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TABLES OF REPRESENTATION AND ROTATION MATRICES FOR THE RELATIVISTIC IRREDUCIBLE REPRESENTATIONS OF 38 POINT GROUPS

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Abstract. Explicit tables of representation and rotation matrices are given for the relativistic irreducible representations of the 32 crystallographic point groups and of the linear and five-fold symmetry groups.

1. INTRODUCTION

Explicit tables of representation and rotation matrices for various double point groups are useful for constructing relativistic molecular orbitals or for assigning them.

The representation matrices for the groups C_{2v}, C_{3v}, D_{3d}, C_{4v}, D_{4h}, T_d, O and O_h were published by Onodera and Okazaki [1] and those for D_{3h} by Toivonen and Pyykkö [2]. The purpose of the present tables is to give for future reference the representation and rotation matrices and the corresponding basis functions for the 38 point groups enumerated in Appendix 1. The eight-fold and the icosahedral groups are missing from the present compilation. Unless otherwise indicated, the treatment is based on and consistent with the tables of Koster *et al.* [3]. The conventions are defined in Appendix 2 and the resulting tables given in Appendix 3.

2. THEORY

Symmetry operations. The group elements are n-fold rotations, C_n, reflexion planes, σ, or rotation reflexions, S_n. The inversion is denoted by I and the identity by E. For the irreducible representations, all the usual labels are given, i.e. the Γ_i notation of Bethe (1929) (also used by Bradley and Cracknell [4] and by Koster et al. [3]), the Griffith [5] notation and the Herzberg [6] notation.

Rotation operators. Consider an operator R giving the coordinates in a rotated system,

$$r' = \mathrm{R}r. \tag{1}$$

Let the operator P_R act on a scalar function $f(r)$ in Hilbert space to make it follow the coordinate system so that

$$f'(r') = (P_R f)(r') \; \{= f(r)\} \tag{2}$$

The left-hand side,

$$f'(r') = (P_R f)(r') \tag{2a}$$

is called the *active interpretation*. Note the use of r' on both sides.

In the *passive interpretation*

$$P_R f(\mathrm{R}r) = f(r), \tag{2b}$$

rewritten as

$$f(r') = (P_R^{-1} f)(r), \tag{3}$$

the operator leaves the function unchanged but changes the coordinates from r to r'.

As an example, consider the effect of an anti-clockwise rotation through α on the the function $f(\phi)$. Then $\mathrm{R}\phi = \phi' = \phi - \alpha$, whence

$$\exp\{im(\phi'+\alpha)\} = \exp(im\alpha)\exp(im\phi') = \exp(im\phi), \tag{4}$$

corresponding to

$$f'(\phi') = P_R f(\phi') = \exp(im\alpha)\exp(im\phi') = f(\phi). \tag{5}$$

Thus the operator for the active interpretation is

$$P_R = \exp(im\alpha). \tag{6}$$

Euler angles. Consider a right-handed coordinate system. Let a positive rotation carry a right-handed screw forward along the rotation axis. The three Euler angles are defined as (i) A rotation around the z axis through α. The new system is $x'y'z'$. Analogously with eq. (5),

$$f'(r') = \exp(i\alpha j_{z'})\, f(r') \tag{7}$$

(ii) A rotation around the new y' through β.
The new system is $x''y''z''$.

(iii) A rotation around the new z'' through γ.
The rotation operator corresponding to an active rotation through the Euler angles $(\alpha\beta\gamma)$ in the "*temporary*" coordinates above is

$$P_R(\alpha\beta\gamma) = \exp(i\gamma j_z)\exp(i\beta j_y)\exp(i\alpha j_z), \tag{8}$$

with the same arguments (xyz) being used on both sides. If "fixed" rotation axes are used instead of the temporary ones, the rotation operators act in the inverse order

$$P_R(\alpha\beta\gamma) = \exp(i\alpha j_z)\exp(i\beta j_y)\exp(i\gamma j_z) \tag{9}$$

The convention used in deriving Appendix 3 is the "active, fixed" one.

Rotation of spherical harmonics. Let now $f = Y_{\ell m}(\theta, \phi)$. In the "active, temporary" interpretation, the transformed functions becomes

$$Z'(\theta', \phi') = \exp(i\gamma j_{z'})\exp(i\beta j_{y'})\exp(i\alpha j_{z'})\, Y_{\ell m}(\theta'\phi'). \tag{10}$$

This is not a spherical harmonic but we know that the $Y_{\ell m}$ with a given ℓ transform into each other under rotations. In the "passive, temporary" interpretation

$$\begin{aligned} Y_{\ell m}(\theta'\phi') &= \exp(-i\alpha j_z)\exp(-i\beta j_y)\exp(-i\gamma j_z)\, Y_{\ell m}(\theta\phi) \\ &\equiv \sum_{m'} D^{\ell}_{m'm}(\alpha\beta\gamma)\, Y_{\ell m'}(\theta\phi). \end{aligned} \tag{11}$$

Thus our convention is that the active, fixed rotations 1.γ, 2.β, 3.α take the (xyz) axes to (x'y'z') while the equation (11) takes the spherical harmonics in the (x'y'z') system back to (xyz). Equation (11) defines the Wigner rotation matrices

$$D^{\ell}_{m'm}(\alpha\beta\gamma) = \langle \ell m' | e^{-i\alpha j_z} e^{-i\beta j_y} e^{-i\gamma j_z} | \ell m \rangle. \tag{12}$$

For half-integer angular momenta, replace ℓ by j:

$$P_R^{-1} | jm > = \sum_{m'} | jm' > D^j_{m'm} (\alpha\beta\gamma). \tag{13}$$

The present conventions correspond to those in Messiah [7], Rose [8] and Tinkman [9]. Replacing the operators j by their eigenvalues m,

$$D^j_{m'm} = e^{-i\alpha m'} d^j_{m'm} e^{-i\gamma m} \tag{14}$$

with

$$d^j_{m'm}(\beta) = < jm' | e^{-i\beta j_y} | jm >. \tag{15}$$

An explicit expression, orginally due to Weyl, is

$$d^j_{m'm}(\beta) = \sum_k \frac{(-)^k \{(j+m)!(j-m)!(j+m')!(j-m')!\}^{1/2}}{k!(j+m-k)!(j-m'-k)!(k+m'-m)!} \left(\cos\frac{\beta}{2}\right)^{2j-2k-m'+m} \left(-\sin\frac{\beta}{2}\right)^{2k+m'-m} \tag{16}$$

The simplified forms for $\beta = 0$ or $\beta = \pi$ are

$$d^j_{m'm}(0) = \delta_{m'm} \tag{17}$$

$$d^j_{m'm}(\pi) = (-)^{-j+m} \delta_{m',-m}. \tag{18}$$

Construction of basis functions. The basis functions ϕ^k_λ, belonging to the row λ of the irreducible representation ("irrep") k are obtained by using the projection operators

$$P^{(k)}_{\lambda\nu} = \frac{n_k}{g} \sum_R \Gamma^{(k)}_{\lambda\nu}(R)^* P_R , \tag{19}$$

where n_k is the dimension of the irrep k, g the order of the double group, $\Gamma^{(k)}(R)$ the representation matrix for the group element R and the irrep k and P_R is the symmetry operation in Hilbert space, corresponding to P_R in eq. (2). Thus we can first project out from an arbitrary function ψ the part transforming as the row λ of k,

$$\phi^k_\lambda = P^{(k)}_{\lambda\lambda} \psi \tag{20}$$

and then construct its partners from the equation (Rosén and Ellis [10])

$$\phi_\nu^k = P_{\nu\lambda}^{(k)} \phi_\lambda^k \tag{21}$$

with

$$P_{\nu\lambda}^{(k)} | j\ell m > = \frac{n_k}{g} \sum_R \Gamma_{\nu\lambda}^{(k)} (R)^* (-)^{\ell\tau_R} \sum_{m'=-j}^{j} | j\ell m' > D_{m'm}^j (\alpha\beta\gamma). \tag{22}$$

where

$$\tau_R = \begin{cases} 1, & \text{R contains an inversion} \\ 0, & \text{otherwise} \end{cases} \tag{23}$$

In analogy with the statement following eq. (11), if the "fixed, active" Euler angles 1. γ, 2. β, 3. α carry out the group operation, then the eq. (3), or in this case (13), takes the transformed function back to the original coordinates.

Barred and unbarred operations. Bethe (1929) arrived at the double-group concept by heuristically including in the group the element $\bar{E}$, corresponding to the rotations through 2π and having the property

$$\bar{E}^2 = E. \tag{24}$$

The new elements $\bar{A} = \bar{E}A$ then double the order of the group G.

For rotations around the same axis

$$C_2 R_i = \begin{cases} \bar{R}_j & \text{for } 0 < R_i < \pi \\ R_j & \text{for } -\pi < R_i < 0 \end{cases} \tag{25}$$

while e.g. in the group C_{3v}

$$C_3 \sigma_v'' = \overline{\sigma_v} . \tag{26}$$

The eq. (25) limits the Euler angles to

$$-\pi < \alpha + \gamma \leqslant \pi \tag{27}$$

$$0 \leqslant \beta \leqslant \pi . \tag{28}$$

The representation and rotation matrices for the barred operations are obtained for the present irreps with half-integer j from

$$\Gamma(\bar{R}) = -\Gamma(R) \tag{29}$$

$$D_{m'm}^j (\bar{R}) = -D_{m'm}^j (R) . \tag{30}$$

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APPENDIX 1.

Index to the tables in Appendix 3

Table(s)	Group(s)
1	C_1
2	C_i
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6	D_2 and C_{2v}
7	D_{2h}
8	C_4 and S_4
9	C_{4h}
10	D_4, C_{4v} and D_{2d}
11	D_{4h}
12	C_3
13	C_{3i}
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25	$C_{\infty v}$ and $D_{\infty h}$
26,27	D_5 and C_{5v}
28	D_{5d}
29,30	D_{5h}

APPENDIX 2.

Definitions of special functions

The spherical harmonics used are defined as

$$Y_{\ell m}(\theta\phi) = (-)^{(m+|m|)/2}\left[\frac{2\ell+1}{4\pi}\,\frac{(\ell-|m|)!}{(\ell+|m|)!}\right]^{1/2} P_{\ell|m|}(\cos\theta)\,e^{im\phi} ,$$

with the associated Legendre polynomial

$$P_{\ell m}(x) = (1-x^2)^{m/2}\, d^m P_\ell(x)/dx^m$$

where the Legendre polynomial

$$P_\ell(x) = \frac{1}{2^\ell \ell!}\,\frac{d^\ell}{dx^\ell}(x^2-1)^\ell .$$

These spherical harmonics have the parity properties

$$Y_{\ell m}(-r) = (-)^\ell Y_{\ell m}(r)$$

$$Y_{\ell m}{}^{*} = (-)^m Y_{\ell,-m} .$$

The ℓs - coupling (as opposed to $s\ell$ - coupling)

$$|\ell sjm\rangle = \sum_{m_\ell m_s} C(\ell\tfrac{1}{2}j;m_\ell m_s m)\,|Y_{\ell m}\rangle\,|\tfrac{1}{2}m_s\rangle$$

with the phase convention

$$C(\ell\tfrac{1}{2}j;m_\ell m_s m) = -\left[\left(\ell-m+\tfrac{1}{2}\right)/(2\ell+1)\right]^{1/2} ,\quad m_s = \tfrac{1}{2},\; j = \ell-\tfrac{1}{2}$$

$$\left[\left(\ell+m+\tfrac{1}{2}\right)/(2\ell+1)\right]^{1/2} ,\quad m_s = \tfrac{1}{2},\; j = \ell+\tfrac{1}{2}$$

$$\text{or}\quad m_s = -\tfrac{1}{2},\; j = \ell-\tfrac{1}{2} .$$

$$+\left[\left(\ell-m+\tfrac{1}{2}\right)/(2\ell+1)\right]^{1/2} ,\quad m_s = -\tfrac{1}{2},\; j = \ell+\tfrac{1}{2} .$$

Table A3.1. C_1

Irrep	Class		Basis
	E	$\bar{E}$	
$\Gamma_2 = \bar{A} = B_{1/2}$	1	-1	$\mid \ell jm >, \forall m$

Table A3.2. C_i

Irrep	Class				Basis
	E	$\bar{E}$	I	$\bar{I}$	
$\Gamma_2^+ = \bar{A}_g = B_{1/2g}$	1	-1	1	-1	$\mid \ell jm >$, even ℓ, $\forall m$
$\Gamma_2^- = \bar{A}_u = B_{1/2u}$	1	-1	-1	1	$\mid \ell jm >$, odd ℓ, $\forall m$

Table A3.3. C_2. The irreps Γ_3 and Γ_4 together form the rep $E_{1/2}$.

Irrep	Class				Basis [a]
	E	$\bar{E}$	C_2	$\bar{C}_2$	
$\Gamma_3 = {}^1\bar{E}$	1	-1	i	-i	$\mid \ell, j, -\frac{1}{2}$ (mod 2) >
$\Gamma_4 = {}^2\bar{E}$	1	-1	-i	i	$\mid \ell, j, \frac{1}{2}$ (mod 2) >
$D^j_{m'm}$	$\delta_{mm'}$	$-\delta_{mm'}$	$e^{-im\pi}\delta_{mm'}$	$-e^{-im\pi}\delta_{mm'}$	

[a] Even ℓ. Interchanged from Koster.

Table A3.4. $C_{1h} = C_s$. The irreps Γ_3 and Γ_4 together form the rep $E_{1/2}$.

Irrep	Class				Basis [a]	
	E	$\bar{E}$	σ	$\bar{\sigma}$	Even ℓ	Odd ℓ
$\Gamma_3 = {}^1\bar{E}$	1	-1	i	-i	$\mid \ell j -\frac{1}{2}$ >	$\mid \ell j \frac{1}{2}$ >
$\Gamma_4 = {}^2\bar{E}$	1	-1	-i	i	$\mid \ell j \ \frac{1}{2}$ >	$\mid \ell, -\frac{1}{2}$ >
$D^j_{m'm}$	$\delta_{mm'}$	$-\delta_{mm'}$	$e^{-im\pi}\delta_{mm'}$	$-e^{-im\pi}\delta_{mm'}$		
Inversion	no	no	yes	yes		

[a] The m quantum number is given mod (2). Koster *et al.* (1963) only give our "odd ℓ" functions.

Table A3.5. C_{2h}. The irreps Γ_3^+ and Γ_4^+ together form the rep $E_{1/2g}$ while Γ_3^- and Γ_4^- together form the rep $E_{1/2u}$.

Irrep	Class				Basis [a]	
	E	C_2	I	σ_h	Even ℓ	Odd ℓ
Γ_3^+	1	i	1	i	$\lvert \ell j -\frac{1}{2}>$	-
Γ_4^+	1	-i	1	-i	$\lvert \ell j \ \frac{1}{2}>$	-
Γ_3^-	1	i	-1	-i	-	$\lvert \ell j -\frac{1}{2}>$
Γ_4^-	1	-i	-1	i	-	$\lvert \ell j \ \frac{1}{2}>$
$D^j_{m'm}$	$\delta_{mm'}$	$e^{-im\pi}\delta_{mm'}$	$\delta_{mm'}$	$e^{-im\pi}\delta_{mm'}$		
Inversion	no	no	yes	yes		

[a] The m quantum number is given mod (2).

Table A3.6. D_2 and C_{2v}.

Irrep	Quantity	Class				Basis [a,b]	
	D_2:	E	$C_2(z)$	$C_2(x)$	$C_2(y)$	D_2	C_{2v}
	C_{2v}:	E	$C_2(z)$	$\sigma_v'(yz)$	$\sigma_v'(xz)$		
$\Gamma_5 = E_{1/2}$	χ	2	0	0	0		
$=E(C_{2v}) = E'(D_2)$	Γ	$\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}$	$\begin{pmatrix}-i & 0\\ 0 & i\end{pmatrix}$	$\begin{pmatrix}0 & -i\\ -i & 0\end{pmatrix}$	$\begin{pmatrix}0 & -1\\ 1 & 0\end{pmatrix}$	$\begin{cases}\lvert \ell j \ \frac{1}{2}> \\ (-)^{\ell}\ s\lvert \ell j -\frac{1}{2}>\end{cases}$	$\begin{cases}\lvert \ell j \ \frac{1}{2}> \\ s\lvert \ell j -\frac{1}{2}>\end{cases}$
	$D^j_{m'm}$ $\delta_{mm'}$ ·	{1	$e^{-im\pi}$	$A \cdot e^{-im\pi}$	1 }[c]		

[a] The m quantum number is given mod (2)

[b] The symbol s is +1 for $j = \ell + \frac{1}{2}$ and -1 for $j = \ell - \frac{1}{2}$.

[c] The symbol $A = (-)^{3j+m}\,\delta_{m,-m'}$.

Table A3.7. D_{2h}

Irrep	Quantity	Class								Basis [a]
		E	$C_2(z)$	$C_2'(y)$	$C_2''(x)$	I	$\sigma_v(xy)$	$\sigma_v'(xz)$	$\sigma_v''(yz)$	
Γ_5^+	χ	2	0	0	0	2	0	0	0	
	Γ	$\begin{pmatrix}1 & 0\\0 & 1\end{pmatrix}$	$\begin{pmatrix}-i & 0\\0 & i\end{pmatrix}$	$\begin{pmatrix}0 & -1\\1 & 0\end{pmatrix}$	$\begin{pmatrix}0 & -i\\-i & 0\end{pmatrix}$	$\begin{pmatrix}1 & 0\\0 & 1\end{pmatrix}$	$\begin{pmatrix}-i & 0\\0 & i\end{pmatrix}$	$\begin{pmatrix}0 & -1\\1 & 0\end{pmatrix}$	$\begin{pmatrix}0 & -i\\-i & 0\end{pmatrix}$	$\left\{\begin{matrix} \lvert \ell j \ \tfrac{1}{2}> \\ s\lvert \ell j -\tfrac{1}{2}> \end{matrix}\right.$ [b]
Γ_5^-	χ	2	0	0	0	-2	0	0	0	
	Γ	$\begin{pmatrix}1 & 0\\0 & 1\end{pmatrix}$	$\begin{pmatrix}-i & 0\\0 & i\end{pmatrix}$	$\begin{pmatrix}0 & -1\\1 & 0\end{pmatrix}$	$\begin{pmatrix}0 & -i\\-i & 0\end{pmatrix}$	$\begin{pmatrix}-1 & 0\\0 & -1\end{pmatrix}$	$\begin{pmatrix}i & 0\\0 & -i\end{pmatrix}$	$\begin{pmatrix}0 & 1\\-1 & 0\end{pmatrix}$	$\begin{pmatrix}0 & i\\i & 0\end{pmatrix}$	$\left\{\begin{matrix} \lvert \ell j \ \tfrac{1}{2}> \\ -s\lvert \ell j -\tfrac{1}{2}> \end{matrix}\right.$ [c]
	$D^j_{m'm}$	A	AC	B	BC	A	AC	B	BC	
	Inv.	no	no	no	no	yes	yes	yes	yes	

[a] The m quantum number is given mod (2).

[b] Even ℓ.

[c] Odd ℓ.

[d] $A = \delta_{mm'}, B = \delta_{m,-m'}(-)^{3j+m}$ and $C = e^{-im\pi}$.

Table A3.8. C_4 and S_4. The quantity $u = \exp(i\pi/4)$.

