Principles of Symmetry, Dynamics, and Spectroscopy - W. G. Harter - Wiley (1993)

Tables

FORMULAS AND TABLES OF GROUP REPRESENTATIONS AND RELATED QUANTITIES

F.1. THE ORTHOGONAL GROUP *O*(3) AND UNITARY UNIMODULAR GROUP SU(2)

The multiplication rules for $O(3)$ and SU(2) may be visualized using Hamilton turns. (See Sections 3.1B, 5.3.C, and 5.5.A.) The common choices for parameters are Darboux axis angles $R[\phi\theta\omega]$ and Euler coordinate angles $R(\alpha\beta\gamma)$. (See Sections 5.3.A and 5.3.B.) The following irreducible representations of Wigner D-functions are derived in Section 5.4 using SU(2) boson algebra:

$$D^j_{mn}(\alpha\beta\gamma) = \left\langle {j \atop m} \middle| R(\alpha\beta\gamma) \middle| {j \atop n} \right\rangle$$
$$= \sum_{k=0} (-1)^k \frac{\sqrt{(j+m)!(j-m)!(j+n)!(j-n)!}}{(j+m-k)!k!(j-n-k)!(n-m+k)!} e^{-i(m\alpha+n\gamma)}$$
$$\times \left(\cos\frac{\beta}{2}\right)^{2j+m-n-2k} \left(\sin\frac{\beta}{2}\right)^{n-m+2k}. \qquad \text{(F.1.1)}$$

Here the rotation operator is expressed in terms of angular momentum generators and Euler angles,

$$R(\alpha\beta\gamma) = e^{-i\alpha J_z/\hbar} e^{-i\beta J_y/\hbar} e^{-i\gamma J_z/\hbar}. \qquad \text{(F.1.2)}$$

Representations $D^j(J_\alpha)$ $(x = x, y, z)$ are derived in Appendix E. Irreducibility, completeness, and orthogonality properties are derived in Appendix G.

Spherical harmonics Y^l_m and multipole functions X^k_q are the $n = 0$ cases of D-functions. They are functions of polar coordinates $(\alpha = \phi, \beta = \theta)$ and (ϕ, θ, r) but not the third Euler angle γ:

$$Y^l_m(\phi\theta) = \sqrt{\frac{2l+1}{4\pi}}\, D^{l*}_{m0}(\phi\theta\,\cdot), \qquad X^k_q(\phi\theta r) = r^k D^{k*}_{q0}(\phi\theta\,\cdot).$$

The multipole functions also have a radial k-power dependence and are kth-degree polynomials of $\{x, y, z\}$. In Table F.1.1 these polynomials are denoted by I^1_q, II^2_q, III^3_q, and IV^4_q for $k = 1, 2, 3$, and 4, respectively. The inverse relations to the kth degree harmonic monomials $x^a y^b z^c$ are also given. The number of harmonic monomials is

$$d(U(3)) = \frac{(k+1)(k+2)}{2},$$

which exceeds the number $(2k + 1)$ of multipole functions in all cases except $k = 0$ and $k = 1$. Therefore the even monomials involve combinations of multipole functions of degree $k, k - 2, \ldots, 2$, and 0 multiplied by r^0, $r^2, \ldots, r^{k-2}$, and r^k, respectively, while the odd monomials combine x^k of degree $k, k - 2, \ldots, 3$, and 1 multiplied by r^0, $r^2, \ldots, r^{k-3}$, and r^{k-1}, respectively. The harmonic monomials can be realized as a basis of a three-dimensional harmonic oscillator and span the symmetric representations of SU(3).

The Clebsch-Gordan and Wigner-3j coupling coefficients are related as described in Section 7.2,

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_2 \end{pmatrix} = \frac{(-1)^{j_1 - j_2 - m_3}}{\sqrt{2j_3 + 1}} C^{\,j_1 \quad j_2 \quad j_3}_{\,m_1 \quad m_2 \quad -m_3} \tag{F.1.3}$$

The standard CG-Dirac notation is

$$C^{\,j_1 \quad j_2 \quad j_3}_{\,m_1 \quad m_2 \quad m_3} = \left\langle \begin{matrix} j_1 & j_2 \\ m_1 & m_2 \end{matrix} \right| \left. j_1 \otimes j_2{}^{j_3}_{m_3} \right\rangle. \tag{F.1.4}$$

The general formula is similar to the one derived in Section 7.2.D:

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_2 \end{pmatrix} = (-1)^{j_1 - j_2 - m_3} \sqrt{\frac{(j_1 + j_2 - j_3)!(j_1 - j_2 + j_3)!(-j_1 + j_2 + j_3)!}{(j_1 + j_2 + j_3 + 1)!}}$$
$$\times (j_1 + m_1)!(j_1 - m_1)!(j_2 + m_2)!(j_2 - m_2)!(j_3 + m_3)!(j_3 - m_3)$$
$$\times \sum_k \frac{(-1)^k}{k!(j_1 + j_2 - j_3 - k)!(j_1 - m_1 - k)!(j_2 + m_2 - k)!(j_3 - j_2 - m_1 + k)!(j_3 - j_1 - m_2 + k)!} \tag{F.1.5}$$

TABLE F.1.1 $R(3)$ Multiple Functions and SU(3) Harmonic Monomials

$\mathrm{I}_1^{(1)} = -\frac{1}{\sqrt{2}}(x+iy)$	$x = \frac{1}{\sqrt{2}}(\mathrm{I}_{-1}^{(1)} - \mathrm{I}_1^{(1)})$
$\mathrm{I}_{-1}^{(1)} = \frac{1}{\sqrt{2}}(x-iy)$	$iy = -\frac{1}{\sqrt{2}}(\mathrm{I}_{-1}^{(1)} + \mathrm{I}_1^{(1)})$
$\mathrm{I}_0^{(1)} = z$	$z = \mathrm{I}_0^{(1)}$
$\mathrm{II}_2^{(2)} = \sqrt{\frac{3}{8}}(x+iy)^2$	$x^2 = \frac{1}{6}(\mathrm{II}_2^{(2)} + \mathrm{II}_{-2}^{(2)}) - \frac{1}{3}\mathrm{II}_0^{(2)} + \frac{1}{3}r^2$
$\mathrm{II}_1^{(2)} = -\sqrt{\frac{3}{2}}z(x+iy)$	$y^2 = -\frac{1}{6}(\mathrm{II}_2^{(2)} + \mathrm{II}_{-2}^{(2)}) - \frac{1}{3}\mathrm{II}_0^{(2)} + \frac{1}{3}r^2$
$\mathrm{II}_0^{(2)} = \frac{1}{2}(3z^2 - r^2)$	$z^2 = -\frac{2}{3}\mathrm{II}_0^{(2)} + \frac{1}{3}r^2$
$\mathrm{II}_{-1}^{(2)} = \sqrt{\frac{3}{2}}z(x-iy)$	$xy = \frac{i}{\sqrt{6}}(\mathrm{II}_2^{(2)} - \mathrm{II}_{-2}^{(2)})$
$\mathrm{II}_{-2}^{(2)} = \sqrt{\frac{3}{8}}(x-iy)^2$	$xz = \frac{1}{\sqrt{6}}(\mathrm{II}_1^{(2)} - \mathrm{II}_{-1}^{(2)})$
	$yz = \frac{i}{\sqrt{6}}(\mathrm{II}_1^{(2)} + \mathrm{II}_{-1}^{(2)})$
$\mathrm{III}_3^{(3)} = -\frac{\sqrt{5}}{4}(x+iy)^3$	$x^3 = \frac{1}{2\sqrt{5}}(\mathrm{III}_{-3}^{(3)} - \mathrm{III}_3^{(3)}) + \frac{\sqrt{3}}{10}(\mathrm{III}_1^{(3)} - \mathrm{III}_{-1}^{(3)}) + \frac{3}{5\sqrt{2}}(\mathrm{I}_{-1}^{(1)} - \mathrm{I}_1^{(1)})r^2$
$\mathrm{III}_2^{(3)} = \sqrt{\frac{15}{8}}z(x+iy)^2$	$iy^3 = \frac{1}{2\sqrt{5}}(\mathrm{III}_{-3}^{(3)} + \mathrm{III}_3^{(3)}) + \frac{\sqrt{3}}{10}(\mathrm{III}_1^{(3)} + \mathrm{III}_{-1}^{(3)}) - \frac{3}{5\sqrt{2}}(\mathrm{I}_{-1}^{(1)} + \mathrm{I}_1^{(1)})r^2$
$\mathrm{III}_1^{(3)} = -\frac{\sqrt{3}}{4}(x+iy)(5z^2 - r^2)$	$z^3 = \frac{2}{5}\mathrm{III}_0^{(3)} + \frac{3}{5}\mathrm{III}_0^{(1)}r^2$
$\mathrm{III}_0^{(3)} = \frac{1}{2}z(5z^2 - 3r^2)$	$ix^2y = -\frac{1}{2\sqrt{5}}(\mathrm{III}_{-3}^{(3)} + \mathrm{III}_3^{(2)}) + \frac{1}{10\sqrt{3}}(\mathrm{III}_1^{(3)} + \mathrm{III}_{-1}^{(3)}) - \frac{1}{3\sqrt{2}}(\mathrm{I}_1^{(1)} + \mathrm{I}_1^{(1)})r^2$
$\mathrm{III}_{-1}^{(3)} = \frac{\sqrt{3}}{4}(x-iy)(5z^2 - r^2)$	$xy^2 = \frac{1}{2\sqrt{5}}(\mathrm{III}_{-3}^{(3)} - \mathrm{III}_3^{(2)}) + \frac{1}{10\sqrt{3}}(\mathrm{III}_1^{(3)} - \mathrm{III}_{-1}^{(3)}) + \frac{3}{3\sqrt{2}}(\mathrm{I}_{-1}^{(1)} - \mathrm{I}_1^{(1)})r^2$
$\mathrm{III}_{-2}^{(3)} = \sqrt{\frac{15}{8}}z(x-iy)^2$	$x^2z = \frac{1}{\sqrt{30}}(\mathrm{III}_2^{(3)} + \mathrm{III}_{-2}^{(3)}) - \frac{1}{20}\mathrm{III}_0^{(3)} + \frac{1}{5}\mathrm{I}_0^{(1)}r^2$
$\mathrm{III}_{-3}^{(3)} = \frac{\sqrt{5}}{4}(x-iy)^3$	$y^2z = -\frac{1}{\sqrt{30}}(\mathrm{III}_2^{(3)} + \mathrm{III}_{-2}^{(3)}) - \frac{1}{20}\mathrm{III}_0^{(3)} + \frac{1}{5}\mathrm{I}_0^{(1)}r^2$
	$xz^2 = -\frac{2}{5\sqrt{3}}(\mathrm{III}_1^{(3)} - \mathrm{III}_{-1}^{(3)}) + \frac{1}{5\sqrt{2}}(\mathrm{I}_{-1}^{(1)} - \mathrm{I}_1^{(1)})r^2$
	$iyz^2 = -\frac{2}{5\sqrt{3}}(\mathrm{III}_1^{(3)} + \mathrm{III}_{-1}^{(3)}) - \frac{1}{5\sqrt{2}}(\mathrm{I}_{-1}^{(1)} + \mathrm{I}_1^{(1)})r^2$
	$ixyz = \frac{1}{\sqrt{30}}(\mathrm{III}_{-2}^{(3)} - \mathrm{III}_2^{(3)})$

