') = \omega_s(R, R')u(RR').$$

The factor system ω_s is the spin factor system. It is determined via the generators and defining relations

$$W_i(A_1, \dots, A_p) = E$$

of the point group K . Then

$$W_i(u(A_1), \dots, u(A_p)) = \lambda_i E,$$

and the factors λ_i fix uniquely the class of the factor system ω_s . These factors are given in the table.

Because $\bar{1}$ is represented by the unit matrix in spin space, the double groups of two isomorphic point groups obtained from each other by replacing the elements $R \in O(3) \setminus SO(3)$ by $-R$ are the same.

The projective representations with factor system ω_s may sometimes be associated with one with a trivial factor system. If this is the case, there are actually no extra representations of the

Table 1.2.6.7. Extra representations of double point groups

222^d Γ_5'	E	$-E$	$\pm A$	$\pm B$	$\pm AB$				
	2	-2	0	0	0				
422^d Γ_6' Γ_7'	E	$-E$	$\pm A^2$	A	$-A$	$\pm B$	$\pm AB$		
	2	-2	0	$\sqrt{2}$	$-\sqrt{2}$	0	0		
	2	-2	0	$-\sqrt{2}$	$\sqrt{2}$	0	0		
622^d Γ_8' Γ_9' Γ_7'	E	$-E$	A^2	$-A^2$	$\pm B$	$\pm A^3$	A^5	$-A^5$	$\pm A^3 B$
	2	-2	1	-1	0	0	$\sqrt{3}$	$-\sqrt{3}$	0
	2	-2	1	-1	0	0	$-\sqrt{3}$	$\sqrt{3}$	0
	2	-2	-2	2	0	0	0	0	0
23^d Γ_5' Γ_6' Γ_7'	E	$-E$	A	$-A$	A^2	$-A^2$	$\pm B$		
	2	-2	1	-1	1	-1	0		
	2	-2	ω	ω^4	ω^2	ω^5	0		
	2	-2	ω^5	ω^2	ω^4	ω	0		
432^d Γ_6' Γ_7' Γ_8'	E	$-E$	B	$-B$	$\pm A^2$	A	$-A$	$\pm AB$	
	2	-2	1	-1	0	$\sqrt{2}$	$-\sqrt{2}$	0	
	2	-2	1	-1	0	$-\sqrt{2}$	$\sqrt{2}$	0	
	4	-4	-1	1	0	0	0	0	

Table 1.2.6.8. Projective spin representations of the 32 crystallographic point groups

Point group	Relations giving λ_i	Double group	Extra representations
$\bar{1}$ $\bar{1}$	$A = E$ $A^2 = E$	1^d	No No
$2, m$ $2/m$	$A^2 = -E$ $A^2 = B^2 = -E, (AB)^2 = E$	2^d	No
$222, 2mm$ mmm	$A^2 = B^2 = (AB)^2 = -E$ $A^2 = B^2 = (AB)^2 = -E$ $C^2 = E, AC = CA, BC = CB$	222^d	Yes
$4, \bar{4}$ $4/m$	$A^4 = -E$ $A^4 = B^2 = -E, AB = BA$	4^d	No
$422, 4mm, \bar{4}2m$ $4/mmm$	$A^4 = B^2 = (AB)^2 = -E$ As above, plus $C^2 = E, AC = CA, BC = CB$	422^d	Yes
$\bar{3}$ $\bar{3}$	$A^3 = -E$ $A^6 = E$	3^d	No
$\bar{3}2, 3m$ $\bar{3}m$	$A^3 = B^2 = (AB)^2 = -E$ $A^6 = E, B^2 = (AB)^2 = -E$	32^d	No
$6, \bar{6}$ $6/m$	$A^6 = -E$ $A^6 = B^2 = -E, AB = BA$	6^d	No
$622, 6mm, \bar{6}2m$ $6/mmm$	$A^6 = B^2 = (AB)^2 = -E$ As above, plus $C^2 = E, AC = CA, BC = CB$	622^d	Yes
23 $m\bar{3}$	$A^3 = B^2 = (AB)^3 = -E$ As above, plus $C^2 = E, AC = CA, BC = CB$	23^d	Yes
$432, \bar{4}3m$ $m\bar{3}m$	$A^4 = B^3 = (AB)^2 = -E$ As above, plus $C^2 = E, AC = CA, BC = CB$	432^d	Yes

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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 \mathbf{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 \mathbf{k} (the group of \mathbf{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				
			$\Gamma^{\otimes 2}$	$\Gamma_s^{\otimes 2}$	$\Gamma^{\otimes 3}$	$\Gamma \otimes \Gamma_s^{\otimes 2}$	$(\Gamma_s^{\otimes 2})_s^{\otimes 2}$
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
$m\bar{3}$	$T \times C_2$		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
$m\bar{3}m$	$O \times C_2$		1	1	0	0	3