Irrep	Class				Basis[a]	
	C_4 : E	C_4	C_2	C_4^{-1}	C_4 and S_4 [b]	S_4 [c]
	S_4 : E	S_4^{-1}	C_2	S_4		
$\Gamma_5 = {}^2\bar{E}_1$	1	u	i	u*	$\lvert \ell j, -\frac{1}{2} >$	$\lvert \ell j, \frac{3}{2} >$
$\Gamma_6 = {}^1\bar{E}_1$	1	u*	-i	u	$\lvert \ell j, \frac{1}{2} >$	$\lvert \ell j, -\frac{3}{2} >$
$\Gamma_7 = {}^2\bar{E}_2$	1	-u	i	-u*	$\lvert \ell j, \frac{3}{2} >$	$\lvert \ell j, -\frac{1}{2} >$
$\Gamma_8 = {}^1\bar{E}_2$	1	-u*	-i	-u	$\lvert \ell j, -\frac{3}{2} >$	$\lvert \ell j, \frac{1}{2} >$
$D^j_{m'm}$	$\delta_{mm'} \cdot \{1$	$e^{-im\pi/2}$	$e^{-im\pi}$	$e^{im\pi/2}\}$		
Inversion (S_4)	no	yes	no	yes		

[a] The m quantum number is given mod (4). [b] Even ℓ. [c] Odd ℓ.

Table A3.9. C_{4h}.

Irrep	Class								Basis [a]
	E	C_4	C_2	C_4^{-1}	I	S_4^{-1}	σ_h	S_4	
Γ_5^+	1	u	i	u*	1	u	i	u*	$\lvert \ell j -\frac{1}{2} >$ [b]
Γ_6^+	1	u*	-i	u	1	u*	-i	u	$\lvert \ell j \ \frac{1}{2} >$ [b]
Γ_7^+	1	-u	i	-u*	1	-u	i	-u*	$\lvert \ell j \ \frac{3}{2} >$ [b]
Γ_8^+	1	-u*	-i	-u	1	-u*	-i	-u	$\lvert \ell j -\frac{3}{2} >$ [b]
Γ_5^-	1	u	i	u*	-1	-u	-i	-u*	$\lvert \ell j -\frac{1}{2} >$ [c]
Γ_6^-	1	u*	-i	u	-1	-u*	i	-u	$\lvert \ell j \ \frac{1}{2} >$ [c]
Γ_7^-	1	-u	i	-u*	-1	u	-i	u*	$\lvert \ell j \ \frac{3}{2} >$ [c]
Γ_8^-	1	-u*	-i	-u	-1	u*	i	u	$\lvert \ell j -\frac{3}{2} >$ [c]
$D^j_{m'm}\ \delta_{mm'} \cdot$	$\{1$	$e^{-im\pi/2}$	$e^{-im\pi}$	$e^{im\pi/2}$	1	$e^{-im\pi/2}$	$e^{-im\pi}$	$e^{im\pi/2}\}$	
Inversion	no	no	no	no	yes	yes	yes	yes	

[a] The m quantum number is given mod (4). [b] Even ℓ. [c] Odd ℓ.

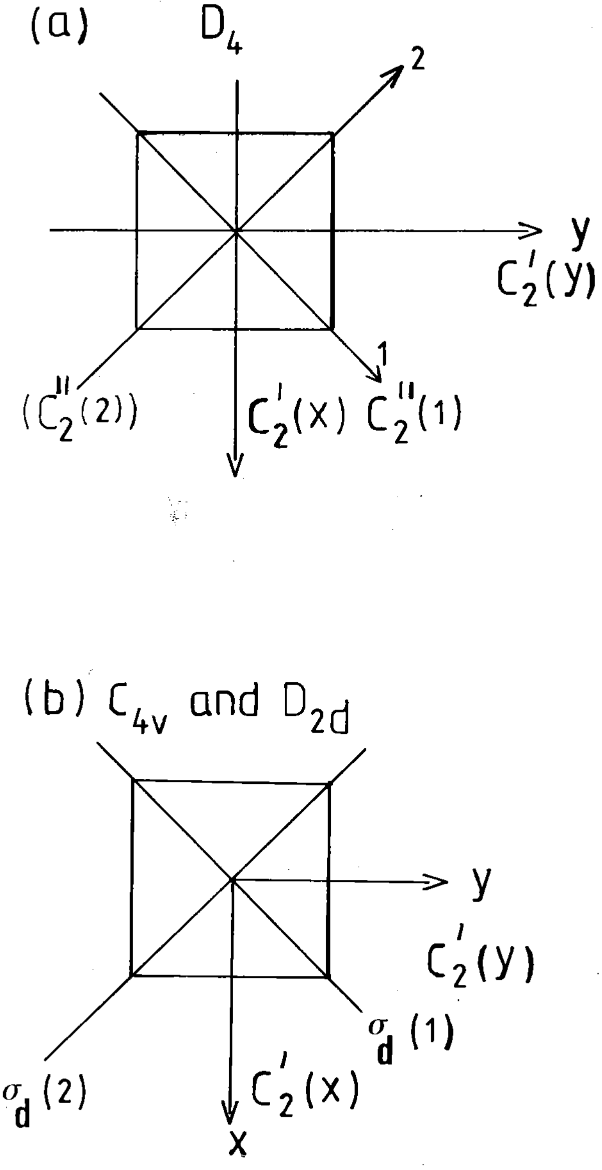

Figure A3.1. Definition of the operations. (a) D_4, (b) C_{4v} and D_{2d}.

Table A3.10. D_4, C_{4v} and D_{2d}. The quantity $u = \exp(i\pi/4)$. For D_4, the C_2 (1) axis bisects x and y. The C_2'' (2) axis bisects y and -x. For C_{4v} and D_{2d}, σ_d (1) = I C_2'' (2) bisects x and y while σ_d (2) = I C_2'' (1) bisects -y and x. (See Fig. A3.1).

Irrep	Quantity	Operation and Class								Basis [a]		
	D_4 :	{ E }	{ C_4	C_4^{-1} }	{ C_2 }	{ $C_2'(x)$	$C_2'(y)$ }	{ $C_2''(1)$	$C_2''(2)$ }	D_4	C_{4v}	D_{2d} [c]
	C_{4v} :	{ E }	{ C_4	C_4^{-1} }	{ C_2 }	{ $\sigma_v(yz)$	$\sigma_v(xz)$ }	{ $\sigma_d(2)$	$\sigma_d(1)$ }		D_{2d} [b]	
	D_{2d} :	{ E }	{ S_4^{-1}	S_4 }	{ C_2 }	{ $C_2'(x)$	$C_2'(y)$ }	{ $\sigma_d(2)$	$\sigma_d(1)$ }			
$\Gamma_6 = E' = \bar{E}_1 = E_{1/2}$	χ	2	2	2	0	0	0	0	0			
	Γ	$\begin{pmatrix}1&0\\0&1\end{pmatrix}$	$\begin{pmatrix}u^*&0\\0&u\end{pmatrix}$	$\begin{pmatrix}u&0\\0&u^*\end{pmatrix}$	$\begin{pmatrix}-i&0\\0&i\end{pmatrix}$	$\begin{pmatrix}0&-i\\-i&0\end{pmatrix}$	$\begin{pmatrix}0&-1\\1&0\end{pmatrix}$	$\begin{pmatrix}0&-u\\u^*&0\end{pmatrix}$	$\begin{pmatrix}0&-u^*\\u&0\end{pmatrix}$	$\begin{cases} \|\ell j\ \frac{1}{2}> \\ (-)^{\ell} s\|\ell j -\frac{1}{2}> \end{cases}$	$\begin{cases} \|\ell j\ \frac{1}{2}> \\ s\|\ell j -\frac{1}{2}> \end{cases}$	$\begin{cases} \|\ell j -\frac{3}{2}> \\ -s\|\ell j\ \frac{3}{2}> \end{cases}$
$\Gamma_7 = E'' = \bar{E}_2 = E_{3/2}$	χ	2	-2	-2	0	0	0	0	0			
	Γ	$\begin{pmatrix}1&0\\0&1\end{pmatrix}$	$\begin{pmatrix}-u^*&0\\0&-u\end{pmatrix}$	$\begin{pmatrix}-u&0\\0&-u^*\end{pmatrix}$	$\begin{pmatrix}-i&0\\0&i\end{pmatrix}$	$\begin{pmatrix}0&-i\\-i&0\end{pmatrix}$	$\begin{pmatrix}0&-1\\1&0\end{pmatrix}$	$\begin{pmatrix}0&u\\-u^*&0\end{pmatrix}$	$\begin{pmatrix}0&u^*\\-u&0\end{pmatrix}$	$\begin{cases} \|\ell j -\frac{3}{2}> \\ (-)^{\ell} s\|\ell j\ \frac{3}{2}> \end{cases}$	$\begin{cases} \|\ell j -\frac{3}{2}> \\ s\|\ell j\ \frac{3}{2}> \end{cases}$	$\begin{cases} \|\ell j\ \frac{1}{2}> \\ -s\|\ell j -\frac{1}{2}> \end{cases}$
	$D^j_{m'm}\ \delta_{mm'}\cdot$	{ 1	$e^{-\pi i m/2}$	$e^{\pi i m/2}$	$e^{-\pi i m}$ } A ·	{ $e^{-\pi i m}$	1	$e^{-\pi i m/2}$	$e^{\pi i m/2}$ }			

[a] The m quantum number is given mod (4). [b] Even ℓ. [c] Odd ℓ. $A = (-)^{3j+m}\delta_{m,-m'}$

Table A3.11. D_{4h}. The quantity $u = \exp(i\pi/4)$. The operations are defined in the previous table.

Irrep	Quantity	{ E }	{C_4	C_4^{-1}}	{ C_2 }	{$C_2'(x)$	$C_2'(y)$}	{$C_2''(1)$	$C_2''(2)$}
Γ_6^+	χ	2	2	2	0	0	0	0	0
	Γ	$\begin{pmatrix}1&0\\0&1\end{pmatrix}$	$\begin{pmatrix}u^*&0\\0&u\end{pmatrix}$	$\begin{pmatrix}u&0\\0&u^*\end{pmatrix}$	$\begin{pmatrix}-i&0\\0&i\end{pmatrix}$	$\begin{pmatrix}0&-i\\-i&0\end{pmatrix}$	$\begin{pmatrix}0&-1\\1&0\end{pmatrix}$	$\begin{pmatrix}0&-u\\u^*&0\end{pmatrix}$	$\begin{pmatrix}0&-u^*\\u&0\end{pmatrix}$
Γ_7^+	χ	2	- 2	- 2	0	0	0	0	0
	Γ	$\begin{pmatrix}1&0\\0&1\end{pmatrix}$	$\begin{pmatrix}-u^*&0\\0&-u\end{pmatrix}$	$\begin{pmatrix}-u&0\\0&-u^*\end{pmatrix}$	$\begin{pmatrix}-i&0\\0&i\end{pmatrix}$	$\begin{pmatrix}0&-i\\-i&0\end{pmatrix}$	$\begin{pmatrix}0&-1\\1&0\end{pmatrix}$	$\begin{pmatrix}0&u\\-u^*&0\end{pmatrix}$	$\begin{pmatrix}0&u^*\\-u&0\end{pmatrix}$
Γ_6^-	χ	2	2	2	0	0	0	0	0
	Γ	$\begin{pmatrix}1&0\\0&1\end{pmatrix}$	$\begin{pmatrix}u^*&0\\0&u\end{pmatrix}$	$\begin{pmatrix}u&0\\0&u^*\end{pmatrix}$	$\begin{pmatrix}-i&0\\0&i\end{pmatrix}$	$\begin{pmatrix}0&-i\\-i&0\end{pmatrix}$	$\begin{pmatrix}0&-1\\1&0\end{pmatrix}$	$\begin{pmatrix}0&-u\\u^*&0\end{pmatrix}$	$\begin{pmatrix}0&-u^*\\u&0\end{pmatrix}$
Γ_7^-	χ	2	- 2	- 2	0	0	0	0	0
	Γ	$\begin{pmatrix}1&0\\0&1\end{pmatrix}$	$\begin{pmatrix}-u^*&0\\0&-u\end{pmatrix}$	$\begin{pmatrix}-u&0\\0&-u^*\end{pmatrix}$	$\begin{pmatrix}-i&0\\0&i\end{pmatrix}$	$\begin{pmatrix}0&-i\\-i&0\end{pmatrix}$	$\begin{pmatrix}0&1\\1&0\end{pmatrix}$	$\begin{pmatrix}0&u\\-u^*&0\end{pmatrix}$	$\begin{pmatrix}0&u^*\\-u&0\end{pmatrix}$
$D^j_{m'm}$	A · { 1		$e^{-\pi im/2}$	$e^{\pi im/2}$	$e^{-\pi im}$ }	B · {$e^{-\pi im}$	1	$e^{-\pi im/2}$	$e^{\pi im/2}$ }

{ I }	{S_4^{-1}	S_4}	{ σ_h }	{$\sigma_v(yz)$	$\sigma_v(xz)$}	{$\sigma_d(2)$	$\sigma_d(1)$}	Basis [a]
2	2	2	0	0	0	0	0	
$\begin{pmatrix}1&0\\0&1\end{pmatrix}$	$\begin{pmatrix}u^*&0\\0&u\end{pmatrix}$	$\begin{pmatrix}u&0\\0&u^*\end{pmatrix}$	$\begin{pmatrix}-i&0\\0&i\end{pmatrix}$	$\begin{pmatrix}0&-i\\-i&0\end{pmatrix}$	$\begin{pmatrix}0&-1\\1&0\end{pmatrix}$	$\begin{pmatrix}0&-u\\u^*&0\end{pmatrix}$	$\begin{pmatrix}0&-u^*\\u&0\end{pmatrix}$	$\begin{cases} \lvert \ell j\ \tfrac{1}{2}\rangle \\ s\lvert \ell j -\tfrac{1}{2}\rangle \end{cases}$ [b]
2	- 2	- 2	0	0	0	0	0	
$\begin{pmatrix}1&0\\0&1\end{pmatrix}$	$\begin{pmatrix}-u^*&0\\0&-u\end{pmatrix}$	$\begin{pmatrix}-u&0\\0&-u^*\end{pmatrix}$	$\begin{pmatrix}-i&0\\0&i\end{pmatrix}$	$\begin{pmatrix}0&-i\\-i&0\end{pmatrix}$	$\begin{pmatrix}0&-1\\1&0\end{pmatrix}$	$\begin{pmatrix}0&u\\-u^*&0\end{pmatrix}$	$\begin{pmatrix}0&u^*\\-u&0\end{pmatrix}$	$\begin{cases} \lvert \ell j -\tfrac{3}{2}\rangle \\ s\lvert \ell j\ \tfrac{3}{2}\rangle \end{cases}$ [b]
- 2	- 2	- 2	0	0	0	0	0	
$\begin{pmatrix}-1&0\\0&-1\end{pmatrix}$	$\begin{pmatrix}-u^*&0\\0&-u\end{pmatrix}$	$\begin{pmatrix}-u&0\\0&-u^*\end{pmatrix}$	$\begin{pmatrix}i&0\\0&-i\end{pmatrix}$	$\begin{pmatrix}0&i\\i&0\end{pmatrix}$	$\begin{pmatrix}0&1\\-1&0\end{pmatrix}$	$\begin{pmatrix}0&u\\-u^*&0\end{pmatrix}$	$\begin{pmatrix}0&u^*\\-u&0\end{pmatrix}$	$\begin{cases} \lvert \ell j\ \tfrac{1}{2}\rangle \\ s\lvert \ell j -\tfrac{1}{2}\rangle \end{cases}$ [c]
- 2	2	2	0	0	0	0	0	
$\begin{pmatrix}-1&0\\0&-1\end{pmatrix}$	$\begin{pmatrix}u^*&0\\0&u\end{pmatrix}$	$\begin{pmatrix}u&0\\0&u^*\end{pmatrix}$	$\begin{pmatrix}i&0\\0&-i\end{pmatrix}$	$\begin{pmatrix}0&i\\i&0\end{pmatrix}$	$\begin{pmatrix}0&1\\-1&0\end{pmatrix}$	$\begin{pmatrix}0&-u\\u^*&0\end{pmatrix}$	$\begin{pmatrix}0&-u^*\\u&0\end{pmatrix}$	$\begin{cases} \lvert \ell j -\tfrac{3}{2}\rangle \\ -s\lvert \ell j\ \tfrac{3}{2}\rangle \end{cases}$ [c]
A · {1	$e^{-\pi im/2}$	$e^{\pi im/2}$	$e^{-\pi im}$}	B · {$e^{-\pi im}$	1	$e^{-\pi im/2}$	$e^{\pi im/2}$ } [d]	

[a] The m quantum number is given mod (4). [b] Even ℓ. [c] Odd ℓ.

[d] The quantity $A = \delta_{mm'}$ and $B = \delta_{m,-m'}(-)^{3j+m'}$.

Table A3.12. C_3. The quantity $w = \exp(i\pi/3)$.

Irrep	Class			Basis [a]
	E	C_3	C_3^{-1}	
Γ_4	1	w	w*	$\lvert \ell j -\frac{1}{2}>$ [b]
Γ_5	1	w*	w	$\lvert \ell j\ \frac{1}{2}>$ [b]
Γ_6	1	-1	-1	$\lvert \ell j\ \frac{3}{2}>$
$D^j_{m'm}$	$\delta_{mm'}$	$e^{-2\pi im/3}\,\delta_{mm'}$	$e^{2\pi im/3}\,\delta_{mm'}$	

[a] The m quantum number is defined mod (3).

[b] Interchanged from Koster. We use active rotations.

Table A3.13. C_{3i}. The quantity $w = \exp(i\pi/3)$.

Irrep	Class						Basis [a]
	E	C_3	C_3^{-1}	I	S_6 [d]	S_6^{-1} [d]	
Γ_4^+	1	w	w*	1	w*	w	$\lvert \ell j -\frac{1}{2}>$ [b]
Γ_5^+	1	w*	w	1	w	w*	$\lvert \ell j\ \frac{1}{2}>$ [b]
Γ_6^+	1	-1	-1	1	-1	-1	$\lvert \ell j\ \frac{3}{2}>$ [b]
Γ_4^-	1	w	w*	-1	-w*	-w	$\lvert \ell j -\frac{1}{2}>$ [c]
Γ_5^-	1	w*	w	-1	-w	-w*	$\lvert \ell j\ \frac{1}{2}>$ [c]
Γ_6^-	1	-1	-1	-1	1	1	$\lvert \ell j\ \frac{3}{2}>$ [c]
$D^j_{m'm}$	$\delta_{mm'}$	$e^{-2\pi im/3}\,\delta_{mm'}$	$e^{2\pi im/3}\,\delta_{mm'}$	$\delta_{mm'}$	$e^{2\pi im/3}\,\delta_{mm'}$	$e^{-2\pi im/3}\,\delta_{mm'}$	

[a] The m quantum number is defined mod (3).

[b] Even ℓ.

[c] Odd ℓ.

[d] Interchanged from Koster.