$$\mathrm{IV}_4^{(4)} = \sqrt{\frac{35}{128}}\,(x + iy)^4$$

$$\mathrm{IV}_3^{(4)} = -\frac{\sqrt{35}}{4}z(x + iy)^3$$

$$\mathrm{IV}_2^{(4)} = \frac{\sqrt{5}}{4\sqrt{2}}(x + iy)^2(7z^2 - r^2)$$

$$\mathrm{IV}_1^{(4)} = -\frac{\sqrt{5}}{4}(x + iy)(7z^3 - 3zr^2)$$

$$\mathrm{IV}_0^{(4)} = \frac{1}{8}(35z^4 - 30z^2r^2 + 3r^4)$$

$$\mathrm{IV}_{-1}^{(4)} = \frac{\sqrt{5}}{4}(x - iy)(7z^3 - 3zr^2)$$

$$\mathrm{IV}_{-2}^{(4)} = \frac{\sqrt{5}}{4\sqrt{2}}(x - iy)^2(7z^3 - r^2)$$

$$\mathrm{IV}_{-3}^{(4)} = \frac{\sqrt{35}}{4}z(x - iy)^3$$

$$\mathrm{IV}_{-4}^{(4)} = \sqrt{\frac{35}{128}}\,(x - iy)^4$$

$$x^4 = \frac{1}{\sqrt{70}}(\mathrm{IV}_4^{(4)} + \mathrm{IV}_{-4}^{(4)}) - \frac{2}{7\sqrt{10}}(\mathrm{IV}_2^{(4)} + \mathrm{IV}_{-2}^{(4)}) + \frac{3}{35}\mathrm{IV}_0^{(4)} + \frac{\sqrt{6}}{7}(\mathrm{II}_2^{(2)} + \mathrm{II}_{-2}^{(2)})r^2 - \frac{2}{7}\mathrm{II}_0^{(2)}r^2 + \frac{1}{5}r^4$$

$$y^4 = \frac{1}{\sqrt{70}}(\mathrm{IV}_4^{(4)} + \mathrm{IV}_{-4}^{(4)}) + \frac{2}{7\sqrt{10}}(\mathrm{IV}_2^{(4)} + \mathrm{IV}_{-2}^{(4)}) + \frac{3}{35}\mathrm{IV}_0^{(4)} - \frac{\sqrt{6}}{7}(\mathrm{II}_2^{(2)} + \mathrm{II}_{-2}^{(2)})r^2 - \frac{2}{7}\mathrm{II}_0^{(2)}r^2 + \frac{1}{5}r^4$$

$$z^4 = \frac{8}{35}\mathrm{IV}_0^{(4)} + \frac{4}{7}\mathrm{II}_0^{(2)}r^2 + \frac{1}{5}r^4$$

$$x^2y^2 = -\frac{1}{\sqrt{70}}(\mathrm{IV}_4^{(4)} + \mathrm{IV}_{-4}^{(4)}) + \frac{1}{35}\mathrm{IV}_0^{(4)} - \frac{2}{21}\mathrm{II}_0^{(2)}r^2 + \frac{1}{15}r^4$$

$$x^2z^2 = \frac{\sqrt{2}}{35}(\mathrm{IV}_2^{(4)} + \mathrm{IV}_{-2}^{(4)}) - \frac{1}{7\sqrt{6}}(\mathrm{IV}_2^{(2)} + \mathrm{IV}_{-2}^{(2)})r^2 - \frac{8}{70}\mathrm{IV}_0^{(4)} + \frac{1}{21}\mathrm{II}_0^{(2)}r^2 + \frac{1}{15}r^4$$

$$y^2z^2 = -\frac{\sqrt{2}}{35}(\mathrm{IV}_2^{(4)} + \mathrm{IV}_{-2}^{(4)}) - \frac{1}{7\sqrt{6}}(\mathrm{IV}_2^{(2)} + \mathrm{IV}_{-2}^{(2)})r^2 - \frac{8}{70}\mathrm{IV}_0^{(4)} + \frac{1}{21}\mathrm{II}_0^{(2)}r^2 + \frac{1}{15}r^4$$

$$ix^2yz = -\frac{1}{2\sqrt{35}}(\mathrm{IV}_3^{(4)} + \mathrm{IV}_{-3}^{(4)}) + \frac{1}{14\sqrt{5}}(\mathrm{IV}_1^{(4)} + \mathrm{IV}_{-1}^{(4)}) - \frac{1}{7\sqrt{6}}(\mathrm{II}_1^{(2)} + \mathrm{II}_{-1}^{(2)})r^2$$

$$xy^2z = +\frac{1}{2\sqrt{35}}(\mathrm{IV}_3^{(4)} - \mathrm{IV}_{-3}^{(4)}) + \frac{1}{14\sqrt{5}}(\mathrm{IV}_1^{(4)} - \mathrm{IV}_{-1}^{(4)}) + \frac{1}{7\sqrt{6}}(\mathrm{II}_1^{(2)} - \mathrm{II}_{-1}^{(2)})r^2$$

$$ixyz^2 = \frac{1}{7}\sqrt{\frac{2}{5}}\,(\mathrm{IV}_2^{(4)} - \mathrm{IV}_{-2}^{(4)}) - \frac{1}{7\sqrt{6}}(\mathrm{I}_2^{(2)} - \mathrm{II}_{-2}^{(2)})r^2$$

$$ix^3y = \frac{1}{\sqrt{70}}(\mathrm{IV}_4^{(4)} - \mathrm{IV}_{-4}^{(4)}) - \frac{1}{7\sqrt{10}}(\mathrm{IV}_2^{(4)} - \mathrm{IV}_{-2}^{(4)}) - \frac{3}{7\sqrt{6}}(\mathrm{II}_2^{(2)} - \mathrm{II}_{-2}^{(2)})r^2$$

$$iy^3x = -\frac{1}{\sqrt{70}}(\mathrm{IV}_4^{(4)} - \mathrm{IV}_{-4}^{(4)}) - \frac{1}{7\sqrt{10}}(\mathrm{IV}_2^{(4)} - \mathrm{IV}_{-2}^{(4)}) - \frac{3}{7\sqrt{6}}(\mathrm{II}_2^{(2)} - \mathrm{II}_{-2}^{(2)})r^2$$

$$x^3z = -\frac{1}{2\sqrt{35}}(\mathrm{IV}_3^{(4)} - \mathrm{IV}_{-3}^{(4)}) + \frac{1}{14\sqrt{5}}(\mathrm{IV}_1^{(4)} - \mathrm{IV}_{-1}^{(4)}) + \frac{3}{7\sqrt{6}}(\mathrm{II}_1^{(2)} - \mathrm{II}_{-1}^{(2)})r^2$$

$$iy^3z = \frac{1}{2\sqrt{35}}(\mathrm{IV}_3^{(4)} + \mathrm{IV}_{-3}^{(4)}) + \frac{3}{14\sqrt{5}}(\mathrm{IV}_1^{(4)} + \mathrm{IV}_{-1}^{(4)}) - \frac{3}{7\sqrt{6}}(\mathrm{II}_1^{(2)} + \mathrm{II}_{-1}^{(2)})r^2$$

$$iz^3y = -\frac{2}{7\sqrt{5}}(\mathrm{IV}_1^{(4)} + \mathrm{IV}_{-1}^{(4)}) - \frac{3}{7\sqrt{6}}(\mathrm{II}_1^{(2)} + \mathrm{II}_{-1}^{(2)})r^2$$

$$z^3x = -\frac{2}{7\sqrt{5}}(\mathrm{IV}_1^{(4)} - \mathrm{IV}_{-1}^{(4)}) + \frac{3}{7\sqrt{6}}(\mathrm{II}_1^{(2)} - \mathrm{II}_{-1}^{(2)})r^2$$

Coupling coefficients are matrix elements of tensor operators according to the Wigner-Eckart theorem. (See Section 7.3.B.)

$$\left\langle \begin{matrix} j_3 \\ m_3 \end{matrix} \middle| T \begin{matrix} j_1 \\ m_1 \end{matrix} \middle| \begin{matrix} j_2 \\ m_2 \end{matrix} \right\rangle = C \begin{matrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{matrix} = \langle j_3 \| j_2 \| j_1 \rangle .$$

Unit tensor operator matrices are given in Tables 7.1 through 7.4, at the end of Chapter 7.

The Racah-6j recoupling coefficient used in Section 7.3.D is given by

$$\begin{Bmatrix} j_1 & j_2 & j_3 \\ l_1 & l_2 & l_3 \end{Bmatrix} = (-1)^{l_1+l_2+j_1+j_2} \Delta(l_1 l_2 j_3) \Delta(j_1 l_2 l_3) \Delta(l_1 j_2 l_3) \Delta(j_1 j_2 j_3)$$

$$\times \sum_k \frac{(-1)^k}{k!(j_1+j_2-j_3-k)!(l_1+l_2-j_3-k)!(j_1+l_2-l_3-k)!}$$

$$\times \frac{(j_1+j_2+l_1+l_2-k+1)!}{(l_1+j_2-l_3-k)!(j_3+l_3-j_1-l_1+k)!(j_3+l_3-j_2-l_2+k)!},$$

where

$$\Delta(jkl) = \sqrt{\frac{(j+k-l)!(j-k+l)!(-j+k+l)!}{(j+k+l+1)!}}. \tag{F.1.6}$$

F.2. THE OCTAHEDRAL GROUPS O AND $O_h = O \times C_i$

The 24 operations of the octahedral O group are shown by Figure 4.1.2. Its multiplication rules can be determined by the Hamilton turns shown in Figures 4.1.3 and 4.1.4. A group multiplication table (Table F.2.1) is given below. It includes $(-)$ signs which are needed to transform half-integral spin particles or spinor bases. Ignore them for vector transformations. The O character table is given in Eq. (4.1.11) and the spinor characters are given in Eq. (5.7.25).