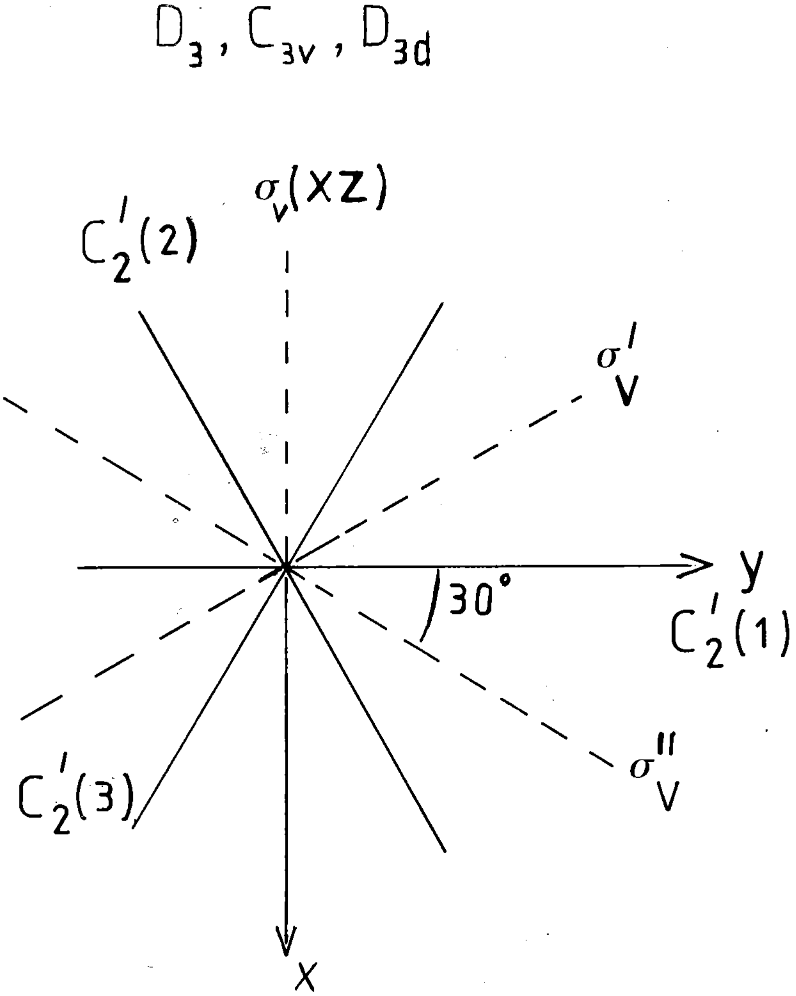

Figure A3.2. Definition for the operations for D_3, C_{3v} and D_{3d}.

Table A3.14. D_3 and C_{3v}. The quantity $w = \exp(i\pi/3)$. $C_2'(1)$ coincides with the y axis, $C_2'(2)$ lies between -x and -y, and $C_2'(3)$ lies between x and -y. σ_v' lies between x and -y. σ_v'' lies between x and y. (See Fig. A3.2).

Irrep	Quantity	Element {and class}					
		D_3 :{E}	{ C_3	C_3^{-1} }	{ $C_2'(1)$	$C_2'(2)$	$C_2'(3)$ }
		C_{3v}:{E}	{ C_3	C_3^{-1} }	{ $\sigma_v(xz)$	σ_v'	σ_v'' }
$\Gamma_4 = E'$	χ	2	1	1	0	0	0
	Γ	$\begin{pmatrix}1 & 0\\0 & 1\end{pmatrix}$	$\begin{pmatrix}w^* & 0\\0 & w\end{pmatrix}$	$\begin{pmatrix}w & 0\\0 & w^*\end{pmatrix}$	$\begin{pmatrix}0 & -1\\1 & 0\end{pmatrix}$	$\begin{pmatrix}0 & w\\-w^* & 0\end{pmatrix}$	$\begin{pmatrix}0 & w^*\\-w & 0\end{pmatrix}$
$\Gamma_5 = \rho_1$	$\chi = \Gamma$	1	-1	-1	i	i	i
$\Gamma_6 = \rho_2$	$\chi = \Gamma$	1	-1	-1	-i	-i	-i
$D^j_{m'm}$	$\delta_{mm'} \cdot$	{1	$e^{-2\pi im/3}$	$e^{2\pi im/3}$}	$A \cdot$ {1	$e^{4\pi im/3}$	$e^{-4\pi im/3}$} [a]

[a] $A = \delta_{m,-m'}(-)^{3j+m}$.

Basis for D_3:

$$\Gamma_4 : \left\{\begin{matrix} |\ell j\ \tfrac{1}{2}> \\ (-)^{\ell}\, s|\ell j - \tfrac{1}{2}> \end{matrix}\right. , \quad \left\{\begin{matrix} |\ell j - \tfrac{5}{2}> \\ (-)^{\ell+1}\, s|\ell j\ \tfrac{5}{2}> \end{matrix}\right.$$

$$\Gamma_5 : \ (-)^{\ell+1}\, s|\ell j\ \tfrac{3}{2}> -i\,|\ell j, -\tfrac{3}{2}>$$

$$\Gamma_6 : \ (-)^{\ell+1}\, s|\ell j\ \tfrac{3}{2}> +i\,|\ell j, -\tfrac{3}{2}>$$

Basis for C_{3v}:

$$\Gamma_4 : \left\{\begin{matrix} |\ell j\ \tfrac{1}{2}> \\ s|\ell j - \tfrac{1}{2}> \end{matrix}\right. , \quad \left\{\begin{matrix} |\ell j - \tfrac{5}{2}> \\ -s|\ell j\ \tfrac{5}{2}> \end{matrix}\right.$$

$$\Gamma_5 : \ -s|\ell j\ \tfrac{3}{2}> -i\,|\ell j, -\tfrac{3}{2}>$$

$$\Gamma_6 : \ -s|\ell j\ \tfrac{3}{2}> +i\,|\ell j - \tfrac{3}{2}> .$$

The m quantum number is defined mod (6).

Table A3.15. D_{3d}. The quantity $w = \exp(i\pi/3)$. The diagonal symmetry planes $\sigma_d(1) = \sigma(xz) \perp C_2'(1)$, $\sigma_d(2) \perp C_2'(2)$, and $\sigma_d(3) \perp C_2'(3)$. The C_2' axes are defined as in the Table A3.14. (See Fig. A3.2).

Irrep	Quantity	Element {and class}											
		{E}	$\{C_3$	$C_3^{-1}\}$	$\{C_2'(1)$	$C_2'(2)$	$C_2'(3)\}$	{I}	$\{S_6^{-1}$	$S_6\}$	$\{\sigma_d(xz)$	$\sigma_d(2)$	$\sigma_d(3)\}$
Γ_4^+	χ	2	1	1	0	0	0	2	1	1	0	0	0
	Γ	$\begin{pmatrix}1 & 0\\0 & 1\end{pmatrix}$	$\begin{pmatrix}w^* & 0\\0 & w\end{pmatrix}$	$\begin{pmatrix}w & 0\\0 & w^*\end{pmatrix}$	$\begin{pmatrix}0 & -1\\1 & 0\end{pmatrix}$	$\begin{pmatrix}0 & w\\-w^* & 0\end{pmatrix}$	$\begin{pmatrix}0 & w^*\\-w & 0\end{pmatrix}$	$\begin{pmatrix}-1 & 0\\0 & -1\end{pmatrix}$	$\begin{pmatrix}w^* & 0\\0 & w\end{pmatrix}$	$\begin{pmatrix}w & 0\\0 & w^*\end{pmatrix}$	$\begin{pmatrix}0 & -1\\1 & 0\end{pmatrix}$	$\begin{pmatrix}0 & w\\-w^* & 0\end{pmatrix}$	$\begin{pmatrix}0 & w^*\\-w & 0\end{pmatrix}$
Γ_5^+	χ	1	-1	-1	i	i	i	1	-1	-1	i	i	i
Γ_6^+	χ	1	-1	-1	-i	-i	-i	1	-1	-1	-i	-i	-i
Γ_4^-	χ	2	1	1	0	0	0	-2	-1	-1	0	0	0
	Γ	$\begin{pmatrix}1 & 0\\0 & 1\end{pmatrix}$	$\begin{pmatrix}w^* & 0\\0 & w\end{pmatrix}$	$\begin{pmatrix}w & 0\\0 & w^*\end{pmatrix}$	$\begin{pmatrix}0 & -1\\1 & 0\end{pmatrix}$	$\begin{pmatrix}0 & w\\-w^* & 0\end{pmatrix}$	$\begin{pmatrix}0 & w^*\\-w & 0\end{pmatrix}$	$\begin{pmatrix}-1 & 0\\0 & -1\end{pmatrix}$	$\begin{pmatrix}-w^* & 0\\0 & -w\end{pmatrix}$	$\begin{pmatrix}-w & 0\\0 & -w^*\end{pmatrix}$	$\begin{pmatrix}0 & 1\\-1 & 0\end{pmatrix}$	$\begin{pmatrix}0 & -w\\w^* & 0\end{pmatrix}$	$\begin{pmatrix}0 & -w^*\\w & 0\end{pmatrix}$
Γ_5^-	χ	1	-1	-1	i	i	i	-1	1	1	-i	-i	-i
Γ_6^-	χ	1	-1	-1	-i	-i	-i	-1	1	1	i	i	i
	$D^j_{m'm}$	$A\cdot\{1$	$e^{-2\pi im/3}$	$e^{2\pi im/3}\}$	$B\cdot\{1$	$e^{4\pi im/3}$	$e^{-4\pi im/3}\}$	$A\cdot\{1$	$e^{-2\pi im/3}$	$e^{2\pi im/3}\}$	$B\cdot\{1$	$e^{4\pi im/3}$	$e^{-4\pi im/3}\}$

$A = \delta_{mm'}$, $B = \delta_{m,-m'} \cdot (-)^{3j+m}$.

Basis: $\Gamma_4^+ : \begin{cases} |\ell j \ \tfrac{1}{2}> \\ s|\ell j - \tfrac{1}{2}> , \end{cases} \begin{cases} |\ell j - \tfrac{5}{2}> \\ -s|\ell j \ \tfrac{5}{2}> . \end{cases}$ $\quad \Gamma_4^- : \begin{cases} |\ell j \ \tfrac{1}{2}> \\ -s|\ell j - \tfrac{1}{2}> , \end{cases} \begin{cases} |\ell j - \tfrac{5}{2}> \\ s|\ell j \ \tfrac{5}{2}> . \end{cases}$

$\Gamma_5^+ : |\tfrac{3}{2}> + is\,|-\tfrac{3}{2}>$,

$\Gamma_5^- : |\tfrac{3}{2}> - is\,|-\tfrac{3}{2}>$

$\Gamma_6^+ : |\tfrac{3}{2}> - is\,|-\tfrac{3}{2}>$

$\Gamma_6^- : |\tfrac{3}{2}> + is\,|-\tfrac{3}{2}>$.

The m quantum number is defined mod (6). The ℓ quantum number is even for Γ_i^+ and odd for Γ_i^-.

Table A3.16. C_6 and C_{3h}. The quantity $v = \exp(i\pi/6)$ and $w = \exp(i\pi/3)$.

Irrep	Element							Basis [a]	
	C_6 :	E	C_6	C_3	C_2	C_3^{-1}	C_6^{-1}	C_6	
	C_{3h} :	E	S_3^{-1}	C_3	σ_h	C_3^{-1}	S_3	C_{3h} [b]	C_{3h} [c]
Γ_7		1	v	w	i	w*	v*	$\|\ell j\ -\frac{1}{2}>$	$\|\ell j\ \frac{5}{2}>$
Γ_8		1	v*	w*	-i	w	v	$\|\ell j\ \frac{1}{2}>$	$\|\ell j\ -\frac{5}{2}>$
Γ_9		1	-v	w	-i	w*	-v*	$\|\ell j\ \frac{5}{2}>$	$\|\ell j\ -\frac{1}{2}>$
Γ_{10}		1	-v*	w*	i	w	-v	$\|\ell j\ -\frac{5}{2}>$	$\|\ell j\ \frac{1}{2}>$
Γ_{11}		1	-i	-1	i	-1	i	$\|\ell j\ \frac{3}{2}>$	$\|\ell j\ -\frac{3}{2}>$
Γ_{12}		1	i	-1	-i	-1	-i	$\|\ell j\ -\frac{3}{2}>$	$\|\ell j\ \frac{3}{2}>$
$D^j_{m'm}$	$\delta_{mm'} \cdot \{$	1	$e^{-im\pi/3}$	$e^{-2im\pi/3}$	$e^{-im\pi}$	$e^{2im\pi/3}$	$e^{im\pi/3}\}$		

[a] The m quantum number is defined mod (6).
[b] Even ℓ.
[c] Odd ℓ.

Table A3.17. C_{6h}. $v = \exp(i\pi/6)$, $w = \exp(i\pi/3)$.

Irrep	Element												Basis [a]
	E	C_6	C_3	C_2	C_3^{-1}	C_6^{-1}	I	S_3^{-1}	S_6^{-1}	σ_h	S_6	S_3	
Γ_7^+	1	v	w	i	w*	v*	1	v	w	i	w*	v*	$\|\ell j\ -\frac{1}{2}>$ [b]
Γ_8^+	1	v*	w*	-i	w	v	1	v*	w*	-i	w	v	$\|\ell j\ \frac{1}{2}>$ [b]
Γ_9^+	1	-v	w	-i	w*	-v*	1	-v	w	-i	w*	-v*	$\|\ell j\ \frac{5}{2}>$ [b]
Γ_{10}^+	1	-v*	w*	i	w	-v	1	-v*	w*	i	w	-v	$\|\ell j\ -\frac{5}{2}>$ [b]
Γ_{11}^+	1	-i	-1	i	-1	i	1	-i	-1	i	-1	i	$\|\ell j\ \frac{3}{2}>$ [b]
Γ_{12}^+	1	i	-1	-i	-1	-i	1	i	-1	-i	-1	-i	$\|\ell j\ -\frac{3}{2}>$ [b]
Γ_7^-	1	v	w	i	w*	v*	-1	-v	-w	-i	-w*	-v*	$\|\ell j\ -\frac{1}{2}>$ [c]
Γ_8^-	1	v*	w*	-i	w	v	-1	-v*	-w*	i	-w	-v	$\|\ell j\ \frac{1}{2}>$ [c]
Γ_9^-	1	-v	w	-i	w*	-v*	-1	v	-w	i	-w*	v*	$\|\ell j\ \frac{5}{2}>$ [c]
Γ_{10}^-	1	-v*	w*	i	w	-v	-1	v*	-w*	-i	-w	v	$\|\ell j\ -\frac{5}{2}>$ [c]
Γ_{11}^-	1	-i	-1	i	-1	i	-1	i	1	-i	1	-i	$\|\ell j\ \frac{3}{2}>$ [c]
Γ_{12}^-	1	i	-1	-i	-1	-i	-1	-i	1	i	1	i	$\|\ell j\ -\frac{3}{2}>$ [c]
$D^j_{m'm}\ \delta_{mm'}\cdot$	{1	$e^{-im\pi/3}$	$e^{-2im\pi/3}$	$e^{-im\pi}$	$e^{2im\pi/3}$	$e^{im\pi/3}$	1	$e^{-im\pi/3}$	$e^{-2im\pi/3}$	$e^{-im\pi}$	$e^{2im\pi/3}$	$e^{im\pi/3}$}	

[a] The m quantum number is defined mod (6). [b] Even ℓ. [c] Odd ℓ.

Table A3.18. D_6, C_{6v} and D_{3h}. $v = \exp(i\pi/6)$, $w = \exp(i\pi/3)$. The elements are defined in Fig. A3.3.

Irrep	Quantity	Element						
	D_6 :	E	C_2	C_3	C_3^{-1}	C_6	C_6^{-1}	$C_2'(1)$
	C_{6v} :	E	C_2	C_3	C_3^{-1}	C_6	C_6^{-1}	$\sigma_d(1)$
	D_{3h} :	E	σ_h	C_3	C_3^{-1}	S_3^{-1}	S_3	$\sigma_v(1)$
$\Gamma_7 = E' = E_{1/2}$	χ	2	0	1	1	3	3	0
	Γ	$\begin{pmatrix}1 & 0\\0 & 1\end{pmatrix}$	$\begin{pmatrix}-i & 0\\0 & i\end{pmatrix}$	$\begin{pmatrix}w^* & 0\\0 & w\end{pmatrix}$	$\begin{pmatrix}w & 0\\0 & w^*\end{pmatrix}$	$\begin{pmatrix}v^* & 0\\0 & v\end{pmatrix}$	$\begin{pmatrix}v & 0\\0 & v^*\end{pmatrix}$	$\begin{pmatrix}0 & -1\\1 & 0\end{pmatrix}$
$\Gamma_8 = E'' = E_{5/2}$	χ	2	0	1	1	-3	-3	0
	Γ	$\begin{pmatrix}1 & 0\\0 & 1\end{pmatrix}$	$\begin{pmatrix}i & 0\\0 & -i\end{pmatrix}$	$\begin{pmatrix}w^* & 0\\0 & w\end{pmatrix}$	$\begin{pmatrix}w & 0\\0 & w^*\end{pmatrix}$	$\begin{pmatrix}-v^* & 0\\0 & -v\end{pmatrix}$	$\begin{pmatrix}-v & 0\\0 & -v^*\end{pmatrix}$	$\begin{pmatrix}0 & 1\\-1 & 0\end{pmatrix}$
$\Gamma_9 = E''' = E_{3/2}$	χ	2	0	-2	-2	0	0	0
	Γ	$\begin{pmatrix}1 & 0\\0 & 1\end{pmatrix}$	$\begin{pmatrix}i & 0\\0 & -i\end{pmatrix}$	$\begin{pmatrix}-1 & 0\\0 & -1\end{pmatrix}$	$\begin{pmatrix}-1 & 0\\0 & -1\end{pmatrix}$	$\begin{pmatrix}-i & 0\\0 & i\end{pmatrix}$	$\begin{pmatrix}i & 0\\0 & -i\end{pmatrix}$	$\begin{pmatrix}0 & -1\\1 & 0\end{pmatrix}$

$D^j_{m'm}$	$A \cdot \{1$	$e^{-\pi i m}$	$e^{-2\pi i m/3}$	$e^{2\pi i m/3}$	$e^{-\pi i m/3}$	$e^{\pi i m/3}\}$	$B \cdot \{1$
γ	0	π	$2\pi/3$	$-2\pi/3$	$\pi/3$	$-\pi/3$	0
β	0	0	0	0	0	0	π
α	0	0	0	0	0	0	0

Table A3.18. (cont.)

Element					Basis [a]		
$C_2'(2)$	$C_2'(3)$	$C_2''(1)$	$C_2''(2)$	$C_2''(3)$	D_{3h} [b]	D_{3h} [c]	D_6
$\sigma_d(2)$	$\sigma_d(3)$	$\sigma_v(1)$	$\sigma_v(2)$	$\sigma_v(3)$	C_{6v}		
$\sigma_v(2)$	$\sigma_v(3)$	$C_2(1)$	$C_2(2)$	$C_2(3)$			
0	0	0	0	0			
$\begin{pmatrix} 0 & w^* \\ -w & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & w \\ -w^* & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & -i \\ -i & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & v \\ -v^* & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & -v^* \\ v & 0 \end{pmatrix}$	$\left\{\begin{matrix} \vert \ell j\ \frac{1}{2}\rangle \\ s\vert \ell j\ -\frac{1}{2}\rangle \end{matrix}\right.$	$\left\{\begin{matrix} \vert \ell j\ -\frac{5}{2}\rangle \\ -s\vert \ell j\ \frac{5}{2}\rangle \end{matrix}\right.$	$\left\{\begin{matrix} \vert \ell j\ \frac{1}{2}\rangle \\ (-)^{\ell} s\vert \ell j\ -\frac{1}{2}\rangle \end{matrix}\right.$
0	0	0	0	0			
$\begin{pmatrix} 0 & -w^* \\ w & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & -w \\ w^* & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & -i \\ -i & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & v \\ -v^* & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & -v^* \\ v & 0 \end{pmatrix}$	$\left\{\begin{matrix} \vert \ell j\ -\frac{5}{2}\rangle \\ s\vert \ell j\ \frac{5}{2}\rangle \end{matrix}\right.$	$\left\{\begin{matrix} \vert \ell j\ \frac{1}{2}\rangle \\ -s\vert \ell j\ -\frac{1}{2}\rangle \end{matrix}\right.$	$\left\{\begin{matrix} \vert \ell j\ -\frac{5}{2}\rangle \\ (-)^{\ell} s\vert \ell j\ \frac{5}{2}\rangle \end{matrix}\right.$
0	0	0	0	0			
$\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix}$	$\left\{\begin{matrix} \vert \ell j\ \frac{3}{2}\rangle \\ -s\vert \ell j\ -\frac{3}{2}\rangle \end{matrix}\right.$	$\left\{\begin{matrix} \vert \ell j\ -\frac{3}{2}\rangle \\ s\vert \ell j\ \frac{3}{2}\rangle \end{matrix}\right.$	$\left\{\begin{matrix} \vert \ell j\ \frac{3}{2}\rangle \\ (-)^{\ell+1} s\vert \ell j\ -\frac{3}{2}\rangle \end{matrix}\right.$
$e^{-4\pi im/3}$	$e^{4\pi im/3}$	$e^{-\pi im}$	$e^{5\pi im/3}$	$e^{\pi im/3}\}^{d}$			
$2\pi/3$	$-2\pi/3$	$\pi/2$	$-5\pi/6$	$-\pi/6$			
π	π	π	π	π			
$-2\pi/3$	$2\pi/3$	$-\pi/2$	$5\pi/6$	$\pi/6$			

[a] The m quantum number is defined mod (6).

[b] Even ℓ.

[c] Odd ℓ.

[d] $A = \delta_{mm'}$, $B = \delta_{m,-m'}(-)^{3j+m}$.

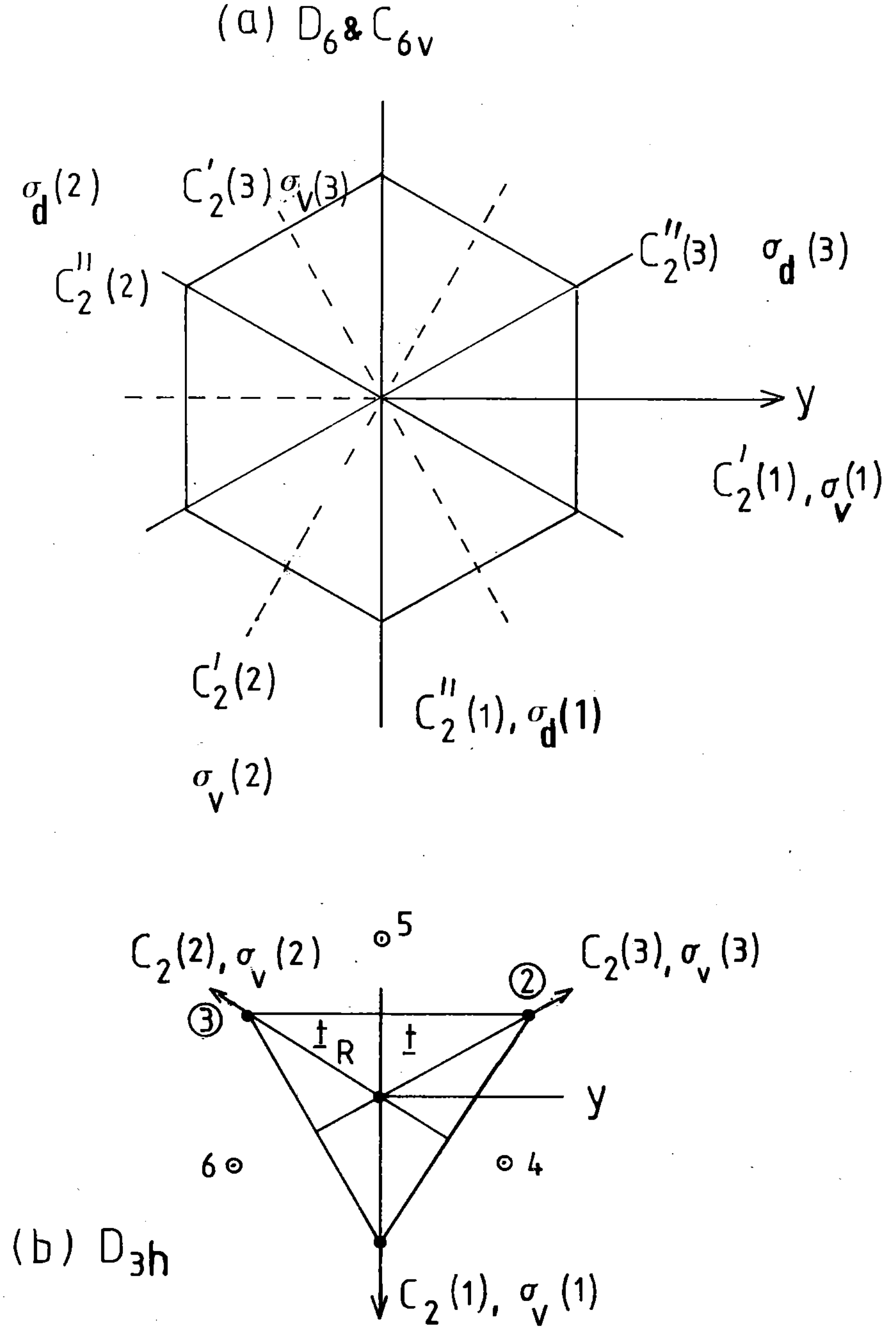

Figure A3.3. The coordinate systems and notations assumed for the double groups D_6 and C_{6v} (a) and D_{3h} (b). In the latter case the site vectors $\underline{t}$ and $\underline{t}_R$, corresponding to the site 2 and the operation $R = C_3$ are shown as an example (see eq. (7.113) in § 7.4.1 of Desclaux and Pyykkö, "Relativistic Theory of Atoms and Molecules" (To be published)).

Table A3.19. D_{6h}. $v = \exp(i\pi/6)$. $w = \exp(i\pi/3)$. The elements are defined in Fig. A3.3 (a).

Irrep	Quantity	Element {and class}					
		{ E }	{ C_2 }	{ C_3	C_3^{-1} }	{ C_6	C_6^{-1} }
Γ_7^+	χ	2	0	1	1	3	3
	Γ	$\begin{pmatrix}1 & 0\\0 & 1\end{pmatrix}$	$\begin{pmatrix}-i & 0\\0 & i\end{pmatrix}$	$\begin{pmatrix}w^* & 0\\0 & w\end{pmatrix}$	$\begin{pmatrix}w & 0\\0 & w^*\end{pmatrix}$	$\begin{pmatrix}v^* & 0\\0 & v\end{pmatrix}$	$\begin{pmatrix}v & 0\\0 & v^*\end{pmatrix}$
Γ_7^-	χ	2	0	1	1	3	3
	Γ	$\begin{pmatrix}1 & 0\\0 & 1\end{pmatrix}$	$\begin{pmatrix}-i & 0\\0 & i\end{pmatrix}$	$\begin{pmatrix}w^* & 0\\0 & w\end{pmatrix}$	$\begin{pmatrix}w & 0\\0 & w^*\end{pmatrix}$	$\begin{pmatrix}v^* & 0\\0 & v\end{pmatrix}$	$\begin{pmatrix}v & 0\\0 & v^*\end{pmatrix}$
Γ_8^+	χ	2	0	1	1	-3	-3
	Γ	$\begin{pmatrix}1 & 0\\0 & 1\end{pmatrix}$	$\begin{pmatrix}-i & 0\\0 & i\end{pmatrix}$	$\begin{pmatrix}w & 0\\0 & w^*\end{pmatrix}$	$\begin{pmatrix}w^* & 0\\0 & w\end{pmatrix}$	$\begin{pmatrix}-v & 0\\0 & -v^*\end{pmatrix}$	$\begin{pmatrix}-v^* & 0\\0 & -v\end{pmatrix}$
Γ_8^-	χ	2	0	1	1	-3	-3
	Γ	$\begin{pmatrix}1 & 0\\0 & 1\end{pmatrix}$	$\begin{pmatrix}-i & 0\\0 & i\end{pmatrix}$	$\begin{pmatrix}w & 0\\0 & w^*\end{pmatrix}$	$\begin{pmatrix}w^* & 0\\0 & w\end{pmatrix}$	$\begin{pmatrix}-v & 0\\0 & -v^*\end{pmatrix}$	$\begin{pmatrix}-v^* & 0\\0 & -v\end{pmatrix}$
Γ_9^+	χ	2	0	-2	-2	0	0
	Γ	$\begin{pmatrix}1 & 0\\0 & 1\end{pmatrix}$	$\begin{pmatrix}i & 0\\0 & -i\end{pmatrix}$	$\begin{pmatrix}-1 & 0\\0 & -1\end{pmatrix}$	$\begin{pmatrix}-1 & 0\\0 & -1\end{pmatrix}$	$\begin{pmatrix}-i & 0\\0 & i\end{pmatrix}$	$\begin{pmatrix}i & 0\\0 & -i\end{pmatrix}$
Γ_9^-	χ	2	0	-2	-2	0	0
	Γ	$\begin{pmatrix}1 & 0\\0 & 1\end{pmatrix}$	$\begin{pmatrix}i & 0\\0 & -i\end{pmatrix}$	$\begin{pmatrix}-1 & 0\\0 & -1\end{pmatrix}$	$\begin{pmatrix}-1 & 0\\0 & -1\end{pmatrix}$	$\begin{pmatrix}-i & 0\\0 & i\end{pmatrix}$	$\begin{pmatrix}i & 0\\0 & -i\end{pmatrix}$
$D^{j}_{m'm}$ [d]		$A \cdot \{\ 1$	$e^{-\pi i m}$	$e^{-2\pi i m/3}$	$e^{2\pi i m/3}$	$e^{-\pi i m/3}$	$e^{\pi i m/3}\ \}$

[d] $A = \delta_{mm'}$, $B = (-)^{3j+m}\,\delta_{m,-m'}$.

cont.

Table A3.19 (cont.)

Irrep	Quantity	Element {and class}								
		$\{C_2'(1)$	$C_2'(2)$	$C_2'(3)\}$	$\{C_2''(1)$	$C_2''(2)$	$C_2''(3)\}$	$\{ I \}$	$\{ \sigma_h \}$	$\{ S_6$
Γ_7^+	χ	0	0	0	0	0	0	2	0	1
	Γ	$\begin{pmatrix}0 & -1\\ 1 & 0\end{pmatrix}$	$\begin{pmatrix}0 & w^*\\ -w & 0\end{pmatrix}$	$\begin{pmatrix}0 & w\\ -w^* & 0\end{pmatrix}$	$\begin{pmatrix}0 & -i\\ -i & 0\end{pmatrix}$	$\begin{pmatrix}0 & v\\ -v^* & 0\end{pmatrix}$	$\begin{pmatrix}0 & -v^*\\ v & 0\end{pmatrix}$	$\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}$	$\begin{pmatrix}-i & 0\\ 0 & i\end{pmatrix}$	$\begin{pmatrix}w & 0\\ 0 & w^*\end{pmatrix}$
Γ_7^-	χ	0	0	0	0	0	0	-2	0	-1
	Γ	$\begin{pmatrix}0 & -1\\ 1 & 0\end{pmatrix}$	$\begin{pmatrix}0 & w^*\\ -w & 0\end{pmatrix}$	$\begin{pmatrix}0 & w\\ -w^* & 0\end{pmatrix}$	$\begin{pmatrix}0 & -i\\ -i & 0\end{pmatrix}$	$\begin{pmatrix}0 & v\\ -v^* & 0\end{pmatrix}$	$\begin{pmatrix}0 & -v^*\\ v & 0\end{pmatrix}$	$\begin{pmatrix}-1 & 0\\ 0 & -1\end{pmatrix}$	$\begin{pmatrix}i & 0\\ 0 & -i\end{pmatrix}$	$\begin{pmatrix}-w & 0\\ 0 & -w^*\end{pmatrix}$
Γ_8^+	χ	0	0	0	0	0	0	2	0	1
	Γ	$\begin{pmatrix}0 & -1\\ 1 & 0\end{pmatrix}$	$\begin{pmatrix}0 & w\\ -w^* & 0\end{pmatrix}$	$\begin{pmatrix}0 & w^*\\ -w & 0\end{pmatrix}$	$\begin{pmatrix}0 & -i\\ -i & 0\end{pmatrix}$	$\begin{pmatrix}0 & -v^*\\ v & 0\end{pmatrix}$	$\begin{pmatrix}0 & v\\ -v^* & 0\end{pmatrix}$	$\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}$	$\begin{pmatrix}-i & 0\\ 0 & i\end{pmatrix}$	$\begin{pmatrix}w^* & 0\\ 0 & w\end{pmatrix}$
Γ_8^-	χ	0	0	0	0	0	0	-2	0	-1
	Γ	$\begin{pmatrix}0 & -1\\ 1 & 0\end{pmatrix}$	$\begin{pmatrix}0 & w\\ -w^* & 0\end{pmatrix}$	$\begin{pmatrix}0 & w^*\\ -w & 0\end{pmatrix}$	$\begin{pmatrix}0 & -i\\ -i & 0\end{pmatrix}$	$\begin{pmatrix}0 & -v^*\\ v & 0\end{pmatrix}$	$\begin{pmatrix}0 & v\\ -v^* & 0\end{pmatrix}$	$\begin{pmatrix}-1 & 0\\ 0 & -1\end{pmatrix}$	$\begin{pmatrix}i & 0\\ 0 & -i\end{pmatrix}$	$\begin{pmatrix}-w^* & 0\\ 0 & -w\end{pmatrix}$
Γ_9^+	χ	0	0	0	0	0	0	2	0	-2
	Γ	$\begin{pmatrix}0 & -1\\ 1 & 0\end{pmatrix}$	$\begin{pmatrix}0 & -1\\ 1 & 0\end{pmatrix}$	$\begin{pmatrix}0 & -1\\ 1 & 0\end{pmatrix}$	$\begin{pmatrix}0 & i\\ i & 0\end{pmatrix}$	$\begin{pmatrix}0 & i\\ i & 0\end{pmatrix}$	$\begin{pmatrix}0 & i\\ i & 0\end{pmatrix}$	$\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}$	$\begin{pmatrix}i & 0\\ 0 & -i\end{pmatrix}$	$\begin{pmatrix}-1 & 0\\ 0 & -1\end{pmatrix}$
Γ_9^-	χ	0	0	0	0	0	0	-2	0	2
	Γ	$\begin{pmatrix}0 & -1\\ 1 & 0\end{pmatrix}$	$\begin{pmatrix}0 & -1\\ 1 & 0\end{pmatrix}$	$\begin{pmatrix}0 & -1\\ 1 & 0\end{pmatrix}$	$\begin{pmatrix}0 & i\\ i & 0\end{pmatrix}$	$\begin{pmatrix}0 & i\\ i & 0\end{pmatrix}$	$\begin{pmatrix}0 & i\\ i & 0\end{pmatrix}$	$\begin{pmatrix}-1 & 0\\ 0 & -1\end{pmatrix}$	$\begin{pmatrix}-i & 0\\ 0 & i\end{pmatrix}$	$\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}$
		B · { 1	$e^{-4\pi i m/3}$	$e^{4\pi i m/3}$	$e^{-\pi i m}$	$e^{5\pi i m/3}$	$e^{\pi i m/3}\}$	A · {1	$e^{-\pi i m}$	$e^{2\pi i m/3}$

Table A3.19 (cont.)

$S_6^{-1}\}$	$\{S_3$	$S_3^{-1}\}$	$\{\sigma_d(1)$	$\sigma_d(2)$	$\sigma_d(3)\}$	$\{\sigma_v(1)$	$\sigma_v(2)$	$\sigma_v(3)\}$	Basis [a]
1	3 ($\sqrt{3}$)	3 ($\sqrt{3}$)	0	0	0	0	0	0	
$\begin{pmatrix} w^* & 0 \\ 0 & w \end{pmatrix}$	$\begin{pmatrix} v & 0 \\ 0 & v^* \end{pmatrix}$	$\begin{pmatrix} v^* & 0 \\ 0 & v \end{pmatrix}$	$\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & w^* \\ -w & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & w \\ -w^* & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & -i \\ -i & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & v \\ -v^* & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & -v^* \\ v & 0 \end{pmatrix}$	$\left\{ \begin{matrix} \mid \ell j \ \frac{1}{2} > \\ s \mid \ell j \ -\frac{1}{2} > \end{matrix} \right.$ [b]
-1	-3 ($-\sqrt{3}$)	-3 ($-\sqrt{3}$)	0	0	0	0	0	0	
$\begin{pmatrix} -w^* & 0 \\ 0 & -w \end{pmatrix}$	$\begin{pmatrix} -v & 0 \\ 0 & -v^* \end{pmatrix}$	$\begin{pmatrix} -v^* & 0 \\ 0 & -v \end{pmatrix}$	$\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & -w^* \\ w & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & -w \\ w^* & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & -v \\ v^* & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & v^* \\ -v & 0 \end{pmatrix}$	$\left\{ \begin{matrix} \mid \ell j \ \frac{1}{2} > \\ -s \mid \ell j \ -\frac{1}{2} > \end{matrix} \right.$ [c]
1	-3 ($-\sqrt{3}$)	-3 ($-\sqrt{3}$)	0	0	0	0	0	0	
$\begin{pmatrix} w & 0 \\ 0 & w^* \end{pmatrix}$	$\begin{pmatrix} -v^* & 0 \\ 0 & -v \end{pmatrix}$	$\begin{pmatrix} -v & 0 \\ 0 & -v^* \end{pmatrix}$	$\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & w \\ -w^* & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & w^* \\ -w & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & -i \\ -i & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & -v^* \\ v & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & v \\ -v^* & 0 \end{pmatrix}$	$\left\{ \begin{matrix} \mid \ell j \ \frac{5}{2} > \\ s \mid \ell j \ -\frac{5}{2} > \end{matrix} \right.$ [b]
-1	3 ($\sqrt{3}$)	3 ($\sqrt{3}$)	0	0	0	0	0	0	
$\begin{pmatrix} -w & 0 \\ 0 & -w^* \end{pmatrix}$	$\begin{pmatrix} v^* & 0 \\ 0 & v \end{pmatrix}$	$\begin{pmatrix} v & 0 \\ 0 & v^* \end{pmatrix}$	$\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & -w \\ w^* & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & -w^* \\ w & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & v^* \\ -v & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & -v \\ v^* & 0 \end{pmatrix}$	$\left\{ \begin{matrix} \mid \ell j \ \frac{5}{2} > \\ -s \mid \ell j \ -\frac{5}{2} > \end{matrix} \right.$ [c]
-2	0	0	0	0	0	0	0	0	
$\begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}$	$\begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix}$	$\begin{pmatrix} -i & 0 \\ 0 & i \end{pmatrix}$	$\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix}$	$\left\{ \begin{matrix} \mid \ell j \ \frac{3}{2} > \\ -s \mid \ell j \ -\frac{3}{2} > \end{matrix} \right.$ [b]
2	0	0	0	0	0	0	0	0	
$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} -i & 0 \\ 0 & i \end{pmatrix}$	$\begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix}$	$\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & -i \\ -i & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & -i \\ -i & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & -i \\ -i & 0 \end{pmatrix}$	$\left\{ \begin{matrix} \mid \ell j \ \frac{3}{2} > \\ s \mid \ell j \ -\frac{3}{2} > \end{matrix} \right.$ [c]
$e^{-2\pi i m/3}$	$e^{\pi i m/3}$	$e^{-\pi i m/3}\}B\cdot$	$\{1$	$e^{-4\pi i m/3}$	$e^{4\pi i m/3}$	$e^{-\pi i m}$	$e^{5\pi i m/3}$	$e^{\pi i m/3}\}$	

[a] The m quantum number is defined mod (6).