The full octahedral group O_h is simply related to the outer product $O \times C_2$ of O and the inversion subgroup $C_i \approx C_2$. Its 48 elements are displayed in Figure 4.1.5, which shows other cubic symmetry groups as well. The full O_h vector character table is given by Eq. (4.1.16) and in Table F.4.1 in this appendix.

A conventional set of irreducible representations is given in Table F.2.2, and the corresponding multipole functions or "Kubic harmonics" are given in Table F.2.3. The remaining representations given in Tables F.2.4 to F.2.7 are defined by various subgroup chains which are described in Section 4.2.

TABLE F.2.1 *O*-Group Table

1	r_1	r_2	r_3	r_4	r_1^2	r_2^2	r_3^2	r_4^2	R_1^2	R_2^2	R_3^2	R_1	R_2	R_3	R_1^3	R_2^3	R_3^3	i_1	i_2	i_3	i_4	i_5	i_6
r_1	r_1^2	$-r_4^2$	$-r_2^2$	$-r_3^2$	-1	$-R_2^2$	$-R_3^2$	$-R_1^2$	$-r_2$	$-r_3$	$-r_4$	i_3	i_6	i_1	$-R_3$	$-R_1$	$-R_2$	R_1^3	i_5	R_2^3	i_2	$-i_4$	R_3^3
r_2	$-r_3^2$	r_2^2	$-r_4^2$	$-r_1^2$	R_2^2	-1	R_1^2	$-R_3^2$	r_1	r_4	$-r_3$	R_3	$-R_1^3$	i_2	i_3	$-i_5$	R_2^3	i_6	R_1	R_2	$-i_1$	R_3^3	i_4
r_3	$-r_4^2$	$-r_1^2$	r_3^2	$-r_2^2$	R_3^2	$-R_1^2$	-1	R_2^2	$-r_4$	r_1	r_2	$-i_4$	R_1	$-R_2^3$	R_3^3	i_6	i_2	i_5	R_1^3	i_1	R_2	$-i_3$	R_3
r_4	$-r_2^2$	$-r_3^2$	$-r_1^2$	r_4^2	R_1^2	R_3^2	$-R_2^2$	-1	r_3	$-r_2$	r_1	$-R_3^3$	$-i_5$	R_2	$-i_4$	R_1^3	i_1	R_1	i_6	$-i_2$	R_2^3	R_3	i_3
r_1^2	-1	R_1^2	R_2^2	R_3^2	$-r_1$	r_3	r_4	r_2	r_4^2	r_2^2	r_3^2	R_2^3	R_3^3	R_1^3	$-i_1$	$-i_3$	$-i_6$	$-R_3$	i_4	R_1	i_5	$-i_2$	$-R_2$
r_2^2	$-R_1^2$	-1	R_3^2	$-R_2^2$	r_4	$-r_2$	r_1	r_3	$-r_3^2$	$-r_1^2$	r_4^2	i_2	$-i_3$	$-R_1$	R_2	$-R_3^3$	$-i_5$	i_4	R_3	R_1^3	$-i_6$	R_2^3	$-i_1$
r_3^2	$-R_2^2$	$-R_3^2$	-1	R_1^2	r_2	r_4	$-r_3$	r_1	r_2^2	$-r_4^2$	$-r_1^2$	$-R_2$	$-i_4$	$-i_6$	i_2	R_3	$-R_1^3$	$-i_3$	R_3^3	i_5	R_1	$-i_1$	$-R_2^3$
r_4^2	$-R_3^2$	R_2^2	$-R_1^2$	-1	r_3	r_1	r_2	$-r_4$	$-r_1^2$	r_3^2	$-r_2^2$	$-i_1$	$-R_3$	$-i_5$	$-R_2^3$	$-i_4$	R_1	$-R_3^3$	i_3	i_6	R_1^3	R_2	$-i_2$
R_1^2	$-r_4$	r_3	$-r_2$	r_1	r_2^2	$-r_1^2$	r_4^2	$-r_3^2$	-1	R_3^2	$-R_2^2$	R_1^3	i_1	$-i_4$	$-R_1$	i_2	$-i_3$	$-R_2$	R_2^3	R_3^3	R_3	$-i_6$	i_5
R_2^2	$-r_2$	r_1	r_4	$-r_3$	r_3^2	$-r_4^2$	$-r_1^2$	r_2^2	$-R_3^2$	-1	R_1^2	$-i_5$	R_2^3	i_3	$-i_6$	$-R_2$	$-i_4$	$-i_2$	i_1	$-R_3$	R_3^3	R_1	R_1^3
R_3^2	$-r_3$	$-r_4$	r_1	r_2	r_4^2	r_3^2	$-r_2^2$	$-r_1^2$	R_2^2	$-R_1^2$	-1	i_6	i_2	R_3^3	$-i_5$	$-i_1$	$-R_3$	R_2^3	$-R_2$	i_4	$-i_3$	R_1^3	$-R_1$
R_1	i_1	$-R_2^3$	$-i_2$	R_2	R_3^3	$-i_3$	$-R_3$	i_4	R_1^3	i_6	i_5	R_1^2	r_1	$-r_4^2$	-1	$-r_3$	r_2^2	$-r_4$	r_2	r_1^2	$-r_3^2$	$-R_2^2$	R_3^2
R_2	i_3	R_3	$-R_3^3$	i_4	R_1^3	i_5	$-i_6$	$-R_1$	$-i_2$	R_2^3	i_1	$-r_2^2$	R_2^2	r_1	r_3^2	-1	$-r_4$	R_1^2	R_3^2	$-r_2$	$-r_3$	$-r_4^2$	r_1^2
R_3	i_6	i_5	R_1	$-R_1^3$	R_2^3	$-R_2$	$-i_2$	$-i_1$	i_3	i_4	R_3^3	r_1	$-r_3^2$	R_3^2	$-r_2$	r_4^2	-1	r_1^2	r_2^2	R_2^2	$-R_1^2$	$-r_4$	$-r_3$
R_1^3	$-R_2$	$-i_2$	R_2^3	i_1	$-i_3$	$-R_3^3$	i_4	R_3	$-R_1$	i_5	$-i_6$	-1	$-r_4$	r_3^2	$-R_1^2$	r_2	$-r_1^2$	$-r_1$	r_3	r_2^2	$-r_4^2$	$-R_3^2$	$-R_2^2$
R_2^3	$-R_3$	i_3	i_4	R_3^3	$-i_6$	R_1	$-R_1^3$	i_5	$-i_1$	$-R_2$	$-i_2$	r_4^2	-1	$-r_2$	$-r_1^2$	$-R_2^2$	r_3	$-R_3^2$	R_1^2	$-r_1$	$-r_4$	$-r_2^2$	r_3^2
R_3^3	$-R_1$	R_1^3	i_6	i_5	$-i_1$	$-i_2$	R_2	$-R_2^3$	i_4	$-i_3$	$-R_3$	$-r_3$	r_2^2	-1	r_4	$-r_1^2$	$-R_3^2$	r_4^2	r_3^2	$-R_1^2$	$-R_2^2$	$-r_2$	$-r_1$
i_1	R_3^3	$-i_4$	i_3	R_3	$-R_1$	$-i_6$	$-i_5$	$-R_1^3$	R_2^3	i_2	$-R_2$	r_1^2	R_3^2	$-r_4$	r_4^2	$-R_1^2$	$-r_1$	-1	$-R_2^2$	$-r_3$	r_2	r_3^2	r_2^2
i_2	i_4	R_3^3	R_3	$-i_3$	$-i_5$	R_1^3	R_1	$-i_6$	R_2	$-i_1$	R_2^3	$-r_3^2$	$-R_1^2$	$-r_3$	$-r_2^2$	$-R_3^2$	$-r_2$	R_2^2	-1	r_4	$-r_1$	r_1^2	r_4^2
i_3	R_1^3	R_1	$-i_5$	i_6	$-R_2$	$-R_2^3$	$-i_1$	i_2	$-R_3$	R_3^3	$-i_4$	$-r_2$	r_1^2	R_1^2	$-r_1$	r_2^2	$-R_2^2$	r_3^2	$-r_4^2$	-1	R_3^2	r_3	$-r_4$
i_4	$-i_5$	i_6	$-R_1^3$	$-R_1$	$-i_2$	i_1	$-R_2^3$	$-R_2$	$-R_3^3$	$-R_3$	i_3	r_4	r_4^2	R_2^2	r_3	r_3^2	R_1^2	$-r_2^2$	r_1^2	$-R_3^3$	-1	r_1	$-r_2$
i_5	i_2	$-R_2$	i_1	$-R_2^3$	i_4	$-R_3$	i_3	$-R_3^3$	i_6	$-R_1^3$	$-R_1$	R_3^2	r_2	r_2^2	R_2^2	r_4	r_4^2	$-r_3$	$-r_1$	$-r_3^2$	$-r_1^2$	-1	$-R_1^2$
i_6	R_2^3	i_1	R_2	i_2	$-R_3$	$-i_4$	$-R_3^3$	$-i_3$	$-i_5$	$-R_1$	R_1^3	R_2^2	$-r_3$	r_1^2	$-R_3^2$	$-r_1$	r_3^2	$-r_2$	$-r_4$	r_4^2	r_2^2	R_1^2	-1

TABLE F.2.2 Conventional O Irreducible Representations. (Cartesian Fourfold Axial Bases)