[b] Even ℓ.

[c] Odd ℓ.

Table A3.20. T and T_h. $\omega = \exp(2\pi i/3)$. $A = \delta_{mm'}$. $B = (-)^{3j+m}\delta_{m,-m'}$. E″ and E‴ together form the rep u′. The elements $C = FI$ ($F \epsilon T$, I = inversion) belong to the group T_h. Their representation matrices $\Gamma(C) = \pm\Gamma(F)$ for representation $\Gamma_i^{\pm}$, i = 5 - 7. The elements are defined in Fig. A3.4.

Irrep	Quantity	{ E }	{ $C_2(z)$	$C_2(y)$	$C_2(x)$}	{ $C_3(1)$	$C_3(2)$
Γ_5=E′	χ	2	0	0	0	1	1
	Γ	$\begin{pmatrix}1 & 0\\0 & 1\end{pmatrix}$	$\begin{pmatrix}-i & 0\\0 & i\end{pmatrix}$	$\begin{pmatrix}0 & -1\\1 & 0\end{pmatrix}$	$\begin{pmatrix}0 & -i\\-i & 0\end{pmatrix}$	$\frac{1+i}{2}\begin{pmatrix}-i & 1\\i & 1\end{pmatrix}$	$\frac{1+i}{2}\begin{pmatrix}1 & i\\1 & -i\end{pmatrix}$
Γ_6=E″	χ	2	0	0	0	ω	ω
	Γ	$\begin{pmatrix}1 & 0\\0 & 1\end{pmatrix}$	$\begin{pmatrix}-i & 0\\0 & i\end{pmatrix}$	$\begin{pmatrix}0 & -1\\1 & 0\end{pmatrix}$	$\begin{pmatrix}0 & -i\\-i & 0\end{pmatrix}$	$\frac{1-\sqrt{3}i}{4}\begin{pmatrix}-1+i & -1-i\\1-i & -1-i\end{pmatrix}$	$\frac{1-\sqrt{3}i}{4}\begin{pmatrix}-1-i & 1-i\\-1-i & 1+i\end{pmatrix}$
Γ_7=E‴=Γ_6^*							
	$D^j_{m'm}$	A	$Ae^{-\pi i m}$	B	$Be^{-\pi i m}$	$d(-\frac{\pi}{2})e^{-\pi i m/2}$	$d(\frac{\pi}{2})e^{\pi i m/2}$
	C	I	$\sigma(xy)$	$\sigma(xz)$	$\sigma(yz)$	$S_6^{-1}(1)$	$S_6^{-1}(2)$

Table A3.20.(cont.)

Element {and class}			
$C_3(3)$	$C_3(4)$ } {	$C_3^{-1}(1)$	$C_3^{-1}(2)$
1	1	1	1
$\frac{1+i}{2}\begin{pmatrix}1 & -i\\ -1 & -i\end{pmatrix}$	$\frac{1+i}{2}\begin{pmatrix}-i & -1\\ -i & 1\end{pmatrix}$	$\frac{1+i}{2}\begin{pmatrix}1 & -1\\ -i & -i\end{pmatrix}$	$\frac{1+i}{2}\begin{pmatrix}-i & -i\\ -1 & 1\end{pmatrix}$
ω	ω	ω^2	ω^2
$\frac{1-\sqrt{3}\,i}{4}\begin{pmatrix}-1-i & -1+i\\ 1+i & -1+i\end{pmatrix}$	$\frac{1-\sqrt{3}\,i}{4}\begin{pmatrix}-1+i & 1+i\\ -1+i & -1-i\end{pmatrix}$	$\frac{1+\sqrt{3}\,i}{4}\begin{pmatrix}-1-i & 1+i\\ -1+i & -1+i\end{pmatrix}$	$\frac{1+\sqrt{3}\,i}{4}\begin{pmatrix}-1+i & -1+i\\ 1+i & -1-i\end{pmatrix}$
$d(-\frac{\pi}{2})e^{\pi i m/2}$	$d(\frac{\pi}{2})e^{-\pi i m/2}$	$d(\frac{\pi}{2})e^{\pi i m'/2}$	$d(-\frac{\pi}{2})e^{-\pi i m'/2}$
$S_6^{-1}(3)$	$S_6^{-1}(4)$	$S_6(1)$	$S_6(2)$

Table A3.20. (cont.)

$C_3^{-1}(3)$	$C_3^{-1}(4)$ }
1	1
$\frac{1+i}{2}\begin{pmatrix}-i & i\\ 1 & 1\end{pmatrix}$	$\frac{1+i}{2}\begin{pmatrix}1 & 1\\ i & -i\end{pmatrix}$
ω^2	ω^2
$\frac{1+\sqrt{3}\,i}{4}\begin{pmatrix}-1+i & 1-i\\ -1-i & -1-i\end{pmatrix}$	$\frac{1+\sqrt{3}\,i}{4}\begin{pmatrix}-1-i & -1-i\\ 1-i & -1+i\end{pmatrix}$
$d(\frac{\pi}{2})e^{-\pi i m'/2}$	$d(-\frac{\pi}{2})e^{\pi i m'/2}$
$S_6(3)$	$S_6(4)$

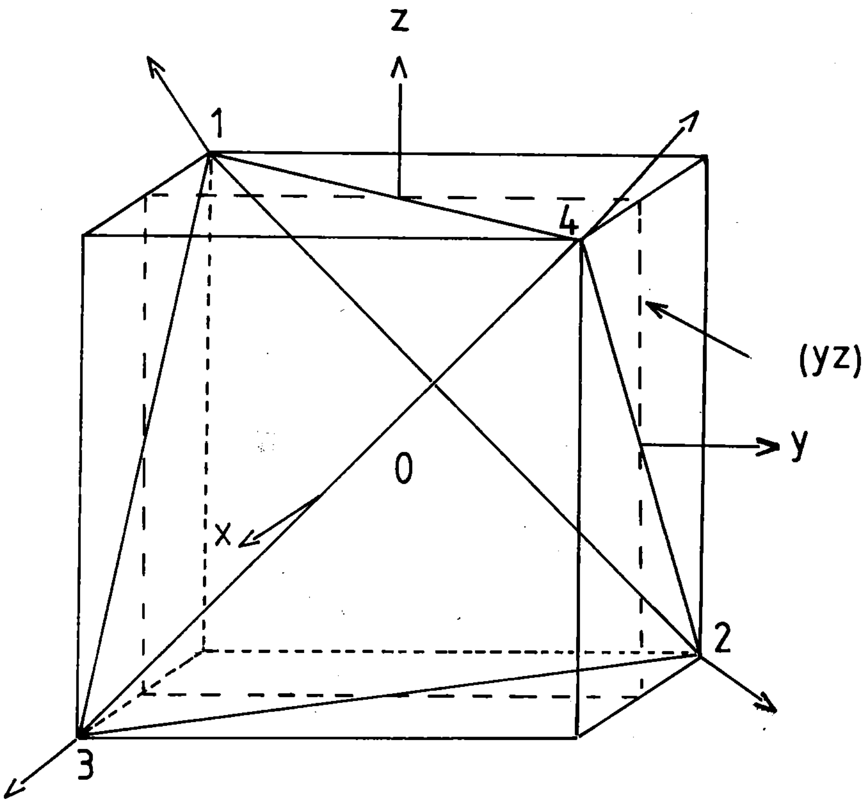

Figure A3.4. The coordinate system and notation assumed for T, T_h, T_d, O and O_h.

Table A3.21. Basis functions for T. For T_h, the functions with even ℓ span Γ_5^+, Γ_6^+ and Γ_7^+ while the functions with odd ℓ span Γ_5^-, Γ_6^- and Γ_7^-.

Irreducible representation	Angular momentum j: $\frac{1}{2}$	$\frac{3}{2}$	$\frac{5}{2}$
$\Gamma_5 = E'$	$\|\frac{1}{2}\rangle$ $\|-\frac{1}{2}\rangle$		$\frac{1}{\sqrt{6}}\left(\|\frac{5}{2}\rangle - \sqrt{5}\|-\frac{3}{2}\rangle\right)$ $\frac{1}{\sqrt{6}}\left(\|-\frac{5}{2}\rangle - \sqrt{5}\|\frac{3}{2}\rangle\right)$
$\Gamma_6 = E''$	-	$-\frac{1}{\sqrt{2}}\left(\|\frac{1}{2}\rangle - i\|-\frac{3}{2}\rangle\right)$ $\frac{1}{\sqrt{2}}\left(\|-\frac{1}{2}\rangle - i\|\frac{3}{2}\rangle\right)$	$\frac{1}{6}\{\sqrt{18}\|\frac{1}{2}\rangle - i(\sqrt{15}\|\frac{5}{2}\rangle +$ $\frac{1}{6}\{\sqrt{18}\|-\frac{1}{2}\rangle - i(\sqrt{15}\|-\frac{5}{2}\rangle +$
$\Gamma_7 = E'''$	-	$\frac{1}{\sqrt{2}}\left(\|-\frac{1}{2}\rangle + i\|\frac{3}{2}\rangle\right)$ $\frac{1}{\sqrt{2}}\left(\|\frac{1}{2}\rangle + i\|-\frac{3}{2}\rangle\right)$	$\frac{1}{6}\{\sqrt{18}\|-\frac{1}{2}\rangle + i(\sqrt{15}\|-\frac{5}{2}\rangle +$ $\frac{1}{6}\{-\sqrt{18}\|\frac{1}{2}\rangle - i(\sqrt{15}\|\frac{5}{2}\rangle +$
$\Gamma_6 + \Gamma_7$	-	$\|\frac{3}{2}\rangle$ $\|\frac{1}{2}\rangle$ $\|-\frac{1}{2}\rangle$ $\|-\frac{3}{2}\rangle$	$\frac{1}{\sqrt{6}}\left(-\|\frac{3}{2}\rangle - \sqrt{5}\|-\frac{5}{2}\rangle\right)$ $\|\frac{1}{2}\rangle$ $-\|-\frac{1}{2}\rangle$ $\frac{1}{\sqrt{6}}\left(\|-\frac{3}{2}\rangle + \sqrt{5}\|\frac{5}{2}\rangle\right)$

cont.

Table A3.21. (cont.)

Irreducible representation	Angular momentum j $\frac{5}{2}$ (cont.)	 $\frac{7}{2}$
$\Gamma_5 = E'$		$\left\{\begin{matrix} \frac{1}{\sqrt{12}}\left(\sqrt{7}\,|\tfrac{1}{2}> + \sqrt{5}\,|-\tfrac{7}{2}>\right) \\ \frac{1}{\sqrt{12}}\left(-\sqrt{7}\,|-\tfrac{1}{2}> - \sqrt{5}\,|\tfrac{7}{2}>\right) \end{matrix}\right.$, $\left\{\begin{matrix} \frac{1}{2}\left(\sqrt{3}\,|\tfrac{5}{2}> - |-\tfrac{3}{2}>\right) \\ \frac{1}{2}\left(-\sqrt{3}\,|-\tfrac{5}{2}> + |\tfrac{3}{2}>\right) \end{matrix}\right.$
$\Gamma_6 = E''$	$+\sqrt{3}\,|-\tfrac{3}{2}>\Big)\Big\}$ $+\sqrt{3}\,|\tfrac{3}{2}>\Big)\Big\}$	$\left\{\begin{matrix} \frac{1}{\sqrt{24}}\left\{\sqrt{5}\,|\tfrac{1}{2}> - \sqrt{7}\,|-\tfrac{7}{2}> + i\left(\sqrt{3}\,|\tfrac{5}{2}> + 3\,|-\tfrac{3}{2}>\right)\right\} \\ \frac{1}{\sqrt{24}}\left\{-\sqrt{5}\,|-\tfrac{1}{2}> + \sqrt{7}\,|\tfrac{7}{2}> - i\left(\sqrt{3}\,|-\tfrac{5}{2}> + 3\,|\tfrac{3}{2}>\right)\right\} \end{matrix}\right.$
$\Gamma_7 = E'''$	$+\sqrt{3}\,|\tfrac{3}{2}>\Big)\Big\}$ $+\sqrt{3}\,|-\tfrac{3}{2}>\Big)\Big\}$	$\left\{\begin{matrix} \frac{1}{\sqrt{24}}\left\{\sqrt{5}\,|-\tfrac{1}{2}> - \sqrt{7}\,|\tfrac{7}{2}> - i\left(\sqrt{3}\,|-\tfrac{5}{2}> + 3\,|\tfrac{3}{2}>\right)\right\} \\ \frac{1}{\sqrt{24}}\left\{\sqrt{5}\,|\tfrac{1}{2}> - \sqrt{7}\,|-\tfrac{7}{2}> - i\left(\sqrt{3}\,|\tfrac{5}{2}> + 3\,|-\tfrac{3}{2}>\right)\right\} \end{matrix}\right.$
$\Gamma_6 + \Gamma_7$		$\left\{\begin{matrix} \frac{1}{2}\left(\sqrt{3}\,|\tfrac{3}{2}> + |-\tfrac{5}{2}>\right) \\ \frac{1}{\sqrt{12}}\left(-\sqrt{5}\,|\tfrac{1}{2}> + \sqrt{7}\,|-\tfrac{7}{2}>\right) \\ \frac{1}{\sqrt{12}}\left(-\sqrt{5}\,|-\tfrac{1}{2}> + \sqrt{7}\,|\tfrac{7}{2}>\right) \\ \frac{1}{2}\left(\sqrt{3}\,|-\tfrac{3}{2}> + |\tfrac{5}{2}>\right) \end{matrix}\right.$

Table A3.22. Representation matrices for T_d, O and O_h from Onodera and Okazaki (1966 b). The elements C = F I (F ∈ O, I = inversion) belong to the group O_h. Their representation matrices Γ (C) = ± Γ (F) for the representations $\Gamma_i^{\pm}$, i = 6-8. The σ_d of T_d and the C_2' of O are labelled by the image of xyz, e.g. $\sigma_d(x\text{-}z\text{-}y)$ maps $\begin{matrix} x \\ y \\ z \end{matrix} \rightarrow \begin{matrix} x \\ -z \\ -y \end{matrix}$. The C_3 axes are labelled as for T and T_h (Fig. A3.4):

Element T_d	Element O	$\Gamma_6 = E' = E_{1/2}$	$\Gamma_7 = E'' = E_{5/2}$	$\Gamma_8 = U' = G_{3/2}$	C
E	E	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 1 & & & \\ & 1 & & \\ & & 1 & \\ & & & 1 \end{pmatrix}$	I
$C_2(x)$	$C_4^2(x)$	$\begin{pmatrix} 0 & -i \\ -i & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & -i \\ -i & 0 \end{pmatrix}$	$\begin{pmatrix} & & & i \\ & & i & \\ & i & & \\ i & & & \end{pmatrix}$	$\sigma_h(yz)$
$C_2(y)$	$C_4^2(y)$	$\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$	$\begin{pmatrix} & & & -1 \\ & & 1 & \\ & -1 & & \\ 1 & & & \end{pmatrix}$	$\sigma_h(xz)$
$C_2(z)$	$C_4^2(z)$	$\begin{pmatrix} -i & 0 \\ 0 & i \end{pmatrix}$	$\begin{pmatrix} -i & 0 \\ 0 & i \end{pmatrix}$	$\begin{pmatrix} i & & & \\ & -i & & \\ & & i & \\ & & & -i \end{pmatrix}$	$\sigma_h(xy)$
$S_4^{-1}(x)$	$C_4(x)$	$\frac{1}{\sqrt{2}}\begin{pmatrix} 1 & -i \\ -i & 1 \end{pmatrix}$	$\frac{1}{\sqrt{2}}\begin{pmatrix} -1 & i \\ i & -1 \end{pmatrix}$	$\frac{1}{\sqrt{8}}\begin{pmatrix} 1 & -\sqrt{3}\,i & -\sqrt{3} & i \\ -\sqrt{3}\,i & -1 & -i & -\sqrt{3} \\ -\sqrt{3} & i & -1 & -\sqrt{3}\,i \\ i & -\sqrt{3} & -\sqrt{3}\,i & 1 \end{pmatrix}$	$S_4^{-1}(x)$
$S_4(x)$	$C_4^{-1}(x)$	$\frac{1}{\sqrt{2}}\begin{pmatrix} 1 & i \\ i & 1 \end{pmatrix}$	$\frac{1}{\sqrt{2}}\begin{pmatrix} -1 & -i \\ -i & -1 \end{pmatrix}$	$\frac{1}{\sqrt{8}}\begin{pmatrix} 1 & \sqrt{3}\,i & -\sqrt{3} & -i \\ \sqrt{3}\,i & -1 & i & -\sqrt{3} \\ -\sqrt{3} & i & -1 & \sqrt{3}\,i \\ -i & -\sqrt{3} & \sqrt{3}\,i & 1 \end{pmatrix}$	$S_4(x)$
$S_4^{-1}(y)$	$C_4(y)$	$\frac{1}{\sqrt{2}}\begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix}$	$\frac{1}{\sqrt{2}}\begin{pmatrix} -1 & 1 \\ -1 & -1 \end{pmatrix}$	$\frac{1}{\sqrt{8}}\begin{pmatrix} 1 & -\sqrt{3} & \sqrt{3} & -1 \\ \sqrt{3} & -1 & -1 & \sqrt{3} \\ \sqrt{3} & 1 & -1 & -\sqrt{3} \\ 1 & \sqrt{3} & \sqrt{3} & 1 \end{pmatrix}$	$S_4^{-1}(y)$
$S_4(y)$	$C_4^{-1}(y)$	$\frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix}$	$\frac{1}{\sqrt{2}}\begin{pmatrix} -1 & -1 \\ 1 & -1 \end{pmatrix}$	$\frac{1}{\sqrt{8}}\begin{pmatrix} 1 & \sqrt{3} & \sqrt{3} & 1 \\ -\sqrt{3} & -1 & 1 & \sqrt{3} \\ \sqrt{3} & -1 & -1 & \sqrt{3} \\ -1 & \sqrt{3} & -\sqrt{3} & 1 \end{pmatrix}$	$S_4(y)$

Table A3.22. (cont.)

T_d	O	Γ_6	Γ_7	Γ_8	C
$S_4^{-1}(z)$	$C_4(z)$	$\frac{1}{\sqrt{2}}\begin{pmatrix} 1\ -i & 0 \\ 0 & 1\ +i \end{pmatrix}$	$\frac{1}{\sqrt{2}}\begin{pmatrix} -1\ +i & 0 \\ 0 & -1\ -i \end{pmatrix}$	$\frac{1}{\sqrt{2}}\begin{pmatrix} -1\ -i & & & \\ & 1\ -i & & \\ & & 1\ +i & \\ & & & -1\ +i \end{pmatrix}$	$S_4^{-1}(z)$
$S_4(z)$	$C_4^{-1}(z)$	$\frac{1}{\sqrt{2}}\begin{pmatrix} 1\ +i & 0 \\ 0 & 1\ -i \end{pmatrix}$	$\frac{1}{\sqrt{2}}\begin{pmatrix} -1\ -i & 0 \\ 0 & -1\ +i \end{pmatrix}$	$\frac{1}{\sqrt{2}}\begin{pmatrix} -1\ +i & & & \\ & 1\ +i & & \\ & & 1\ -i & \\ & & & -1\ -i \end{pmatrix}$	$S_4(z)$
$\sigma_d(x\text{-}z\text{-}y)$	$C_2'(-xzy)$	$\frac{1}{\sqrt{2}}\begin{pmatrix} -i & -1 \\ 1 & i \end{pmatrix}$	$\frac{1}{\sqrt{2}}\begin{pmatrix} i & 1 \\ -1 & -i \end{pmatrix}$	$\frac{1}{\sqrt{8}}\begin{pmatrix} i & \sqrt{3} & -\sqrt{3}\,i & -1 \\ -\sqrt{3} & i & -1 & \sqrt{3}\,i \\ -\sqrt{3}\,i & 1 & -i & \sqrt{3} \\ 1 & \sqrt{3}\,i & -\sqrt{3} & -i \end{pmatrix}$	$\sigma_d(x\text{-}z\text{-}y)$
$\sigma_d(xzy)$	$C_2'(-x\text{-}z\text{-}y)$	$\frac{1}{\sqrt{2}}\begin{pmatrix} i & -1 \\ 1 & -i \end{pmatrix}$	$\frac{1}{\sqrt{2}}\begin{pmatrix} -i & 1 \\ -1 & i \end{pmatrix}$	$\frac{1}{\sqrt{8}}\begin{pmatrix} -i & \sqrt{3} & \sqrt{3}\,i & -1 \\ -\sqrt{3} & -i & -1 & -\sqrt{3}\,i \\ \sqrt{3}\,i & 1 & i & \sqrt{3} \\ 1 & -\sqrt{3}\,i & -\sqrt{3} & i \end{pmatrix}$	$\sigma_d(xzy)$
$\sigma_d(-zy\text{-}x)$	$C_2'(z\text{-}yx)$	$\frac{i}{\sqrt{2}}\begin{pmatrix} -1 & -1 \\ -1 & 1 \end{pmatrix}$	$\frac{i}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$	$\frac{i}{\sqrt{8}}\begin{pmatrix} 1 & \sqrt{3} & \sqrt{3} & 1 \\ \sqrt{3} & 1 & -1 & -\sqrt{3} \\ \sqrt{3} & -1 & -1 & \sqrt{3} \\ 1 & -\sqrt{3} & \sqrt{3} & -1 \end{pmatrix}$	$\sigma_d(-zy\text{-}x)$
$\sigma_d(zyx)$	$C_2'(-z\text{-}y\text{-}x)$	$\frac{i}{\sqrt{2}}\begin{pmatrix} -1 & 1 \\ 1 & 1 \end{pmatrix}$	$\frac{i}{\sqrt{2}}\begin{pmatrix} 1 & -1 \\ -1 & -1 \end{pmatrix}$	$\frac{i}{\sqrt{8}}\begin{pmatrix} 1 & -\sqrt{3} & \sqrt{3} & -1 \\ -\sqrt{3} & 1 & 1 & -\sqrt{3} \\ \sqrt{3} & 1 & -1 & -\sqrt{3} \\ -1 & -\sqrt{3} & -\sqrt{3} & -1 \end{pmatrix}$	$\sigma_d(zyx)$

Table A3.22. (cont.)

T_d	O	Γ_6	Γ_7	Γ_8	C
$\sigma_d(\text{-y-xz})$	$C_2'(\text{yx-z})$	$\frac{1}{\sqrt{2}}\begin{pmatrix} 0 & -1\ -i \\ 1\ -i & 0 \end{pmatrix}$	$\frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 1\ +i \\ -1\ +i & 0 \end{pmatrix}$	$\frac{1}{\sqrt{2}}\begin{pmatrix} & & & 1\ -i \\ & & 1\ +i & \\ & -1\ +i & & \\ -1\ -i & & & \end{pmatrix}$	$\sigma_2(\text{yxz})$
$\sigma_d(\text{yxz})$	$C_2'(\text{-y-x-z})$	$\frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 1\ -i \\ -1\ -i & 0 \end{pmatrix}$	$\frac{1}{\sqrt{2}}\begin{pmatrix} 0 & -1\ +i \\ 1\ +i & 0 \end{pmatrix}$	$\frac{1}{\sqrt{2}}\begin{pmatrix} & & & -1\ -i \\ & & -1\ +i & \\ & 1\ +i & & \\ 1\ -i & & & \end{pmatrix}$	$\sigma_d(\text{yxz})$
$C_3(1)$	$C_3(1)$	$\frac{1\ +i}{2}\begin{pmatrix} -i & 1 \\ i & 1 \end{pmatrix}$	$\frac{1\ +i}{2}\begin{pmatrix} -i & 1 \\ i & 1 \end{pmatrix}$	$\frac{1\ +i}{4}\begin{pmatrix} -1 & -\sqrt{3}\,i & \sqrt{3} & i \\ \sqrt{3} & i & 1 & \sqrt{3}\,i \\ -\sqrt{3} & i & -1 & \sqrt{3}\,i \\ 1 & -\sqrt{3}\,i & -\sqrt{3} & i \end{pmatrix}$	$S_6^{-1}(1)$
$C_3(2)$	$C_3(2)$	$\frac{1\ +i}{2}\begin{pmatrix} 1 & i \\ 1 & -i \end{pmatrix}$	$\frac{1\ +i}{2}\begin{pmatrix} 1 & i \\ 1 & -i \end{pmatrix}$	$\frac{1\ +i}{4}\begin{pmatrix} i & -\sqrt{3} & -\sqrt{3}\,i & 1 \\ \sqrt{3}\,i & -1 & i & -\sqrt{3} \\ \sqrt{3}\,i & 1 & i & \sqrt{3} \\ i & \sqrt{3} & -\sqrt{3}\,i & -1 \end{pmatrix}$	$S_6^{-1}(2)$
$C_3(3)$	$C_3(3)$	$\frac{1\ +i}{2}\begin{pmatrix} 1 & -i \\ -1 & -i \end{pmatrix}$	$\frac{1\ +i}{2}\begin{pmatrix} 1 & -i \\ -1 & -i \end{pmatrix}$	$\frac{1\ +i}{4}\begin{pmatrix} i & \sqrt{3} & -\sqrt{3}\,i & -1 \\ -\sqrt{3}\,i & -1 & -i & -\sqrt{3} \\ \sqrt{3}\,i & -1 & i & -\sqrt{3} \\ -i & \sqrt{3} & \sqrt{3}\,i & -1 \end{pmatrix}$	$S_6^{-1}(3)$
$C_3(4)$	$C_3(4)$	$\frac{1\ +i}{2}\begin{pmatrix} -i & -1 \\ -i & 1 \end{pmatrix}$	$\frac{1\ +i}{2}\begin{pmatrix} -i & -1 \\ -i & 1 \end{pmatrix}$	$\frac{1\ +i}{4}\begin{pmatrix} -1 & \sqrt{3}\,i & \sqrt{3} & -i \\ -\sqrt{3} & i & -1 & \sqrt{3}\,i \\ -\sqrt{3} & -i & -1 & -\sqrt{3}\,i \\ -1 & -\sqrt{3}\,i & \sqrt{3} & i \end{pmatrix}$	$S_6^{-1}(4)$

Table A3.22. (cont.)

T_d	O	Γ_6	Γ_7	Γ_8	C
$C_3^{-1}(1)$	$C_3^{-1}(1)$	$\frac{1+i}{2}\begin{pmatrix} 1 & -1 \\ -i & -i \end{pmatrix}$	$\frac{1+i}{2}\begin{pmatrix} 1 & -1 \\ -i & -i \end{pmatrix}$	$\frac{1+i}{4}\begin{pmatrix} i & -\sqrt{3}\,i & \sqrt{3}\,i & -i \\ \sqrt{3} & -1 & -1 & \sqrt{3} \\ -\sqrt{3}\,i & -i & i & \sqrt{3}\,i \\ -1 & -\sqrt{3} & -\sqrt{3} & -1 \end{pmatrix}$	$S_6(1)$
$C_3^{-1}(2)$	$C_3^{-1}(2)$	$\frac{1+i}{2}\begin{pmatrix} -i & -i \\ -1 & 1 \end{pmatrix}$	$\frac{1+i}{2}\begin{pmatrix} -i & -i \\ -1 & 1 \end{pmatrix}$	$\frac{1+i}{4}\begin{pmatrix} -1 & -\sqrt{3} & -\sqrt{3} & -1 \\ \sqrt{3}\,i & i & -i & -\sqrt{3}\,i \\ \sqrt{3} & -1 & -1 & \sqrt{3} \\ -i & \sqrt{3}\,i & -\sqrt{3}\,i & i \end{pmatrix}$	$S_6(2)$
$C_3^{-1}(3)$	$C_3^{-1}(3)$	$\frac{1+i}{2}\begin{pmatrix} -i & i \\ 1 & 1 \end{pmatrix}$	$\frac{1+i}{2}\begin{pmatrix} -i & i \\ 1 & 1 \end{pmatrix}$	$\frac{1+i}{4}\begin{pmatrix} -1 & \sqrt{3} & -\sqrt{3} & 1 \\ -\sqrt{3}\,i & i & i & -\sqrt{3}\,i \\ \sqrt{3} & 1 & -1 & -\sqrt{3} \\ i & \sqrt{3}\,i & \sqrt{3}\,i & i \end{pmatrix}$	$S_6(3)$
$C_3^{-1}(4)$	$C_3^{-1}(4)$	$\frac{1+i}{2}\begin{pmatrix} 1 & 1 \\ i & -i \end{pmatrix}$	$\frac{1+i}{2}\begin{pmatrix} 1 & 1 \\ i & -i \end{pmatrix}$	$\frac{1+i}{4}\begin{pmatrix} i & \sqrt{3}\,i & \sqrt{3}\,i & i \\ -\sqrt{3} & -1 & 1 & \sqrt{3} \\ -\sqrt{3}\,i & i & i & \sqrt{3}\,i \\ 1 & -\sqrt{3} & \sqrt{3} & -1 \end{pmatrix}$	$S_6(4)$

Table A3.23. Characters of T_d, O and O_h.

Irrep	Class				
T_d :	E	$8C_3$	$3C_2,\ 3\bar{C}_2$	$6S_4$	$6\sigma_d,\ 6\bar{\sigma}_d$
O :	E	$8C_3$	$3C_2,\ 3\bar{C}_2$	$6C_4$	$6C_2',\ 6\bar{C}_2'$
$\Gamma_6 = E' = E_{1/2}$	2	1	0	2	0
$\Gamma_7 = E'' = E_{5/2}$	2	1	0	- 2	0
$\Gamma_8 = U' = G_{3/2}$	4	- 1	0	0	0

Table A3.24. Basis functions for T_d, O and O_h.[a]

Group	Irrep	AO	Basis
O_h	Γ_6^+	$s_{1/2}$	$\|\frac{1}{2}>$
			$\|-\frac{1}{2}>$
		$g_{7/2}$	$-\sqrt{\frac{7}{12}}\ \|\frac{1}{2}> - \sqrt{\frac{5}{12}}\ \|-\frac{7}{2}>$
			$\sqrt{\frac{7}{12}}\ \|-\frac{1}{2}> + \sqrt{\frac{5}{12}}\ \|\frac{7}{2}>$
		$g_{9/2}$	$\sqrt{\frac{1}{24}}\ \|-\frac{7}{2}> + \sqrt{\frac{14}{24}}\ \|\frac{1}{2}> + \sqrt{\frac{9}{24}}\ \|\frac{9}{2}>$
			$\sqrt{\frac{1}{24}}\ \|\frac{7}{2}> + \sqrt{\frac{14}{24}}\ \|-\frac{1}{2}> + \sqrt{\frac{9}{24}}\ \|-\frac{9}{2}>$
	Γ_6^-	$p_{1/2}$	$i\|\frac{1}{2}>$
			$i\|-\frac{1}{2}>$
		$f_{7/2}$	$i\left(-\sqrt{\frac{7}{12}}\ \|\frac{1}{2}> - \sqrt{\frac{5}{12}}\ \|-\frac{7}{2}>\right)$
			$i\left(\sqrt{\frac{7}{12}}\ \|-\frac{1}{2}> + \sqrt{\frac{5}{12}}\ \|\frac{7}{2}>\right)$

[a] These relative phases are consistent with the model systems MH_6 (O_h) and MH_4 (T_d). The corresponding proton fields are given by Pyykkö and Desclaux (1978) (Chem.Phys. *34*, 261).

Table A3.24. (cont.)

Group	Irrep	AO	Basis
O_h	Γ_8^+	$d_{3/2}$	$-\lvert -\frac{3}{2}\rangle$
			$-\lvert -\frac{1}{2}\rangle$
			$-\lvert \frac{1}{2}\rangle$
			$-\lvert \frac{3}{2}\rangle$
		$d_{5/2}$	$\sqrt{\frac{1}{6}}\,\lvert -\frac{3}{2}\rangle + \sqrt{\frac{5}{6}}\,\lvert \frac{5}{2}\rangle$
			$-\lvert -\frac{1}{2}\rangle$
			$\lvert \frac{1}{2}\rangle$
			$-\sqrt{\frac{1}{6}}\,\lvert \frac{3}{2}\rangle - \sqrt{\frac{5}{6}}\,\lvert -\frac{5}{2}\rangle$
		$g_{7/2}$	$-\frac{1}{2}\,\lvert \frac{5}{2}\rangle - \frac{\sqrt{3}}{2}\,\lvert -\frac{3}{2}\rangle$
			$\sqrt{\frac{5}{12}}\,\lvert -\frac{1}{2}\rangle - \sqrt{\frac{7}{12}}\,\lvert \frac{7}{2}\rangle$
			$\sqrt{\frac{5}{12}}\,\lvert \frac{1}{2}\rangle - \sqrt{\frac{7}{12}}\,\lvert -\frac{7}{2}\rangle$
			$-\frac{1}{2}\,\lvert -\frac{5}{2}\rangle - \frac{\sqrt{3}}{2}\,\lvert \frac{3}{2}\rangle$
		$g_{9/2}$	$\sqrt{\frac{3}{10}}\,\lvert -\frac{3}{2}\rangle + \sqrt{\frac{7}{10}}\,\lvert \frac{5}{2}\rangle$
			$\sqrt{\frac{50}{120}}\,\lvert -\frac{1}{2}\rangle - \sqrt{\frac{7}{120}}\,\lvert \frac{7}{2}\rangle - \sqrt{\frac{63}{120}}\,\lvert -\frac{9}{2}\rangle$
			$-\sqrt{\frac{50}{120}}\,\lvert \frac{1}{2}\rangle + \sqrt{\frac{7}{120}}\,\lvert -\frac{7}{2}\rangle + \sqrt{\frac{63}{120}}\,\lvert \frac{9}{2}\rangle$
			$-\sqrt{\frac{3}{10}}\,\lvert \frac{3}{2}\rangle - \sqrt{\frac{7}{10}}\,\lvert -\frac{5}{2}\rangle$

Table A3.24. (cont.)

Group	Irrep	Basis
O_h	Γ_8^-	$p_{3/2}\left\{\begin{array}{l} i\left\vert\ \frac{1}{2}\right> \\ -i\left\vert\ \frac{3}{2}\right> \\ -i\left\vert -\frac{3}{2}\right> \\ i\left\vert -\frac{1}{2}\right> \end{array}\right.$ $\quad f_{5/2}:\left\{\begin{array}{l} -i\left\vert\ \frac{1}{2}\right> \\ -i\left(\sqrt{\frac{5}{6}}\left\vert -\frac{5}{2}\right> + \sqrt{\frac{1}{6}}\left\vert\ \frac{3}{2}\right>\right) \\ i\left(\sqrt{\frac{5}{6}}\left\vert\ \frac{5}{2}\right> + \sqrt{\frac{1}{6}}\left\vert -\frac{3}{2}\right>\right) \\ i\left\vert -\frac{1}{2}\right> \end{array}\right.$ $\quad f_{7/2}:\left\{\begin{array}{l} i\left(\sqrt{\frac{5}{12}}\left\vert\ \frac{1}{2}\right> - \sqrt{\frac{7}{12}}\left\vert -\frac{7}{2}\right>\right) \\ \frac{i}{2}\left(\left\vert -\frac{5}{2}\right> + \sqrt{3}\left\vert\ \frac{3}{2}\right>\right) \\ \frac{i}{2}\left(\left\vert\ \frac{5}{2}\right> + \sqrt{3}\left\vert -\frac{3}{2}\right>\right) \\ i\left(\sqrt{\frac{5}{12}}\left\vert -\frac{1}{2}\right> - \sqrt{\frac{7}{12}}\left\vert\ \frac{7}{2}\right>\right) \end{array}\right.$
T_d	Γ_6	$s_{1/2}:\Gamma_6^+(O_h)$ $\quad f_{5/2}:\left\{\begin{array}{l} i\left(\sqrt{\frac{1}{6}}\left\vert\ \frac{5}{2}\right> - \sqrt{\frac{5}{6}}\left\vert -\frac{3}{2}\right>\right) \\ i\left(\sqrt{\frac{1}{6}}\left\vert -\frac{5}{2}\right> - \sqrt{\frac{5}{6}}\left\vert\ \frac{3}{2}\right>\right) \end{array}\right.$ $\quad f_{7/2}:\left\{\begin{array}{l} \frac{i}{2}\left(-\sqrt{3}\left\vert\ \frac{5}{2}\right> + \left\vert -\frac{3}{2}\right>\right) \\ \frac{i}{2}\left(\sqrt{3}\left\vert -\frac{5}{2}\right> - \left\vert\ \frac{3}{2}\right>\right) \end{array}\right.$
	Γ_7	$p_{1/2}:\Gamma_6^-(O_h)$ $\quad d_{5/2}:\left\{\begin{array}{l} -\sqrt{\frac{1}{6}}\left\vert\ \frac{5}{2}\right> + \sqrt{\frac{5}{6}}\left\vert -\frac{3}{2}\right> \\ -\sqrt{\frac{1}{6}}\left\vert -\frac{5}{2}\right> + \sqrt{\frac{5}{6}}\left\vert\ \frac{3}{2}\right> \end{array}\right.$ $\quad f_{7/2}:\ \Gamma_6^-(O_h)$
	Γ_8	$p_{3/2}:\Gamma_8^-(O_h)$ $\quad d_{3/2}:-\Gamma_8^+(O_h)$ $\quad d_{5/2}:\Gamma_8^+(O_h)$ $\quad f_{5/2}:\ \Gamma_8^-(O_h)$ $\quad f_{7/2}:\ \Gamma_8^-(O_h)$.

Table A3.25. Basis functions for $C_{\infty v}$ and $D_{\infty h}$.

Group	Irrep	Basis[a]			
$D_{\infty h}$	$\Gamma_{1/2g}$	$s_{1/2}: \left\{ \begin{array}{l} \|\tfrac{1}{2}\rangle \\ \|-\tfrac{1}{2}\rangle \end{array} \right.$	$d_{3/2}: \left\{ \begin{array}{l} -\|\tfrac{1}{2}\rangle \\ \|-\tfrac{1}{2}\rangle \end{array} \right.$	$d_{5/2}: \left\{ \begin{array}{l} \|\tfrac{1}{2}\rangle \\ \|-\tfrac{1}{2}\rangle \end{array} \right.$	
	$\Gamma_{1/2u}$	$p_{1/2}: \left\{ \begin{array}{l} -\|\tfrac{1}{2}\rangle \\ \|-\tfrac{1}{2}\rangle \end{array} \right.$	$p_{3/2}: \left\{ \begin{array}{l} \|\tfrac{1}{2}\rangle \\ \|-\tfrac{1}{2}\rangle \end{array} \right.$	$f_{5/2}: \left\{ \begin{array}{l} -\|\tfrac{1}{2}\rangle \\ \|-\tfrac{1}{2}\rangle \end{array} \right.$	$f_{7/2}: \left\{ \begin{array}{l} \|\tfrac{1}{2}\rangle \\ \|-\tfrac{1}{2}\rangle \end{array} \right.$

[a] These coefficients for Γ_m are -1 for $j = \ell - \frac{1}{2}$ and $m_s = +\frac{1}{2}$ $(m = m_\ell + m_s)$, and $+1$ otherwise.