(a) Vector Representation T_1

$$\mathscr{D}^{T_1}(1) = \begin{vmatrix} 1 & \cdot & \cdot \\ \cdot & 1 & \cdot \\ \cdot & \cdot & 1 \end{vmatrix} \quad R_1^2 = \begin{vmatrix} 1 & \cdot & \cdot \\ \cdot & -1 & \cdot \\ \cdot & \cdot & -1 \end{vmatrix} \quad r_1 = \begin{vmatrix} \cdot & \cdot & 1 \\ 1 & \cdot & \cdot \\ \cdot & 1 & \end{vmatrix} \quad r_2 = \begin{vmatrix} \cdot & \cdot & -1 \\ 1 & \cdot & \cdot \\ \cdot & -1 & \cdot \end{vmatrix} \quad r_1^2 = \begin{vmatrix} \cdot & 1 & \cdot \\ \cdot & \cdot & 1 \\ 1 & \cdot & \cdot \end{vmatrix} \quad r_2^2 = \begin{vmatrix} \cdot & 1 & \cdot \\ \cdot & \cdot & -1 \\ -1 & \cdot & \cdot \end{vmatrix}$$

$$\mathscr{D}^{T_1}(R_3^2) = \begin{vmatrix} -1 & \cdot & \cdot \\ \cdot & -1 & \cdot \\ \cdot & \cdot & 1 \end{vmatrix} \quad R_2^2 = \begin{vmatrix} -1 & \cdot & \cdot \\ \cdot & 1 & \cdot \\ \cdot & \cdot & -1 \end{vmatrix} \quad r_4 = \begin{vmatrix} \cdot & \cdot & 1 \\ -1 & \cdot & \cdot \\ \cdot & -1 & \end{vmatrix} \quad r_3 = \begin{vmatrix} \cdot & \cdot & -1 \\ -1 & \cdot & \cdot \\ \cdot & 1 & \end{vmatrix} \quad r_3^2 = \begin{vmatrix} \cdot & -1 & \cdot \\ \cdot & \cdot & 1 \\ -1 & \cdot & \cdot \end{vmatrix} \quad r_4^2 = \begin{vmatrix} \cdot & -1 & \cdot \\ \cdot & \cdot & -1 \\ 1 & \cdot & \cdot \end{vmatrix}$$

$$\mathscr{D}^{T_1}(R_3) = \begin{vmatrix} \cdot & -1 & \cdot \\ 1 & \cdot & \cdot \\ \cdot & \cdot & 1 \end{vmatrix} \quad i_4 = \begin{vmatrix} \cdot & -1 & \cdot \\ -1 & \cdot & \cdot \\ \cdot & \cdot & -1 \end{vmatrix} \quad i_1 = \begin{vmatrix} \cdot & \cdot & 1 \\ \cdot & -1 & \cdot \\ 1 & \cdot & \cdot \end{vmatrix} \quad i_2 = \begin{vmatrix} \cdot & \cdot & -1 \\ \cdot & -1 & \cdot \\ -1 & \cdot & \cdot \end{vmatrix} \quad R_1^3 = \begin{vmatrix} 1 & \cdot & \cdot \\ \cdot & \cdot & 1 \\ \cdot & -1 & \cdot \end{vmatrix} \quad R_1 = \begin{vmatrix} 1 & \cdot & \cdot \\ \cdot & \cdot & -1 \\ \cdot & 1 & \cdot \end{vmatrix}$$

$$\begin{matrix} O: \\ D_4: \\ C_2: \end{matrix} \left| \begin{matrix} T_1 \\ E \\ B_1 \end{matrix} \right\rangle \left| \begin{matrix} T_1 \\ E \\ B_2 \end{matrix} \right\rangle \left| \begin{matrix} T_1 \\ A_2 \\ A_2 \end{matrix} \right\rangle \text{basis}$$

$$\mathscr{D}^{T_1}(R_3^3) = \begin{vmatrix} \cdot & 1 & \cdot \\ -1 & \cdot & \cdot \\ \cdot & \cdot & 1 \end{vmatrix} \quad i_3 = \begin{vmatrix} \cdot & 1 & \cdot \\ 1 & \cdot & \cdot \\ \cdot & \cdot & -1 \end{vmatrix} \quad R_2 = \begin{vmatrix} \cdot & \cdot & 1 \\ \cdot & 1 & \cdot \\ -1 & \cdot & \cdot \end{vmatrix} \quad R_2^3 = \begin{vmatrix} \cdot & \cdot & -1 \\ \cdot & 1 & \cdot \\ 1 & \cdot & \cdot \end{vmatrix} \quad i_6 = \begin{vmatrix} -1 & \cdot & \cdot \\ \cdot & \cdot & 1 \\ \cdot & 1 & \cdot \end{vmatrix} \quad i_5 = \begin{vmatrix} -1 & \cdot & \cdot \\ \cdot & \cdot & -1 \\ \cdot & -1 & \cdot \end{vmatrix}$$

(b) Second-Rank Tensor $T_2 = T_1 \otimes A_2$ Representation (T_2 is T_1 with R, R^3, and i Operations Negated.)

$$\mathscr{D}^{T_2}(1) = \begin{vmatrix} 1 & \cdot & \cdot \\ \cdot & 1 & \cdot \\ \cdot & \cdot & 1 \end{vmatrix} \quad R_1^2 = \begin{vmatrix} 1 & \cdot & \cdot \\ \cdot & -1 & \cdot \\ \cdot & \cdot & -1 \end{vmatrix} \quad r_1 = \begin{vmatrix} \cdot & \cdot & 1 \\ 1 & \cdot & \cdot \\ \cdot & 1 & \cdot \end{vmatrix} \quad r_2 = \begin{vmatrix} \cdot & \cdot & -1 \\ 1 & \cdot & \cdot \\ \cdot & -1 & \cdot \end{vmatrix} \quad r_1^2 = \begin{vmatrix} \cdot & 1 & \cdot \\ \cdot & \cdot & 1 \\ 1 & \cdot & \cdot \end{vmatrix} \quad r_2^2 = \begin{vmatrix} \cdot & 1 & \cdot \\ \cdot & \cdot & -1 \\ -1 & \cdot & \cdot \end{vmatrix}$$

$$\mathscr{D}^{T_2}(R_3^2) = \begin{vmatrix} -1 & \cdot & \cdot \\ \cdot & -1 & \cdot \\ \cdot & \cdot & 1 \end{vmatrix} \quad R_2^2 = \begin{vmatrix} -1 & \cdot & \cdot \\ \cdot & 1 & \cdot \\ \cdot & \cdot & -1 \end{vmatrix} \quad r_4 = \begin{vmatrix} \cdot & \cdot & 1 \\ -1 & \cdot & \cdot \\ \cdot & -1 & \cdot \end{vmatrix} \quad r_3 = \begin{vmatrix} \cdot & \cdot & -1 \\ -1 & \cdot & \cdot \\ \cdot & 1 & \cdot \end{vmatrix} \quad r_3^2 = \begin{vmatrix} \cdot & -1 & \cdot \\ \cdot & \cdot & 1 \\ -1 & \cdot & \cdot \end{vmatrix} \quad r_4^2 = \begin{vmatrix} \cdot & -1 & \cdot \\ \cdot & \cdot & -1 \\ 1 & \cdot & \cdot \end{vmatrix}$$

$$\mathscr{D}^{T_2}(R_3) = \begin{vmatrix} \cdot & 1 & \cdot \\ -1 & \cdot & \cdot \\ \cdot & \cdot & -1 \end{vmatrix} \quad i_4 = \begin{vmatrix} \cdot & 1 & \cdot \\ 1 & \cdot & \cdot \\ \cdot & \cdot & 1 \end{vmatrix} \quad i_1 = \begin{vmatrix} \cdot & \cdot & -1 \\ \cdot & 1 & \cdot \\ -1 & \cdot & \cdot \end{vmatrix} \quad i_2 = \begin{vmatrix} \cdot & \cdot & 1 \\ \cdot & 1 & \cdot \\ 1 & \cdot & \cdot \end{vmatrix} \quad R_1^3 = \begin{vmatrix} -1 & \cdot & \cdot \\ \cdot & \cdot & -1 \\ \cdot & 1 & \cdot \end{vmatrix} \quad R_1 = \begin{vmatrix} -1 & \cdot & \cdot \\ \cdot & \cdot & 1 \\ \cdot & -1 & \cdot \end{vmatrix}$$

$$\begin{matrix} O: \\ D_4: \\ C_2: \end{matrix} \begin{vmatrix} T_2 \\ E \\ B_1 \end{vmatrix}\Bigg\rangle - \begin{vmatrix} T_2 \\ E \\ B_2 \end{vmatrix}\Bigg\rangle \begin{vmatrix} T_2 \\ B_2 \\ A_2 \end{vmatrix}\Bigg\rangle \text{basis}$$

$$\mathscr{D}^{T_2}(R_3^3) = \begin{vmatrix} \cdot & -1 & \cdot \\ 1 & \cdot & \cdot \\ \cdot & \cdot & -1 \end{vmatrix} \quad i_3 = \begin{vmatrix} \cdot & -1 & \cdot \\ -1 & \cdot & \cdot \\ \cdot & \cdot & 1 \end{vmatrix} \quad R_2 = \begin{vmatrix} \cdot & \cdot & -1 \\ \cdot & -1 & \cdot \\ 1 & \cdot & \cdot \end{vmatrix} \quad R_2^3 = \begin{vmatrix} \cdot & \cdot & 1 \\ \cdot & -1 & \cdot \\ -1 & \cdot & \cdot \end{vmatrix} \quad i_6 = \begin{vmatrix} 1 & \cdot & \cdot \\ \cdot & \cdot & -1 \\ \cdot & -1 & \cdot \end{vmatrix} \quad i_5 = \begin{vmatrix} 1 & \cdot & \cdot \\ \cdot & \cdot & 1 \\ \cdot & 1 & \cdot \end{vmatrix}$$