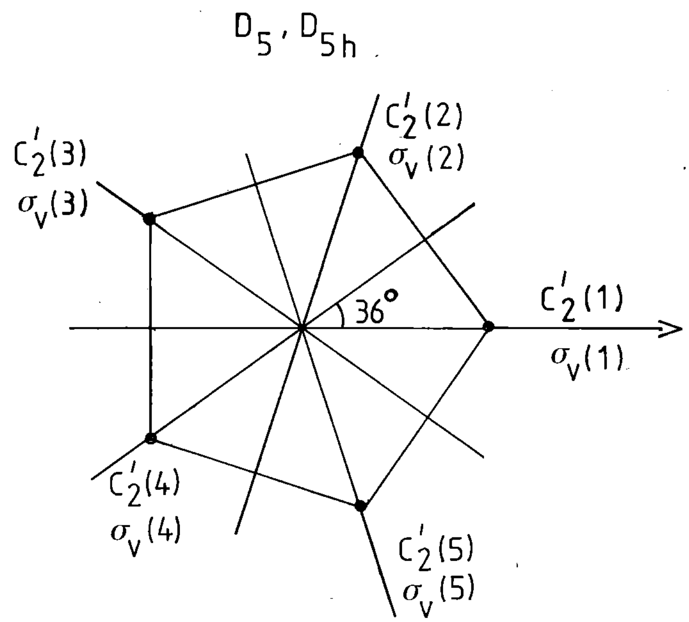

Figure A3.5. Definition of the operations for D_5 and D_{5h}.

Table A3.26. D_5 and C_{5v}. $w = \exp(i\pi/5)$. The elements are defined in Fig. A3.5. The symmetry planes $\sigma_v(i)$ are perpendicular against $C_2'(i)$. The irreps ρ_1 and ρ_2 together form $E''' = E_{5/2}$.

Irrep	Quantity	Elements {and class}				
	D_5 :	{ E }	{ C_5	C_5^{-1} }	{ C_5^2	C_5^{-2} }
	C_{5v} :	{ E }	{ C_5	C_5^{-1} }	{ C_5^2	C_5^{-2} }
$\Gamma_5 = E' = E_{1/2}$	χ	2	$\frac{1}{2}(1+\sqrt{5})$	$\frac{1}{2}(1+\sqrt{5})$	$\frac{1}{2}(-1+\sqrt{5})$	$\frac{1}{2}(-1+\sqrt{5})$
	Γ	$\begin{pmatrix}1 & 0\\0 & 1\end{pmatrix}$	$\begin{pmatrix}w^* & 0\\0 & w\end{pmatrix}$	$\begin{pmatrix}w & 0\\0 & w^*\end{pmatrix}$	$\begin{pmatrix}w^{*2} & 0\\0 & w^2\end{pmatrix}$	$\begin{pmatrix}w^2 & 0\\0 & w^{*2}\end{pmatrix}$
$\Gamma_6 = E'' = E_{3/2}$	χ	2	$\frac{1}{2}(1-\sqrt{5})$	$\frac{1}{2}(1-\sqrt{5})$	$-\frac{1}{2}(1+\sqrt{5})$	$-\frac{1}{2}(1+\sqrt{5})$
	Γ	$\begin{pmatrix}1 & 0\\0 & 1\end{pmatrix}$	$\begin{pmatrix}-w^2 & 0\\0 & -w^{*2}\end{pmatrix}$	$\begin{pmatrix}-w^{*2} & 0\\0 & -w^2\end{pmatrix}$	$\begin{pmatrix}-w^* & 0\\0 & -w\end{pmatrix}$	$\begin{pmatrix}-w & 0\\0 & -w^*\end{pmatrix}$
$\Gamma_7 = \rho_1$		1	-1	-1	1	1
$\Gamma_8 = \rho_2$		1	-1	-1	1	1
	$D^j_{m'm}$ $\delta_{m'm}$ ·	{ 1	$e^{-2\pi im/5}$	$e^{2\pi im/5}$	$e^{-4\pi im/5}$	$e^{4\pi im/5}$ }

$A = \delta_{m,-m'} (-)^{3j+m}$.

Table A3.26. (cont.)

Irrep	Quantity	Elements {and class}				
	D_5 :	{ $C_2'(1)$	$C_2'(2)$	$C_2'(3)$	$C_2'(4)$	$C_2'(5)$ }
	C_{5v} :	{ $\sigma_v(1)$	$\sigma_v(2)$	$\sigma_v(3)$	$\sigma_v(4)$	$\sigma_v(5)$ }
$\Gamma_5 = E' = E_{1/2}$	χ	0	0	0	0	0
	Γ	$\begin{pmatrix}0 & -1\\1 & 0\end{pmatrix}$	$\begin{pmatrix}0 & -w^{*2}\\w^2 & 0\end{pmatrix}$	$\begin{pmatrix}0 & w\\-w^* & 0\end{pmatrix}$	$\begin{pmatrix}0 & w^*\\-w & 0\end{pmatrix}$	$\begin{pmatrix}0 & -w^2\\w^{*2} & 0\end{pmatrix}$
$\Gamma_6 = E'' = E_{3/2}$	χ	0	0	0	0	0
	Γ	$\begin{pmatrix}0 & -1\\1 & 0\end{pmatrix}$	$\begin{pmatrix}0 & w^*\\-w & 0\end{pmatrix}$	$\begin{pmatrix}0 & -w^{*2}\\w^2 & 0\end{pmatrix}$	$\begin{pmatrix}0 & -w^2\\w^{*2} & 0\end{pmatrix}$	$\begin{pmatrix}0 & w\\-w^* & 0\end{pmatrix}$
$\Gamma_7 = \rho_1$		i	i	i	i	i
$\Gamma_8 = \rho_2$		-i	-i	-i	-i	-i
	A ·	{ 1	$e^{4\pi im/5}$	$e^{8\pi im/5}$	$e^{-8\pi im/5}$	$e^{-4\pi im/5}$ }

Table A3.27. Basis functions for D_5 and C_{5v}. The m quantum number is defined mod (10).

Irrep	Basis: D_5	Basis: C_{5v}
Γ_5	$\left\{ \begin{array}{r} \|\ell j \ \frac{1}{2}> \\ (-)^{\ell} s\|\ell j -\frac{1}{2}> \end{array} \right.$, $\left\{ \begin{array}{r} \|\ell j -\frac{9}{2}> \\ (-)^{\ell+1} s\|\ell j \ \frac{9}{2}> \end{array} \right.$	$\left\{ \begin{array}{r} \|\ell j \ \frac{1}{2}> \\ s\|\ell j -\frac{1}{2}> \end{array} \right.$, $\left\{ \begin{array}{r} \|\ell j -\frac{9}{2}> \\ -s\|\ell j \ \frac{9}{2}> \end{array} \right.$
Γ_6	$\left\{ \begin{array}{r} \|\ell j \ \frac{3}{2}> \\ (-)^{\ell+1} s\|\ell j -\frac{3}{2}> \end{array} \right.$, $\left\{ \begin{array}{r} \|\ell j -\frac{7}{2}> \\ (-)^{\ell} s\|\ell j \ \frac{7}{2}> \end{array} \right.$	$\left\{ \begin{array}{r} \|\ell j \ \frac{3}{2}> \\ -s\|\ell j -\frac{3}{2}> \end{array} \right.$, $\left\{ \begin{array}{r} \|\ell j -\frac{7}{2}> \\ s\|\ell j \ \frac{7}{2}> \end{array} \right.$
Γ_7	$(-)^{\ell} s\|\ell j \ \frac{5}{2}> - i \ \|\ell j -\frac{5}{2}>$	$s\|\ell j \ \frac{5}{2}> - i \ \|\ell j -\frac{5}{2}>$
Γ_8	$(-)^{\ell} s\|\ell j \ \frac{5}{2}> + i \ \|\ell j -\frac{5}{2}>$	$s\|\ell j \ \frac{5}{2}> + i \ \|\ell j -\frac{5}{2}>$

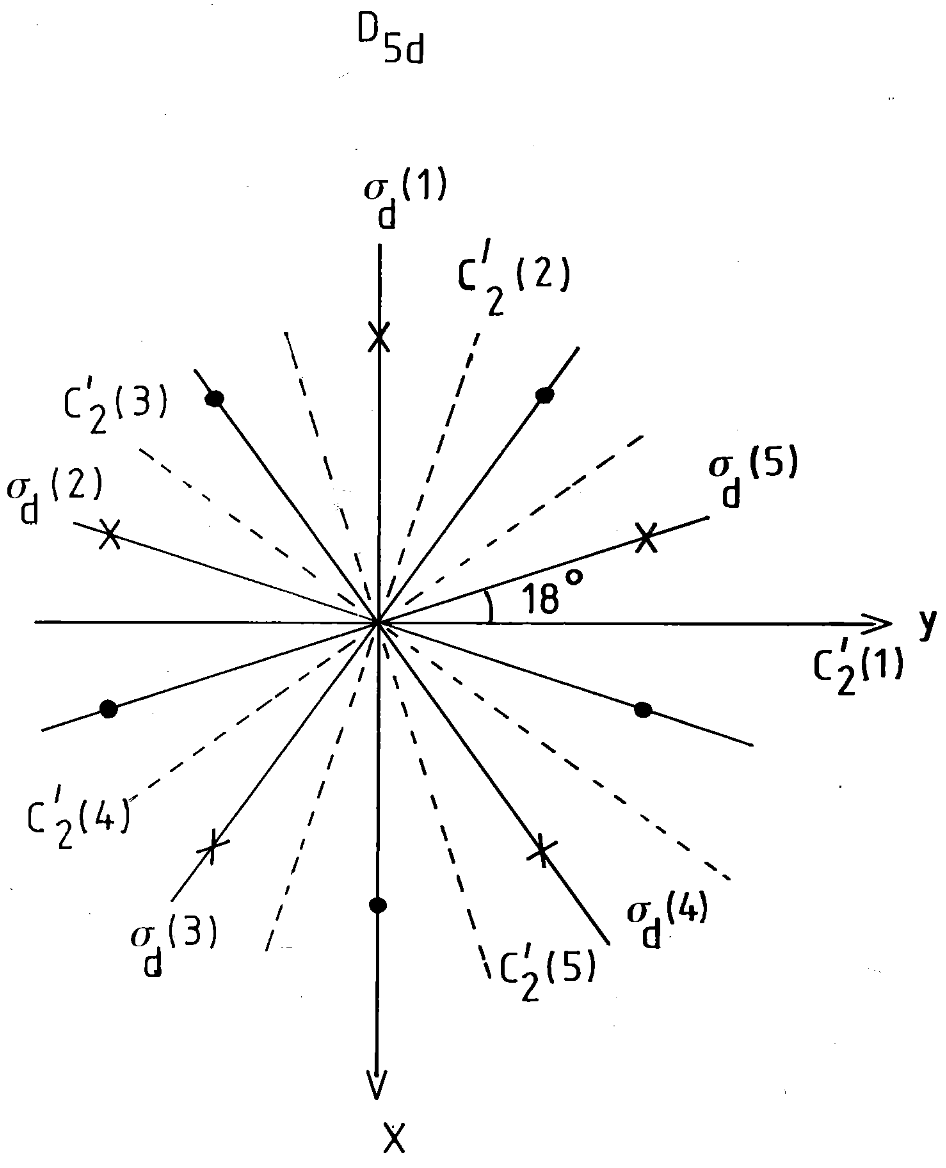

Figure A3.6. Definition of the operations for D_{5d}.

Table A3.28. D_{5d}. $w = \exp(i\pi/5)$. The elements are defined in Fig. A3.6.

Irrep	Quantity	Element				
		E	C_5	C_5^{-1}	C_5^2	C_5^{-2}
Γ_5^+	χ	2	$\frac{1}{2}(1+\sqrt{5})$	$\frac{1}{2}(1+\sqrt{5})$	$\frac{1}{2}(-1+\sqrt{5})$	$\frac{1}{2}(-1+\sqrt{5})$
	Γ	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} w^* & 0 \\ 0 & w \end{pmatrix}$	$\begin{pmatrix} w & 0 \\ 0 & w^* \end{pmatrix}$	$\begin{pmatrix} w^{*2} & 0 \\ 0 & w^2 \end{pmatrix}$	$\begin{pmatrix} w^2 & 0 \\ 0 & w^{*2} \end{pmatrix}$
Γ_5^-	χ	2	$\frac{1}{2}(1+\sqrt{5})$	$\frac{1}{2}(1+\sqrt{5})$	$\frac{1}{2}(-1+\sqrt{5})$	$\frac{1}{2}(-1+\sqrt{5})$
	Γ	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} w^* & 0 \\ 0 & w \end{pmatrix}$	$\begin{pmatrix} w & 0 \\ 0 & w^* \end{pmatrix}$	$\begin{pmatrix} w^{*2} & 0 \\ 0 & w^2 \end{pmatrix}$	$\begin{pmatrix} w^2 & 0 \\ 0 & w^{*2} \end{pmatrix}$
Γ_6^+	χ	2	$\frac{1}{2}(1-\sqrt{5})$	$\frac{1}{2}(1-\sqrt{5})$	$-\frac{1}{2}(1+\sqrt{5})$	$-\frac{1}{2}(1+\sqrt{5})$
	Γ	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} -w^2 & 0 \\ 0 & -w^{*2} \end{pmatrix}$	$\begin{pmatrix} -w^{*2} & 0 \\ 0 & -w^2 \end{pmatrix}$	$\begin{pmatrix} -w^* & 0 \\ 0 & -w \end{pmatrix}$	$\begin{pmatrix} -w & 0 \\ 0 & -w^* \end{pmatrix}$
Γ_6^-	χ	2	$\frac{1}{2}(-1+\sqrt{5})$	$\frac{1}{2}(-1+\sqrt{5})$	$\frac{1}{2}(1+\sqrt{5})$	$\frac{1}{2}(1+\sqrt{5})$
	Γ	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} -w^2 & 0 \\ 0 & -w^{*2} \end{pmatrix}$	$\begin{pmatrix} -w^{*2} & 0 \\ 0 & -w^2 \end{pmatrix}$	$\begin{pmatrix} -w^* & 0 \\ 0 & -w \end{pmatrix}$	$\begin{pmatrix} -w & 0 \\ 0 & -w^* \end{pmatrix}$
Γ_7^+		1	-1	-1	1	1
Γ_7^-		1	-1	-1	1	1
Γ_8^+		1	-1	-1	1	1
Γ_8^-		1	-1	-1	1	1
$D^j_{m'm}\,\delta_{mm'}$ {		1	$e^{-2\pi i m/5}$	$e^{2\pi i m/5}$	$e^{-4\pi i m/5}$	$e^{4\pi i m/5}$

Table A3.28. (cont.)

Irrep	Quantity	Element				
		S_{10}	S_{10}^{-1}	S_{10}^{3}	S_{10}^{-3}	S_2
Γ_5^+	χ	$\frac{1}{2}(-1+\sqrt{5})$	$\frac{1}{2}(-1+\sqrt{5})$	$\frac{1}{2}(1+\sqrt{5})$	$\frac{1}{2}(1+\sqrt{5})$	2
	Γ	$\begin{pmatrix} w^2 & 0 \\ 0 & w^{*2} \end{pmatrix}$	$\begin{pmatrix} w^{*2} & 0 \\ 0 & w^2 \end{pmatrix}$	$\begin{pmatrix} w & 0 \\ 0 & w^* \end{pmatrix}$	$\begin{pmatrix} w^* & 0 \\ 0 & w \end{pmatrix}$	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$
Γ_5^-	χ	$\frac{1}{2}(1-\sqrt{5})$	$\frac{1}{2}(1-\sqrt{5})$	$-\frac{1}{2}(1+\sqrt{5})$	$-\frac{1}{2}(1+\sqrt{5})$	-2
	Γ	$\begin{pmatrix} -w^2 & 0 \\ 0 & -w^{*2} \end{pmatrix}$	$\begin{pmatrix} -w^{*2} & 0 \\ 0 & -w^2 \end{pmatrix}$	$\begin{pmatrix} -w & 0 \\ 0 & -w^* \end{pmatrix}$	$\begin{pmatrix} -w^* & 0 \\ 0 & -w \end{pmatrix}$	$\begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}$
Γ_6^+	χ	$-\frac{1}{2}(1+\sqrt{5})$	$-\frac{1}{2}(1+\sqrt{5})$	$\frac{1}{2}(1-\sqrt{5})$	$\frac{1}{2}(1-\sqrt{5})$	2
	Γ	$\begin{pmatrix} -w & 0 \\ 0 & -w^* \end{pmatrix}$	$\begin{pmatrix} -w^* & 0 \\ 0 & -w \end{pmatrix}$	$\begin{pmatrix} -w^{*2} & 0 \\ 0 & -w^2 \end{pmatrix}$	$\begin{pmatrix} -w^2 & 0 \\ 0 & -w^{*2} \end{pmatrix}$	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$
Γ_6^-	χ	$\frac{1}{2}(1+\sqrt{5})$	$\frac{1}{2}(1+\sqrt{5})$	$\frac{1}{2}(-1+\sqrt{5})$	$\frac{1}{2}(-1+\sqrt{5})$	-2
	Γ	$\begin{pmatrix} w & 0 \\ 0 & w^* \end{pmatrix}$	$\begin{pmatrix} w^* & 0 \\ 0 & w \end{pmatrix}$	$\begin{pmatrix} w^{*2} & 0 \\ 0 & w^2 \end{pmatrix}$	$\begin{pmatrix} w^2 & 0 \\ 0 & w^{*2} \end{pmatrix}$	$\begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}$
Γ_7^+		1	1	-1	-1	1
Γ_7^-		-1	-1	1	1	-1
Γ_8^+		1	1	-1	-1	1
Γ_8^-		-1	-1	1	1	-1
		$e^{4\pi i m/5}$	$e^{-4\pi i m/5}$	$e^{2\pi i m/5}$	$e^{-2\pi i m/5}$	1 }

Table A3.28. (cont.)