TABLE F.2.2 *(Continued)*

(c) Second-rank Tensor E Representation

$\mathscr{D}^E(1)$	$R_1^2 =$	$r_1 =$	$r_2 =$	$r_1^2 =$	$r_2^2 =$
$\begin{vmatrix} 1 & 0 \\ 0 & 1 \end{vmatrix}$	$\begin{vmatrix} 1 & 0 \\ 0 & 1 \end{vmatrix}$	$\begin{vmatrix} \frac{-1}{2} & \frac{-\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & \frac{-1}{2} \end{vmatrix}$	$\begin{vmatrix} \frac{-1}{2} & \frac{-\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & \frac{-1}{2} \end{vmatrix}$	$\begin{vmatrix} \frac{-1}{2} & \frac{\sqrt{3}}{2} \\ \frac{-\sqrt{3}}{2} & \frac{-1}{2} \end{vmatrix}$	$\begin{vmatrix} \frac{-1}{2} & \frac{\sqrt{3}}{2} \\ \frac{-\sqrt{3}}{2} & \frac{-1}{2} \end{vmatrix}$
$\mathscr{D}^E(R_3^2)$	$R_2^2 =$	$r_4 =$	$r_3 =$	$r_3^2 =$	$r_4^2 =$
$\begin{vmatrix} 1 & 0 \\ 0 & 1 \end{vmatrix}$	$\begin{vmatrix} 1 & 0 \\ 0 & 1 \end{vmatrix}$	$\begin{vmatrix} \frac{-1}{2} & \frac{-\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & \frac{-1}{2} \end{vmatrix}$	$\begin{vmatrix} \frac{-1}{2} & \frac{-\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & \frac{-1}{2} \end{vmatrix}$	$\begin{vmatrix} \frac{-1}{2} & \frac{\sqrt{3}}{2} \\ \frac{-\sqrt{3}}{2} & \frac{-1}{2} \end{vmatrix}$	$\begin{vmatrix} \frac{-1}{2} & \frac{\sqrt{3}}{2} \\ \frac{-\sqrt{3}}{2} & \frac{-1}{2} \end{vmatrix}$
$\mathscr{D}^E(R_3)$	$i_4 =$	$i_1 =$	$i_2 =$	$R_1^3 =$	$R_1 =$
$\begin{vmatrix} 1 & 0 \\ 0 & -1 \end{vmatrix}$	$\begin{vmatrix} 1 & 0 \\ 0 & -1 \end{vmatrix}$	$\begin{vmatrix} \frac{-1}{2} & \frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & \frac{1}{2} \end{vmatrix}$	$\begin{vmatrix} \frac{-1}{2} & \frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & \frac{1}{2} \end{vmatrix}$	$\begin{vmatrix} \frac{-1}{2} & \frac{-\sqrt{3}}{2} \\ \frac{-\sqrt{3}}{2} & \frac{1}{2} \end{vmatrix}$	$\begin{vmatrix} \frac{-1}{2} & \frac{-\sqrt{3}}{2} \\ \frac{-\sqrt{3}}{2} & \frac{1}{2} \end{vmatrix}$
$\mathscr{D}^E(R_3^3)$	$i_3 =$	$R_2 =$	$R_2^3 =$	$i_6 =$	$i_5 =$
$\begin{vmatrix} 1 & 0 \\ 0 & -1 \end{vmatrix}$	$\begin{vmatrix} 1 & 0 \\ 0 & -1 \end{vmatrix}$	$\begin{vmatrix} \frac{-1}{2} & \frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & \frac{1}{2} \end{vmatrix}$	$\begin{vmatrix} \frac{-1}{2} & \frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & \frac{1}{2} \end{vmatrix}$	$\begin{vmatrix} \frac{-1}{2} & \frac{-\sqrt{3}}{2} \\ \frac{-\sqrt{3}}{2} & \frac{1}{2} \end{vmatrix}$	$\begin{vmatrix} \frac{-1}{2} & \frac{-\sqrt{3}}{2} \\ \frac{-\sqrt{3}}{2} & \frac{1}{2} \end{vmatrix}$

O: $\left|T_2\right\rangle \left|T_2\right\rangle$; D_4: $\left|A_1\right\rangle \left|B_1\right\rangle$; C_2: $\left|A_1\right\rangle \left|A_1\right\rangle$ basis

For scalar (A_1) $\left|\begin{matrix} A_1 \\ A_1 \\ A_1 \end{matrix}\right\rangle$ and pseudoscalar (A_2) $\left|\begin{matrix} A_2 \\ B_1 \\ A_1 \end{matrix}\right\rangle$ representations, see the O character table.

TABLE F.2.3 Octahedral Multipole Functions and Harmonic Monomials

$I_1^{T_{1u}} = x \quad I_1^{T_{1g}} = J_x$	
$I_2^{T_{1u}} = y \quad I_2^{T_{1g}} = J_y$	
$I_3^{T_{1u}} = z \quad I_3^{T_{1g}} = J_z$	
$II^{A_{1g}} = x^2 + y^2 + z^2$	$x^2 = \frac{1}{3} II^{A_{1g}} - \frac{1}{6} II_1^{E_g} + \frac{1}{2\sqrt{3}} II_2^{E_g}$
$II_1^{E_g} = -x^2 - y^2 + 2z^2$	$y^2 = \frac{1}{3} II^{A_{1g}} - \frac{1}{6} II_1^{E_g} - \frac{1}{2\sqrt{3}} II_2^{E_g}$
$II_2^{E_g} = \sqrt{3}(x^2 - y^2)$	$z^2 = \frac{1}{3} II^{A_{1g}} + \frac{1}{3} II_1^{E_g}$
$II_1^{T_{2g}} = yz$	$yz = II_1^{T_{2g}}$
$II_2^{T_{2g}} = xz$	$xz = II_2^{T_{2g}}$
$II_3^{T_{2g}} = xy$	$xy = II_3^{T_{2g}}$
$III^{A_{2u}} = xyz$	$x^3 = III_1^{T_{1u}}$
$III_1^{T_{1u}} = x^3$	$y^3 = III_2^{T_{1u}}$
$III_2^{T_{1u}} = y^3$	$z^3 = III_3^{T_{1u}}$
$III_3^{T_{1u}} = z^3$	$xy^2 = \frac{1}{2} III'^{T_{1u}}_1 + \frac{1}{2} III_1^{T_{2u}}$
$III'^{T_{1u}}_1 = xy^2 + xz^2$	$xz^2 = \frac{1}{2} III'^{T_{1u}}_1 - \frac{1}{2} III_1^{T_{2u}}$
$III'^{T_{1u}}_2 = yz^2 + yx^2$	$yx^2 = \frac{1}{2} III'^{T_{1u}}_2 - \frac{1}{2} III_2^{T_{2u}}$
$III'^{T_{1u}}_3 = zx^2 + zy^2$	$yz^2 = \frac{1}{2} III'^{T_{1u}}_2 + \frac{1}{2} III_2^{T_{2u}}$
$III_1^{T_{2u}} = xy^2 - xz^2$	$zx^2 = \frac{1}{2} III'^{T_{1u}}_3 + \frac{1}{2} III_3^{T_{2u}}$
$III_2^{T_{2u}} = yz^2 - yx^2$	$zy^2 = \frac{1}{2} III'^{T_{1u}}_3 - \frac{1}{2} III_3^{T_{2u}}$
$III_3^{T_{2u}} = zx^2 - zy^2$	$xyz = III^{A_{2u}}$

TABLE F.2.3 *(Continued)*

$IV^{A_{1g}} = x^4 + y^4 + z^4$	$x^4 = \frac{1}{3}IV^{A_{1g}} - \frac{1}{6}IV_1^{E_g} + \frac{1}{2\sqrt{3}}IV_2^{E_g}$
$IV'^{A_{1g}} = x^2y^2 + x^2z^2 + y^2z^2$	$y^4 = \frac{1}{3}IV^{A_{1g}} - \frac{1}{6}IV_1^{E_g} - \frac{1}{2\sqrt{3}}IV_2^{E_g}$
$IV_1^{E_g} = -x^4 - y^4 + 2z^4$	$z^4 = \frac{1}{3}IV^{A_{1g}} + \frac{1}{3}IV_1^{E_g}$
$IV_2^{E_g} = \sqrt{3}(x^4 - y^4)$	$y^2z^2 = \frac{1}{3}IV'^{A_{1g}} - \frac{1}{6}IV_1'^{E_g} + \frac{1}{2\sqrt{3}}IV_2'^{E_g}$
$IV_1'^{E_g} = 2x^2y^2 - x^2z^2 - y^2z^2$	$x^2z^2 = \frac{1}{3}IV'^{A_{1g}} - \frac{1}{6}IV_1'^{E_g} - \frac{1}{2\sqrt{3}}IV_2'^{E_g}$
$IV_2'^{E_g} = \sqrt{3}(-x^2z^2 + y^2z^2)$	$x^2y^2 = \frac{1}{3}IV'^{A_{1g}} + \frac{1}{3}IV_1'^{E_g}$
$IV_1^{T_{1g}} = y^3z - z^3y$	$xy^3 = \frac{1}{2}IV_3'^{T_{2g}} - \frac{1}{2}IV_3^{T_{1g}}$
$IV_2^{T_{1g}} = z^3x - x^3z$	$yx^3 = \frac{1}{2}IV_3'^{T_{2g}} - \frac{1}{2}IV_3^{T_{1g}}$
$IV_3^{T_{1g}} = x^3y - y^3x$	$xz^3 = \frac{1}{2}IV_2'^{T_{2g}} + \frac{1}{2}IV_2^{T_{1g}}$
$IV_1^{T_{2g}} = x^2yz$	$zx^3 = \frac{1}{2}IV_2'^{T_{2g}} - \frac{1}{2}IV_2^{T_{1g}}$
$IV_2^{T_{2g}} = xy^2z$	$yz^3 = \frac{1}{2}IV_1'^{T_{2g}} - \frac{1}{2}IV_1^{T_{1g}}$
$IV_3^{T_{2g}} = xyz^2$	$zy^3 = \frac{1}{2}IV_1'^{T_{2g}} + \frac{1}{2}IV_1^{T_{1g}}$
$IV_1'^{T_{2g}} = y^3z + z^3y$	$x^2yz = IV_1^{T_{2g}}$
$IV_2'^{T_{2g}} = z^3x + x^3z$	$xy^2z = IV_2^{T_{2g}}$
$IV_3'^{T_{2u}} = x^3y + y^3x$	$xyz^2 = IV_3^{T_{2g}}$

TABLE F.2.4 $O \supset D_4 \supset D_2$ **Subgroup Chain Labeled Irreducible Representations (Fourfold Standing-Wave Bases)**

(a) Vector Representations

$$\mathscr{D}^{T_1}(1) = \begin{vmatrix} 1 & \cdot & \cdot \\ \cdot & 1 & \cdot \\ \cdot & \cdot & 1 \end{vmatrix} \quad R_1^2 = \begin{vmatrix} 1 & \cdot & \cdot \\ \cdot & -1 & \cdot \\ \cdot & \cdot & -1 \end{vmatrix} \quad r_1 = \begin{vmatrix} \cdot & \cdot & 1 \\ 1 & \cdot & \cdot \\ \cdot & 1 & \cdot \end{vmatrix} \quad r_2 = \begin{vmatrix} \cdot & \cdot & -1 \\ 1 & \cdot & \cdot \\ \cdot & -1 & \cdot \end{vmatrix} \quad r_1^2 = \begin{vmatrix} \cdot & 1 & \cdot \\ \cdot & \cdot & 1 \\ 1 & \cdot & \cdot \end{vmatrix} \quad r_2^2 = \begin{vmatrix} \cdot & 1 & \cdot \\ \cdot & \cdot & -1 \\ -1 & \cdot & \cdot \end{vmatrix}$$

$$\mathscr{D}^{T_1}(R_3^2) = \begin{vmatrix} -1 & \cdot & \cdot \\ \cdot & -1 & \cdot \\ \cdot & \cdot & 1 \end{vmatrix} \quad R_2^2 = \begin{vmatrix} -1 & \cdot & \cdot \\ \cdot & 1 & \cdot \\ \cdot & \cdot & -1 \end{vmatrix} \quad r_4 = \begin{vmatrix} \cdot & \cdot & 1 \\ -1 & \cdot & \cdot \\ \cdot & -1 & \cdot \end{vmatrix} \quad r_3 = \begin{vmatrix} \cdot & \cdot & -1 \\ -1 & \cdot & \cdot \\ \cdot & 1 & \cdot \end{vmatrix} \quad r_3^2 = \begin{vmatrix} \cdot & -1 & \cdot \\ \cdot & \cdot & 1 \\ -1 & \cdot & \cdot \end{vmatrix} \quad r_4^2 = \begin{vmatrix} \cdot & -1 & \cdot \\ \cdot & \cdot & -1 \\ 1 & \cdot & \cdot \end{vmatrix}$$