Irrep	Quantity	Element						
		$C_2'(1)$	$C_2'(2)$	$C_2'(3)$	$C_2'(4)$	C_2' 5)	$\sigma_d(1)$	$\sigma_d(2)$
Γ_5^+	χ	0	0	0	0	0	0	0
	Γ	$\begin{pmatrix}0 & -1\\ 1 & 0\end{pmatrix}$	$\begin{pmatrix}0 & -w^{*2}\\ w^2 & 0\end{pmatrix}$	$\begin{pmatrix}0 & w\\ -w^* & 0\end{pmatrix}$	$\begin{pmatrix}0 & w^*\\ -w & 0\end{pmatrix}$	$\begin{pmatrix}0 & -w^2\\ w^{*2} & 0\end{pmatrix}$	$\begin{pmatrix}0 & -1\\ 1 & 0\end{pmatrix}$	$\begin{pmatrix}0 & -w^{*2}\\ w^2 & 0\end{pmatrix}$
Γ_5^-	χ	0	0	0	0	0	0	0
	Γ	$\begin{pmatrix}0 & -1\\ 1 & 0\end{pmatrix}$	$\begin{pmatrix}0 & -w^{*2}\\ w^2 & 0\end{pmatrix}$	$\begin{pmatrix}0 & w\\ -w^* & 0\end{pmatrix}$	$\begin{pmatrix}0 & w^*\\ -w & 0\end{pmatrix}$	$\begin{pmatrix}0 & -w^2\\ w^{*2} & 0\end{pmatrix}$	$\begin{pmatrix}0 & 1\\ -1 & 0\end{pmatrix}$	$\begin{pmatrix}0 & w^{*2}\\ -w^2 & 0\end{pmatrix}$
Γ_6^+	χ	0	0	0	0	0	0	0
	Γ	$\begin{pmatrix}0 & -1\\ 1 & 0\end{pmatrix}$	$\begin{pmatrix}0 & w^*\\ -w & 0\end{pmatrix}$	$\begin{pmatrix}0 & -w^{*2}\\ w^2 & 0\end{pmatrix}$	$\begin{pmatrix}0 & -w^2\\ w^{*2} & 0\end{pmatrix}$	$\begin{pmatrix}0 & w\\ -w^* & 0\end{pmatrix}$	$\begin{pmatrix}0 & -1\\ 1 & 0\end{pmatrix}$	$\begin{pmatrix}0 & w^*\\ -w & 0\end{pmatrix}$
Γ_6^-	χ	0	0	0	0	0	0	0
	Γ	$\begin{pmatrix}0 & -1\\ 1 & 0\end{pmatrix}$	$\begin{pmatrix}0 & w^*\\ -w & 0\end{pmatrix}$	$\begin{pmatrix}0 & -w^{*2}\\ w^2 & 0\end{pmatrix}$	$\begin{pmatrix}0 & -w^2\\ w^{*2} & 0\end{pmatrix}$	$\begin{pmatrix}0 & w\\ -w^* & 0\end{pmatrix}$	$\begin{pmatrix}0 & 1\\ -1 & 0\end{pmatrix}$	$\begin{pmatrix}0 & -w^*\\ w & 0\end{pmatrix}$
Γ_7^+		i	i	i	i	i	i	i
Γ_7^-		i	i	i	i	i	–i	–i
Γ_8^+		–i	–i	–i	–i	–i	–i	–i
Γ_8^-		–i	–i	–i	–i	–i	i	i
$\delta_{m,-m'}(-)^{3j+m}\cdot\{$		1	$e^{4\pi im/5}$	$e^{8\pi im/5}$	$e^{-8\pi im/5}$	$e^{-4\pi im/5}$	1	$e^{4\pi im/5}$

Table A3.28. (cont.)

Irrep	Quantity	Element $\sigma_d(3)$	$\sigma_d(4)$	$\sigma_d(5)$	Basis[a]
Γ_5^+	χ	0	0	0	
	Γ	$\begin{pmatrix} 0 & w \\ -w^* & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & w^* \\ -w & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & -w^* \\ w^{*2} & 0 \end{pmatrix}$	$\left\{\begin{matrix} \mid \ell j, 1/2 > \\ s \mid \ell j, -1/2 > \end{matrix}\right.^{b}, \left\{\begin{matrix} \mid \ell j, -9/2 > \\ -s \mid \ell j, 9/2 > \end{matrix}\right.^{b}$
Γ_5^-	χ	0	0	0	
	Γ	$\begin{pmatrix} 0 & -w \\ w^* & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & -w^* \\ w & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & w^* \\ -w^{*2} & 0 \end{pmatrix}$	$\left\{\begin{matrix} \mid \ell j, 1/2 > \\ -s \mid \ell j, -1/2 > \end{matrix}\right.^{c}, \left\{\begin{matrix} \mid \ell j, -9/2 > \\ s \mid \ell j, 9/2 > \end{matrix}\right.^{c}$
Γ_6^+	χ	0	0	0	
	Γ	$\begin{pmatrix} 0 & -w^{*2} \\ v^2 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & -w^2 \\ w^{*2} & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & w \\ -w^* & 0 \end{pmatrix}$	$\left\{\begin{matrix} \mid \ell j, 3/2 > \\ -s \mid \ell j, -3/2 > \end{matrix}\right.^{b}, \left\{\begin{matrix} \mid \ell j, -7/2 > \\ s \mid \ell j, 7/2 > \end{matrix}\right.^{b}$
Γ_6^-	χ	0	0	0	
	Γ	$\begin{pmatrix} 0 & w^{*2} \\ -w^2 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & w^2 \\ -w^{*2} & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & -w \\ w^* & 0 \end{pmatrix}$	$\left\{\begin{matrix} \mid \ell j, 3/2 > \\ s \mid \ell j, -3/2 > \end{matrix}\right.^{c}, \left\{\begin{matrix} \mid \ell j, -7/2 > \\ -s \mid \ell j, 7/2 > \end{matrix}\right.^{c}$
Γ_7^+		i	i	i	$s \mid \ell j, 5/2 > -i \mid \ell j, -5/2 >^{b}$
Γ_7^-		–i	–i	–i	$s \mid \ell j, 5/2 > +i \mid \ell j, -5/2 >^{c}$
Γ_8^+		–i	–i	–i	$s \mid \ell j, 5/2 > +i \mid \ell j, -5/2 >^{b}$
Γ_8^-		i	i	i	$s \mid \ell j, 5/2 > -i \mid \ell j, -5/2 >^{c}$
		$e^{8\pi i m/5}$	$e^{-8\pi i m/5}$	$e^{-4\pi i m/5}$ }	

[a] The m quantum number is defined mod (10).

[b] Even ℓ.

[c] Odd ℓ.

Table A3.29. D_{5h}. $v = \exp(i\pi/10)$. $w = \exp(i\pi/5)$. The elements are defined in Fig. A3.5.

Irrep	Element									
	E	C_5	C_5^{-1}	C_5^{2}	C_5^{-2}	σ_h	S_5	S_5^{-1}	S_5^{2}	S_5^{-2}
Γ_9	$\begin{pmatrix}1&0\\0&1\end{pmatrix}$	$\begin{pmatrix}w^*&0\\0&w\end{pmatrix}$	$\begin{pmatrix}w&0\\0&w^*\end{pmatrix}$	$\begin{pmatrix}w^{*2}&0\\0&w^2\end{pmatrix}$	$\begin{pmatrix}w^2&0\\0&w^{*2}\end{pmatrix}$	$\begin{pmatrix}-i&0\\0&i\end{pmatrix}$	$\begin{pmatrix}v^3&0\\0&v^{*3}\end{pmatrix}$	$\begin{pmatrix}v^{*3}&0\\0&v^3\end{pmatrix}$	$\begin{pmatrix}v&0\\0&v^*\end{pmatrix}$	$\begin{pmatrix}v^*&0\\0&v\end{pmatrix}$
Γ_{10}	$\begin{pmatrix}1&0\\0&1\end{pmatrix}$	$\begin{pmatrix}w^*&0\\0&w\end{pmatrix}$	$\begin{pmatrix}w&0\\0&w^*\end{pmatrix}$	$\begin{pmatrix}w^{*2}&0\\0&w^2\end{pmatrix}$	$\begin{pmatrix}w^2&0\\0&w^{*2}\end{pmatrix}$	$\begin{pmatrix}i&0\\0&-i\end{pmatrix}$	$\begin{pmatrix}-v^3&0\\0&-v^{*3}\end{pmatrix}$	$\begin{pmatrix}-v^{*3}&0\\0&-v^3\end{pmatrix}$	$\begin{pmatrix}-v&0\\0&-v^*\end{pmatrix}$	$\begin{pmatrix}-v^*&0\\0&-v\end{pmatrix}$
Γ_{11}	$\begin{pmatrix}1&0\\0&1\end{pmatrix}$	$\begin{pmatrix}-w^2&0\\0&-w^{*2}\end{pmatrix}$	$\begin{pmatrix}-w^{*2}&0\\0&-w^2\end{pmatrix}$	$\begin{pmatrix}-w^*&0\\0&-w\end{pmatrix}$	$\begin{pmatrix}-w&0\\0&-w^*\end{pmatrix}$	$\begin{pmatrix}i&0\\0&-i\end{pmatrix}$	$\begin{pmatrix}-v^*&0\\0&-v\end{pmatrix}$	$\begin{pmatrix}-v&0\\0&-v^*\end{pmatrix}$	$\begin{pmatrix}v^3&0\\0&v^{*3}\end{pmatrix}$	$\begin{pmatrix}v^{*3}&0\\0&v^3\end{pmatrix}$
Γ_{12}	$\begin{pmatrix}1&0\\0&1\end{pmatrix}$	$\begin{pmatrix}-w^2&0\\0&-w^{*2}\end{pmatrix}$	$\begin{pmatrix}-w^{*2}&0\\0&-w^2\end{pmatrix}$	$\begin{pmatrix}-w^*&0\\0&-w\end{pmatrix}$	$\begin{pmatrix}-w&0\\0&-w^*\end{pmatrix}$	$\begin{pmatrix}-i&0\\0&i\end{pmatrix}$	$\begin{pmatrix}v^*&0\\0&v\end{pmatrix}$	$\begin{pmatrix}v&0\\0&v^*\end{pmatrix}$	$\begin{pmatrix}-v^3&0\\0&-v^{*3}\end{pmatrix}$	$\begin{pmatrix}-v^{*3}&0\\0&-v^3\end{pmatrix}$
Γ_{13}	$\begin{pmatrix}1&0\\0&1\end{pmatrix}$	$\begin{pmatrix}-1&0\\0&-1\end{pmatrix}$	$\begin{pmatrix}-1&0\\0&-1\end{pmatrix}$	$\begin{pmatrix}1&0\\0&1\end{pmatrix}$	$\begin{pmatrix}1&0\\0&1\end{pmatrix}$	$\begin{pmatrix}-i&0\\0&i\end{pmatrix}$	$\begin{pmatrix}-i&0\\0&i\end{pmatrix}$	$\begin{pmatrix}i&0\\0&-i\end{pmatrix}$	$\begin{pmatrix}i&0\\0&-i\end{pmatrix}$	$\begin{pmatrix}-i&0\\0&i\end{pmatrix}$
$D^j_{m'm}\,\delta_{mm'}\cdot\{$	1	$e^{-2\pi im/5}$	$e^{2\pi im/5}$	$e^{-4\pi im/5}$	$e^{4\pi im/5}$	$e^{-\pi im}$	$e^{3\pi im/5}$	$e^{-3\pi im/5}$	$e^{\pi im/5}$	$e^{-\pi im/5}\,\}$

Table A3.29. (cont.)

Irrep	Element						
	$C_2'(1)$	$C_2'(2)$	$C_2'(3)$	$C_2'(4)$	$C_2'(5)$	$\sigma_v(1)$	$\sigma_v(2)$
Γ_9	$\begin{pmatrix}0 & -1\\ 1 & 0\end{pmatrix}$	$\begin{pmatrix}0 & -w^{*2}\\ w^2 & 0\end{pmatrix}$	$\begin{pmatrix}0 & w\\ -w^* & 0\end{pmatrix}$	$\begin{pmatrix}0 & w^*\\ -w & 0\end{pmatrix}$	$\begin{pmatrix}0 & -w^2\\ w^{*2} & 0\end{pmatrix}$	$\begin{pmatrix}0 & -i\\ -i & 0\end{pmatrix}$	$\begin{pmatrix}0 & -v\\ v^* & 0\end{pmatrix}$
Γ_{10}	$\begin{pmatrix}0 & -1\\ 1 & 0\end{pmatrix}$	$\begin{pmatrix}0 & -w^{*2}\\ w^2 & 0\end{pmatrix}$	$\begin{pmatrix}0 & w\\ -w^* & 0\end{pmatrix}$	$\begin{pmatrix}0 & w^*\\ -w & 0\end{pmatrix}$	$\begin{pmatrix}0 & -w^2\\ w^{*2} & 0\end{pmatrix}$	$\begin{pmatrix}0 & i\\ i & 0\end{pmatrix}$	$\begin{pmatrix}0 & v\\ -v^* & 0\end{pmatrix}$
Γ_{11}	$\begin{pmatrix}0 & -1\\ 1 & 0\end{pmatrix}$	$\begin{pmatrix}0 & w^*\\ -w & 0\end{pmatrix}$	$\begin{pmatrix}0 & -w^{*2}\\ w^2 & 0\end{pmatrix}$	$\begin{pmatrix}0 & -w^2\\ w^{*2} & 0\end{pmatrix}$	$\begin{pmatrix}0 & w\\ -w^* & 0\end{pmatrix}$	$\begin{pmatrix}0 & i\\ i & 0\end{pmatrix}$	$\begin{pmatrix}0 & -v^3\\ v^{*3} & 0\end{pmatrix}$
Γ_{12}	$\begin{pmatrix}0 & -1\\ 1 & 0\end{pmatrix}$	$\begin{pmatrix}0 & w^*\\ -w & 0\end{pmatrix}$	$\begin{pmatrix}0 & -w^{*2}\\ w^2 & 0\end{pmatrix}$	$\begin{pmatrix}0 & -w^2\\ w^{*2} & 0\end{pmatrix}$	$\begin{pmatrix}0 & w\\ -w^* & 0\end{pmatrix}$	$\begin{pmatrix}0 & -i\\ -i & 0\end{pmatrix}$	$\begin{pmatrix}0 & v^3\\ -v^{*3} & 0\end{pmatrix}$
Γ_{13}	$\begin{pmatrix}0 & -1\\ 1 & 0\end{pmatrix}$	$\begin{pmatrix}0 & -1\\ 1 & 0\end{pmatrix}$	$\begin{pmatrix}0 & -1\\ 1 & 0\end{pmatrix}$	$\begin{pmatrix}0 & -1\\ 1 & 0\end{pmatrix}$	$\begin{pmatrix}0 & -1\\ 1 & 0\end{pmatrix}$	$\begin{pmatrix}0 & -i\\ -i & 0\end{pmatrix}$	$\begin{pmatrix}0 & -i\\ -i & 0\end{pmatrix}$
$\delta_{m,-m'}(-)^{3j+m}\cdot\{1$	$e^{4\pi im/5}$	$e^{8\pi im/5}$	$e^{-8\pi im/5}$	$e^{-4\pi im/5}$	$e^{-\pi im}$	$e^{-\pi im/5}$	

Table A3.29. (cont.)

Irrep	Element			Basis [a]	
	$\sigma_v(3)$	$\sigma_v(4)$	$\sigma_v(5)$	Even ℓ	Odd ℓ
Γ_9	$\begin{pmatrix}0 & -v^{*3}\\ v^3 & 0\end{pmatrix}$	$\begin{pmatrix}0 & v^3\\ -v^{*3} & 0\end{pmatrix}$	$\begin{pmatrix}0 & v^*\\ -v & 0\end{pmatrix}$	$\begin{cases}\lvert \ell j, 1/2 >\\ s\lvert \ell j, -1/2 >\end{cases}$	$\begin{cases}\lvert \ell j, -9/2 >\\ s\lvert \ell j, 9/2 >\end{cases}$
Γ_{10}	$\begin{pmatrix}0 & v^{*3}\\ -v^3 & 0\end{pmatrix}$	$\begin{pmatrix}0 & -v^3\\ v^{*3} & 0\end{pmatrix}$	$\begin{pmatrix}0 & -v^*\\ v & 0\end{pmatrix}$	$\begin{cases}\lvert \ell j, -9/2 >\\ -s\lvert \ell j, 9/2 >\end{cases}$	$\begin{cases}\lvert \ell j, 1/2 >\\ -s\lvert \ell j, -1/2 >\end{cases}$
Γ_{11}	$\begin{pmatrix}0 & v\\ -v^* & 0\end{pmatrix}$	$\begin{pmatrix}0 & -v^*\\ v & 0\end{pmatrix}$	$\begin{pmatrix}0 & v^{*3}\\ -v^3 & 0\end{pmatrix}$	$\begin{cases}\lvert \ell j, 3/2 >\\ -s\lvert \ell j, -3/2 >\end{cases}$	$\begin{cases}\lvert \ell j, -7/2 >\\ -s\lvert \ell j, 7/2 >\end{cases}$
Γ_{12}	$\begin{pmatrix}0 & -v\\ v^* & 0\end{pmatrix}$	$\begin{pmatrix}0 & v^*\\ -v & 0\end{pmatrix}$	$\begin{pmatrix}0 & -v^{*3}\\ v^3 & 0\end{pmatrix}$	$\begin{cases}\lvert \ell j, -7/2 >\\ s\lvert \ell j, 7/2 >\end{cases}$	$\begin{cases}\lvert \ell j, 3/2 >\\ s\lvert \ell j, -3/2 >\end{cases}$
Γ_{13}	$\begin{pmatrix}0 & -i\\ -i & 0\end{pmatrix}$	$\begin{pmatrix}0 & -i\\ -i & 0\end{pmatrix}$	$\begin{pmatrix}0 & -i\\ -i & 0\end{pmatrix}$	$\begin{cases}\lvert \ell j, 5/2 >\\ s\lvert \ell j, -5/2 >\end{cases}$	$\begin{cases}\lvert \ell j, -5/2 >\\ s\lvert \ell j, 5/2 >\end{cases}$
	$e^{3\pi im/5}$	$e^{7\pi im/5}$	$e^{-9\pi im/5}\}$		

[a] The m quantum number is defined mod (10).

Table A3.30. Characters for D_{5h}.

D_{5h}	E	$2C_5$	$2C_5^2$	σ_h / $\bar{\sigma}_h$	$2S_5$	$2S_5^2$	$5C_2'$ / $5\bar{C}_2'$	$5\sigma_v$ / $5\bar{\sigma}_v$	$\bar{E}$	$2\bar{C}_5$	$2\bar{C}_5^{\,2}$	$2\bar{S}_5$	$2\bar{S}_5^{\,2}$
Γ_1	1	1	1	1	1	1	1	1	1	1	1	1	1
Γ_2	1	1	1	1	1	1	-1	-1	1	1	1	1	1
Γ_3	1	1	1	-1	-1	-1	1	-1	1	1	1	-1	-1
Γ_4	1	1	1	-1	-1	-1	-1	1	1	1	1	-1	-1
Γ_5	2	a	b	2	a	b	0	0	2	a	b	a	b
Γ_6	2	a	b	-2	-a	-b	0	0	2	a	b	-a	-b
Γ_7	2	b	a	2	b	a	0	0	2	b	a	b	a
Γ_8	2	b	a	-2	-b	-a	0	0	2	b	a	-b	-a
Γ_9	2	-b	a	0	d	c	0	0	-2	b	-a	-d	-c
Γ_{10}	2	-b	a	0	-d	-c	0	0	-2	b	-a	d	c
Γ_{11}	2	-a	b	0	-c	d	0	0	-2	a	-b	c	-d
Γ_{12}	2	-a	b	0	c	-d	0	0	-2	a	-b	-c	d
Γ_{13}	2	-2	2	0	0	0	0	0	-2	2	-2	0	0

$a = 2\cos\left(\frac{2\pi}{5}\right) = \frac{1}{2}(-1+\sqrt{5})$. $b = 2\cos\left(\frac{4\pi}{5}\right) = -\frac{1}{2}(1+\sqrt{5})$.

$c = 2\cos\left(\frac{\pi}{10}\right) = \sqrt{(5+\sqrt{5})/2}$. $d = 2\cos\left(\frac{3\pi}{10}\right) = ac$.

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