$$\mathscr{D}^{T_1}(R_3) = \begin{vmatrix} \cdot & -1 & \cdot \\ 1 & \cdot & \cdot \\ \cdot & \cdot & 1 \end{vmatrix} \quad i_4 = \begin{vmatrix} \cdot & -1 & \cdot \\ -1 & \cdot & \cdot \\ \cdot & \cdot & -1 \end{vmatrix} \quad i_1 = \begin{vmatrix} \cdot & \cdot & 1 \\ \cdot & -1 & \cdot \\ 1 & \cdot & \cdot \end{vmatrix} \quad i_2 = \begin{vmatrix} \cdot & \cdot & -1 \\ \cdot & -1 & \cdot \\ -1 & \cdot & \cdot \end{vmatrix} \quad R_1^3 = \begin{vmatrix} 1 & \cdot & \cdot \\ \cdot & \cdot & 1 \\ \cdot & -1 & \cdot \end{vmatrix} \quad R_1 = \begin{vmatrix} 1 & \cdot & \cdot \\ \cdot & \cdot & -1 \\ \cdot & 1 & \cdot \end{vmatrix}$$

$$\begin{matrix} O: \\ D_4: \\ D_2: \end{matrix} \left| \begin{matrix} T_1 \\ E \\ B_1 \end{matrix} \right\rangle \left| \begin{matrix} T_1 \\ E \\ B_2 \end{matrix} \right\rangle \left| \begin{matrix} T_1 \\ A_2 \\ A_2 \end{matrix} \right\rangle \text{ basis}$$

$$\mathscr{D}^{T_1}(R_3^3) = \begin{vmatrix} \cdot & 1 & \cdot \\ -1 & \cdot & \cdot \\ \cdot & \cdot & 1 \end{vmatrix} \quad i_3 = \begin{vmatrix} \cdot & 1 & \cdot \\ 1 & \cdot & \cdot \\ \cdot & \cdot & -1 \end{vmatrix} \quad R_2 = \begin{vmatrix} \cdot & \cdot & 1 \\ \cdot & 1 & \cdot \\ -1 & \cdot & \cdot \end{vmatrix} \quad R_2^3 = \begin{vmatrix} \cdot & \cdot & -1 \\ \cdot & 1 & \cdot \\ 1 & \cdot & \cdot \end{vmatrix} \quad i_6 = \begin{vmatrix} -1 & \cdot & \cdot \\ \cdot & \cdot & 1 \\ \cdot & 1 & \cdot \end{vmatrix} \quad i_5 = \begin{vmatrix} -1 & \cdot & \cdot \\ \cdot & \cdot & -1 \\ \cdot & -1 & \cdot \end{vmatrix}$$

TABLE F.2.4 *(Continued)*

(b) Second-Rank Tensor Representations

$$\mathscr{D}^{T_2}(1) = \begin{vmatrix} 1 & \cdot & \cdot \\ \cdot & 1 & \cdot \\ \cdot & \cdot & 1 \end{vmatrix} \quad R_1^2 = \begin{vmatrix} 1 & \cdot & \cdot \\ \cdot & -1 & \cdot \\ \cdot & \cdot & -1 \end{vmatrix} \quad r_1 = \begin{vmatrix} \cdot & \cdot & 1 \\ -1 & \cdot & \cdot \\ \cdot & -1 & \cdot \end{vmatrix} \quad r_2 = \begin{vmatrix} \cdot & \cdot & -1 \\ -1 & \cdot & \cdot \\ \cdot & 1 & \cdot \end{vmatrix} \quad r_1^2 = \begin{vmatrix} \cdot & -1 & \cdot \\ \cdot & \cdot & -1 \\ 1 & \cdot & \cdot \end{vmatrix} \quad r_2^2 = \begin{vmatrix} \cdot & -1 & \cdot \\ \cdot & \cdot & 1 \\ -1 & \cdot & \cdot \end{vmatrix}$$

$$\mathscr{D}^{T_2}(R_3^2) = \begin{vmatrix} -1 & \cdot & \cdot \\ \cdot & -1 & \cdot \\ \cdot & \cdot & 1 \end{vmatrix} \quad R_2^2 = \begin{vmatrix} -1 & \cdot & \cdot \\ \cdot & 1 & \cdot \\ \cdot & \cdot & -1 \end{vmatrix} \quad r_4 = \begin{vmatrix} \cdot & \cdot & 1 \\ 1 & \cdot & \cdot \\ \cdot & 1 & \cdot \end{vmatrix} \quad r_3 = \begin{vmatrix} \cdot & \cdot & -1 \\ 1 & \cdot & \cdot \\ \cdot & -1 & \cdot \end{vmatrix} \quad r_3^2 = \begin{vmatrix} \cdot & 1 & \cdot \\ \cdot & \cdot & -1 \\ -1 & \cdot & \cdot \end{vmatrix} \quad r_4^2 = \begin{vmatrix} \cdot & 1 & \cdot \\ \cdot & \cdot & 1 \\ 1 & \cdot & \cdot \end{vmatrix}$$

$$\mathscr{D}^{T_2}(R_3) = \begin{vmatrix} \cdot & -1 & \cdot \\ 1 & \cdot & \cdot \\ \cdot & \cdot & -1 \end{vmatrix} \quad i_4 = \begin{vmatrix} \cdot & -1 & \cdot \\ -1 & \cdot & \cdot \\ \cdot & \cdot & 1 \end{vmatrix} \quad i_1 = \begin{vmatrix} \cdot & \cdot & -1 \\ \cdot & 1 & \cdot \\ -1 & \cdot & \cdot \end{vmatrix} \quad i_2 = \begin{vmatrix} \cdot & \cdot & 1 \\ \cdot & 1 & \cdot \\ 1 & \cdot & \cdot \end{vmatrix} \quad R_1^3 = \begin{vmatrix} -1 & \cdot & \cdot \\ \cdot & \cdot & 1 \\ \cdot & -1 & \cdot \end{vmatrix} \quad R_1 = \begin{vmatrix} -1 & \cdot & \cdot \\ \cdot & \cdot & -1 \\ \cdot & 1 & \cdot \end{vmatrix}$$

$$\begin{matrix} O: \\ D_4: \\ D_2: \end{matrix} \left| \begin{matrix} T_2 \\ E \\ B_1 \end{matrix} \right\rangle \left| \begin{matrix} T_2 \\ E \\ B_2 \end{matrix} \right\rangle \left| \begin{matrix} T_2 \\ B_2 \\ A_2 \end{matrix} \right\rangle \text{basis}$$

$$\mathscr{D}^{T_2}(R_3^3) = \begin{vmatrix} \cdot & 1 & \cdot \\ -1 & \cdot & \cdot \\ \cdot & \cdot & -1 \end{vmatrix} \quad i_3 = \begin{vmatrix} \cdot & 1 & \cdot \\ 1 & \cdot & \cdot \\ \cdot & \cdot & 1 \end{vmatrix} \quad R_2 = \begin{vmatrix} \cdot & \cdot & -1 \\ \cdot & -1 & \cdot \\ 1 & \cdot & \cdot \end{vmatrix} \quad R_2^3 = \begin{vmatrix} \cdot & \cdot & 1 \\ \cdot & -1 & \cdot \\ -1 & \cdot & \cdot \end{vmatrix} \quad i_6 = \begin{vmatrix} 1 & \cdot & \cdot \\ \cdot & \cdot & 1 \\ \cdot & 1 & \cdot \end{vmatrix} \quad i_5 = \begin{vmatrix} 1 & \cdot & \cdot \\ \cdot & \cdot & -1 \\ \cdot & -1 & \cdot \end{vmatrix}$$

$$\mathscr{D}^E(1)\ \begin{vmatrix} 1 & 0 \\ 0 & 1 \end{vmatrix} \quad R_1^2 = \begin{vmatrix} 1 & 0 \\ 0 & 1 \end{vmatrix} \quad r_1 = \begin{vmatrix} \frac{-1}{2} & \frac{-\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & \frac{-1}{2} \end{vmatrix} \quad r_2 = \begin{vmatrix} \frac{-1}{2} & \frac{-\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & \frac{-1}{2} \end{vmatrix} \quad r_1^2 = \begin{vmatrix} \frac{-1}{2} & \frac{\sqrt{3}}{2} \\ \frac{-\sqrt{3}}{2} & \frac{-1}{2} \end{vmatrix} \quad r_2^2 = \begin{vmatrix} \frac{-1}{2} & \frac{\sqrt{3}}{2} \\ \frac{-\sqrt{3}}{2} & \frac{-1}{2} \end{vmatrix}$$

$$\mathscr{D}^E(R_3^2)\ \begin{vmatrix} 1 & 0 \\ 0 & 1 \end{vmatrix} \quad R_2^2 = \begin{vmatrix} 1 & 0 \\ 0 & 1 \end{vmatrix} \quad r_4 = \begin{vmatrix} \frac{-1}{2} & \frac{-\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & \frac{-1}{2} \end{vmatrix} \quad r_3 = \begin{vmatrix} \frac{-1}{2} & \frac{-\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & \frac{-1}{2} \end{vmatrix} \quad r_3^2 = \begin{vmatrix} \frac{-1}{2} & \frac{\sqrt{3}}{2} \\ \frac{-\sqrt{3}}{2} & \frac{-1}{2} \end{vmatrix} \quad r_4^2 = \begin{vmatrix} \frac{-1}{2} & \frac{\sqrt{3}}{2} \\ \frac{-\sqrt{3}}{2} & \frac{-1}{2} \end{vmatrix}$$

$$\mathscr{D}^E(R_3)\ \begin{vmatrix} 1 & 0 \\ 0 & -1 \end{vmatrix} \quad i_4 = \begin{vmatrix} 1 & 0 \\ 0 & -1 \end{vmatrix} \quad i_1 = \begin{vmatrix} \frac{-1}{2} & \frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & \frac{1}{2} \end{vmatrix} \quad i_2 = \begin{vmatrix} \frac{-1}{2} & \frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & \frac{1}{2} \end{vmatrix} \quad R_1^3 = \begin{vmatrix} \frac{-1}{2} & \frac{-\sqrt{3}}{2} \\ \frac{-\sqrt{3}}{2} & \frac{1}{2} \end{vmatrix} \quad R_1 = \begin{vmatrix} \frac{-1}{2} & \frac{-\sqrt{3}}{2} \\ \frac{-\sqrt{3}}{2} & \frac{1}{2} \end{vmatrix} \quad \begin{matrix} O: \\ D_4: \\ D_2: \end{matrix} \left| \begin{matrix} E \\ A_1 \\ A_1 \end{matrix} \right\rangle \left| \begin{matrix} E \\ B_1 \\ A_1 \end{matrix} \right\rangle \text{basis}$$

$$\mathscr{D}^E(R_3^3)\ \begin{vmatrix} 1 & 0 \\ 0 & -1 \end{vmatrix} \quad i_3 = \begin{vmatrix} 1 & 0 \\ 0 & -1 \end{vmatrix} \quad R_2 = \begin{vmatrix} \frac{-1}{2} & \frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & \frac{1}{2} \end{vmatrix} \quad R_2^3 = \begin{vmatrix} \frac{-1}{2} & \frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & \frac{1}{2} \end{vmatrix} \quad i_6 = \begin{vmatrix} \frac{-1}{2} & \frac{-\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & \frac{1}{2} \end{vmatrix} \quad i_5 = \begin{vmatrix} \frac{-1}{2} & \frac{-\sqrt{3}}{2} \\ \frac{-\sqrt{3}}{2} & \frac{1}{2} \end{vmatrix}$$

For scalar (A_1) $\left| \begin{matrix} A_1 \\ A_1 \\ A_1 \end{matrix} \right\rangle$ and pseudoscalar (A_2) $\left| \begin{matrix} A_2 \\ B_1 \\ A_1 \end{matrix} \right\rangle$ representations, see the O character table.

TABLE F.2.5 $O \supset D_3 \supset C_2$ Labeled Irreducible Representations (Yamanouchi Threefold Standing-Wave Bases)

(a) Vector Representation in Bases $\begin{matrix} O: \\ D_3: \\ C_2: \end{matrix} \left| \begin{matrix} T_1 \\ E \\ A \end{matrix} \right\rangle \left| \begin{matrix} T_1 \\ E \\ B \end{matrix} \right\rangle \left| \begin{matrix} T_1 \\ A_2 \\ B \end{matrix} \right\rangle$

$\mathscr{D}^{T_1}(1) =$
$$\begin{vmatrix} 1 & \cdot & \cdot \\ \cdot & 1 & \cdot \\ \cdot & \cdot & 1 \end{vmatrix}$$

$i_4 = [12]$
$$\begin{vmatrix} 1 & \cdot & \cdot \\ \cdot & -1 & \cdot \\ \cdot & \cdot & -1 \end{vmatrix}$$

$R_1^2 = [13][24]$
$$\begin{vmatrix} \cdot & \frac{\sqrt{3}}{3} & \frac{\sqrt{6}}{3} \\ \frac{\sqrt{3}}{3} & \frac{-2}{3} & \frac{\sqrt{2}}{3} \\ \frac{\sqrt{6}}{3} & \frac{\sqrt{2}}{3} & \frac{-1}{3} \end{vmatrix}$$

$R_3 = [1423]$
$$\begin{vmatrix} \cdot & \frac{-\sqrt{3}}{3} & \frac{-\sqrt{6}}{3} \\ \frac{\sqrt{3}}{3} & \frac{2}{3} & \frac{-\sqrt{2}}{3} \\ \frac{\sqrt{6}}{3} & \frac{-\sqrt{2}}{3} & \frac{1}{3} \end{vmatrix}$$

$r_1 = [132]$
$$\begin{vmatrix} \frac{-1}{2} & \frac{-\sqrt{3}}{2} & \cdot \\ \frac{\sqrt{3}}{2} & \frac{-1}{2} & \cdot \\ \cdot & \cdot & 1 \end{vmatrix}$$

$i_5 = [13]$
$$\begin{vmatrix} \frac{-1}{2} & \frac{-\sqrt{3}}{2} & \cdot \\ \frac{-\sqrt{3}}{2} & \frac{1}{2} & \cdot \\ \cdot & \cdot & -1 \end{vmatrix}$$

$r_4 = [234]$
$$\begin{vmatrix} \frac{1}{2} & \frac{-\sqrt{3}}{6} & \frac{\sqrt{6}}{3} \\ \frac{-\sqrt{3}}{2} & \frac{-1}{6} & \frac{\sqrt{2}}{3} \\ \cdot & \frac{-\sqrt{8}}{3} & \frac{-1}{3} \end{vmatrix}$$

$i_6 = [24]$
$$\begin{vmatrix} \frac{-1}{2} & \frac{\sqrt{3}}{6} & \frac{-\sqrt{6}}{3} \\ \frac{\sqrt{3}}{6} & \frac{-5}{6} & \frac{-\sqrt{2}}{3} \\ \frac{-\sqrt{6}}{3} & \frac{-\sqrt{2}}{3} & \frac{1}{3} \end{vmatrix}$$

$r_1^2 = [123]$
$$\begin{vmatrix} \frac{-1}{2} & \frac{\sqrt{3}}{2} & \cdot \\ \frac{-\sqrt{3}}{2} & \frac{-1}{2} & \cdot \\ \cdot & \cdot & 1 \end{vmatrix}$$

$i_2 = [23]$
$$\begin{vmatrix} \frac{-1}{2} & \frac{\sqrt{3}}{2} & \cdot \\ \frac{\sqrt{3}}{2} & \frac{1}{2} & \cdot \\ \cdot & \cdot & -1 \end{vmatrix}$$

$r_2^2 = [142]$
$$\begin{vmatrix} \frac{-1}{2} & \frac{-\sqrt{3}}{6} & \frac{\sqrt{6}}{3} \\ \frac{\sqrt{3}}{6} & \frac{5}{6} & \frac{\sqrt{2}}{3} \\ \frac{-\sqrt{6}}{3} & \frac{\sqrt{2}}{3} & \frac{-1}{3} \end{vmatrix}$$

$R_2^3 = [1342]$
$$\begin{vmatrix} \frac{1}{2} & \frac{\sqrt{3}}{6} & \frac{-\sqrt{6}}{3} \\ \frac{-\sqrt{3}}{2} & \frac{1}{6} & \frac{-\sqrt{2}}{3} \\ \cdot & \frac{\sqrt{8}}{3} & \frac{1}{3} \end{vmatrix}$$

$R_2^2 = [14][23]$
$$\begin{vmatrix} \cdot & \frac{-\sqrt{3}}{3} & \frac{-\sqrt{6}}{3} \\ \frac{-\sqrt{3}}{3} & \frac{-2}{3} & \frac{\sqrt{2}}{3} \\ \frac{-\sqrt{6}}{3} & \frac{\sqrt{2}}{3} & \frac{-1}{3} \end{vmatrix}$$

$R_3^3 = [1324]$
$$\begin{vmatrix} \cdot & \frac{\sqrt{3}}{3} & \frac{\sqrt{6}}{3} \\ \frac{-\sqrt{3}}{3} & \frac{2}{3} & \frac{-\sqrt{2}}{3} \\ \frac{-\sqrt{6}}{3} & \frac{-\sqrt{2}}{3} & \frac{1}{3} \end{vmatrix}$$

$R_3^2 = [12][34]$
$$\begin{vmatrix} -1 & \cdot & \cdot \\ \cdot & \frac{1}{3} & \frac{-\sqrt{8}}{3} \\ \cdot & \frac{-\sqrt{8}}{3} & \frac{-1}{3} \end{vmatrix}$$

$i_3 = [34]$
$$\begin{vmatrix} -1 & \cdot & \cdot \\ \cdot & \frac{-1}{3} & \frac{\sqrt{8}}{3} \\ \cdot & \frac{\sqrt{8}}{3} & \frac{1}{3} \end{vmatrix}$$

$r_2 = [124]$
$$\begin{vmatrix} \frac{-1}{2} & \frac{\sqrt{3}}{6} & \frac{-\sqrt{6}}{3} \\ \frac{-\sqrt{3}}{6} & \frac{5}{6} & \frac{\sqrt{2}}{3} \\ \frac{\sqrt{6}}{3} & \frac{\sqrt{2}}{3} & \frac{-1}{3} \end{vmatrix}$$

$R_1 = [1234]$
$$\begin{vmatrix} \frac{1}{2} & \frac{-\sqrt{3}}{6} & \frac{\sqrt{6}}{3} \\ \frac{\sqrt{3}}{2} & \frac{1}{6} & \frac{-\sqrt{2}}{3} \\ \cdot & \frac{\sqrt{8}}{3} & \frac{1}{3} \end{vmatrix}$$

$r_3 = [143]$
$$\begin{vmatrix} \frac{1}{2} & \frac{\sqrt{3}}{2} & \cdot \\ \frac{\sqrt{3}}{6} & \frac{-1}{6} & \frac{-\sqrt{8}}{3} \\ \frac{-\sqrt{6}}{3} & \frac{\sqrt{2}}{3} & \frac{-1}{3} \end{vmatrix}$$

$R_1^3 = [1432]$
$$\begin{vmatrix} \frac{1}{2} & \frac{\sqrt{3}}{2} & \cdot \\ \frac{-\sqrt{3}}{6} & \frac{1}{6} & \frac{\sqrt{8}}{3} \\ \frac{\sqrt{6}}{3} & \frac{-\sqrt{2}}{3} & \frac{1}{3} \end{vmatrix}$$

$r_3^2 = [134]$
$$\begin{vmatrix} \frac{1}{2} & \frac{\sqrt{3}}{6} & \frac{-\sqrt{6}}{3} \\ \frac{\sqrt{3}}{2} & \frac{-1}{6} & \frac{\sqrt{2}}{3} \\ \cdot & \frac{-\sqrt{8}}{3} & \frac{-1}{3} \end{vmatrix}$$

$i_1 = [14]$
$$\begin{vmatrix} \frac{-1}{2} & \frac{-\sqrt{3}}{6} & \frac{\sqrt{6}}{3} \\ \frac{-\sqrt{3}}{6} & \frac{-5}{6} & \frac{-\sqrt{2}}{3} \\ \frac{\sqrt{6}}{3} & \frac{-\sqrt{2}}{3} & \frac{1}{3} \end{vmatrix}$$

$r_4^2 = [243]$
$$\begin{vmatrix} \frac{1}{2} & \frac{-\sqrt{3}}{2} & \cdot \\ \frac{-\sqrt{3}}{6} & \frac{-1}{6} & \frac{-\sqrt{8}}{3} \\ \frac{\sqrt{6}}{3} & \frac{\sqrt{2}}{3} & \frac{-1}{3} \end{vmatrix}$$

$R_2 = [1243]$
$$\begin{vmatrix} \frac{1}{2} & \frac{-\sqrt{3}}{2} & \cdot \\ \frac{\sqrt{3}}{6} & \frac{1}{6} & \frac{\sqrt{8}}{3} \\ \frac{-\sqrt{6}}{3} & \frac{-\sqrt{2}}{3} & \frac{1}{3} \end{vmatrix}$$

(b) Tensor Representation T_2 in Bases $\begin{matrix} O: \\ D_3: \\ C_2: \end{matrix}\left|\begin{matrix} T_2 \\ A_1 \\ A \end{matrix}\right\rangle \left|\begin{matrix} T_2 \\ E \\ A \end{matrix}\right\rangle \left|\begin{matrix} T_2 \\ E \\ B \end{matrix}\right\rangle$ and E in Bases $\begin{matrix} O: \\ D_3: \\ C_2: \end{matrix}\left|\begin{matrix} E \\ E \\ A \end{matrix}\right\rangle \left|\begin{matrix} E \\ E \\ B \end{matrix}\right\rangle$

$\mathscr{D}^{T_2}(1) = \begin{vmatrix} 1 & \cdot & \cdot \\ \cdot & 1 & \cdot \\ \cdot & \cdot & 1 \end{vmatrix}$

$i_4 = [12]$ $\begin{vmatrix} 1 & \cdot & \cdot \\ \cdot & 1 & \cdot \\ \cdot & \cdot & -1 \end{vmatrix}$

$R_1^2 = [13][24]$ $\begin{vmatrix} \frac{-1}{3} & \frac{-\sqrt{2}}{3} & \frac{\sqrt{6}}{3} \\ \frac{-\sqrt{2}}{3} & \frac{-2}{3} & \frac{-\sqrt{3}}{3} \\ \frac{\sqrt{6}}{3} & \frac{-\sqrt{3}}{3} & \cdot \end{vmatrix}$

$R_3 = [1423]$ $\begin{vmatrix} \frac{-1}{3} & \frac{-\sqrt{2}}{3} & \frac{-\sqrt{6}}{3} \\ \frac{-\sqrt{2}}{3} & \frac{-2}{3} & \frac{\sqrt{3}}{3} \\ \frac{\sqrt{6}}{3} & \frac{-\sqrt{3}}{3} & \cdot \end{vmatrix}$

$r_1 = [132]$ $\begin{vmatrix} 1 & \cdot & \cdot \\ \cdot & \frac{-1}{2} & \frac{-\sqrt{3}}{2} \\ \cdot & \frac{\sqrt{3}}{2} & \frac{-1}{2} \end{vmatrix}$

$i_5 = [13]$ $\begin{vmatrix} 1 & \cdot & \cdot \\ \cdot & \frac{-1}{2} & \frac{-\sqrt{3}}{2} \\ \cdot & \frac{-\sqrt{3}}{2} & \frac{1}{2} \end{vmatrix}$

$r_4 = [234]$ $\begin{vmatrix} \frac{-1}{3} & \frac{\sqrt{8}}{3} & \cdot \\ \frac{-\sqrt{2}}{3} & \frac{-1}{6} & \frac{\sqrt{3}}{2} \\ \frac{\sqrt{6}}{3} & \frac{\sqrt{3}}{6} & \frac{1}{2} \end{vmatrix}$

$i_6 = [24]$ $\begin{vmatrix} \frac{-1}{3} & \frac{-\sqrt{2}}{3} & \frac{\sqrt{6}}{3} \\ \frac{-\sqrt{2}}{3} & \frac{5}{6} & \frac{\sqrt{3}}{6} \\ \frac{\sqrt{6}}{3} & \frac{\sqrt{3}}{6} & \frac{1}{2} \end{vmatrix}$

$r_1^2 = [123]$ $\begin{vmatrix} 1 & \cdot & \cdot \\ \cdot & \frac{-1}{2} & \frac{\sqrt{3}}{2} \\ \cdot & \frac{-\sqrt{3}}{2} & \frac{-1}{2} \end{vmatrix}$

$i_2 = [23]$ $\begin{vmatrix} 1 & \cdot & \cdot \\ \cdot & \frac{-1}{2} & \frac{\sqrt{3}}{2} \\ \cdot & \frac{\sqrt{3}}{2} & \frac{1}{2} \end{vmatrix}$

$r_2^2 = [142]$ $\begin{vmatrix} \frac{-1}{3} & \frac{-\sqrt{2}}{3} & \frac{-\sqrt{6}}{3} \\ \frac{-\sqrt{2}}{3} & \frac{5}{6} & \frac{-\sqrt{3}}{6} \\ \frac{\sqrt{6}}{3} & \frac{\sqrt{3}}{6} & \frac{-1}{2} \end{vmatrix}$

$R_2^3 = [1342]$ $\begin{vmatrix} \frac{-1}{3} & \frac{\sqrt{8}}{3} & \cdot \\ \frac{-\sqrt{2}}{3} & \frac{-1}{6} & \frac{-\sqrt{3}}{2} \\ \frac{\sqrt{6}}{3} & \frac{\sqrt{3}}{6} & \frac{-1}{2} \end{vmatrix}$

$R_2^2 = [14][23]$ $\begin{vmatrix} \frac{-1}{3} & \frac{-\sqrt{2}}{3} & \frac{-\sqrt{6}}{3} \\ \frac{-\sqrt{2}}{3} & \frac{-2}{3} & \frac{\sqrt{3}}{3} \\ \frac{-\sqrt{6}}{3} & \frac{\sqrt{3}}{3} & \cdot \end{vmatrix}$

$R_3^3 = [1324]$ $\begin{vmatrix} \frac{-1}{3} & \frac{-\sqrt{2}}{3} & \frac{\sqrt{6}}{3} \\ \frac{-\sqrt{2}}{3} & \frac{-2}{3} & -\frac{\sqrt{3}}{3} \\ \frac{-\sqrt{6}}{3} & \frac{\sqrt{3}}{3} & \cdot \end{vmatrix}$

$R_3^2 = [12][34]$ $\begin{vmatrix} \frac{-1}{3} & \frac{\sqrt{8}}{3} & \cdot \\ \frac{\sqrt{8}}{3} & \frac{1}{3} & \cdot \\ \cdot & \cdot & -1 \end{vmatrix}$

$i_3 = [34]$ $\begin{vmatrix} \frac{-1}{3} & \frac{\sqrt{8}}{3} & \cdot \\ \frac{\sqrt{8}}{3} & \frac{1}{3} & \cdot \\ \cdot & \cdot & 1 \end{vmatrix}$

$r_2 = [124]$ $\begin{vmatrix} \frac{-1}{3} & \frac{-\sqrt{2}}{3} & \frac{\sqrt{6}}{3} \\ \frac{-\sqrt{2}}{3} & \frac{5}{6} & \frac{\sqrt{3}}{6} \\ \frac{-\sqrt{6}}{3} & \frac{-\sqrt{3}}{6} & \frac{-1}{2} \end{vmatrix}$

$R_1 = [1234]$ $\begin{vmatrix} \frac{-1}{3} & \frac{\sqrt{8}}{3} & \cdot \\ \frac{-\sqrt{2}}{3} & \frac{-1}{6} & \frac{\sqrt{3}}{2} \\ \frac{-\sqrt{6}}{3} & \frac{-\sqrt{3}}{6} & \frac{-1}{2} \end{vmatrix}$

$r_3 = [143]$ $\begin{vmatrix} \frac{-1}{3} & \frac{-\sqrt{2}}{3} & \frac{-\sqrt{6}}{3} \\ \frac{\sqrt{8}}{3} & \frac{-1}{6} & \frac{-\sqrt{3}}{6} \\ \cdot & \frac{-\sqrt{3}}{2} & \frac{1}{2} \end{vmatrix}$

$R_1^3 = [1432]$ $\begin{vmatrix} \frac{-1}{3} & \frac{-\sqrt{2}}{3} & \frac{-\sqrt{6}}{3} \\ \frac{\sqrt{8}}{3} & \frac{-1}{6} & \frac{-\sqrt{3}}{6} \\ \cdot & \frac{\sqrt{3}}{2} & \frac{-1}{2} \end{vmatrix}$

$r_3^2 = [134]$ $\begin{vmatrix} \frac{-1}{3} & \frac{\sqrt{8}}{3} & \cdot \\ \frac{-\sqrt{2}}{3} & \frac{-1}{6} & \frac{-\sqrt{3}}{2} \\ \frac{-\sqrt{6}}{3} & \frac{-\sqrt{3}}{6} & \frac{1}{2} \end{vmatrix}$

$i_1 = [14]$ $\begin{vmatrix} \frac{-1}{3} & \frac{-\sqrt{2}}{3} & \frac{-\sqrt{6}}{3} \\ \frac{-\sqrt{2}}{3} & \frac{5}{6} & \frac{-\sqrt{3}}{6} \\ \frac{-\sqrt{6}}{3} & \frac{-\sqrt{3}}{6} & \frac{1}{2} \end{vmatrix}$

$r_4^2 = [243]$ $\begin{vmatrix} \frac{-1}{3} & \frac{-\sqrt{2}}{3} & \frac{\sqrt{6}}{3} \\ \frac{\sqrt{8}}{3} & \frac{-1}{6} & \frac{\sqrt{3}}{6} \\ \cdot & \frac{\sqrt{3}}{2} & \frac{1}{2} \end{vmatrix}$

$R_2 = [1243]$ $\begin{vmatrix} \frac{-1}{3} & \frac{-\sqrt{2}}{3} & \frac{\sqrt{6}}{3} \\ \frac{\sqrt{8}}{3} & \frac{-1}{6} & \frac{\sqrt{3}}{6} \\ \cdot & \frac{-\sqrt{3}}{2} & \frac{-1}{2} \end{vmatrix}$

TABLE F.2.5 *(Continued)*

$\mathscr{D}^E(1) =$ $\begin{vmatrix} 1 & 0 \\ 0 & 1 \end{vmatrix}$	$i_4 = [12]$ $\begin{vmatrix} 1 & 0 \\ 0 & -1 \end{vmatrix}$	$R_1^2 = [13][24]$ $\begin{vmatrix} 1 & 0 \\ 0 & 1 \end{vmatrix}$	$R_3 = [1423]$ $\begin{vmatrix} 1 & 0 \\ 0 & -1 \end{vmatrix}$
$r_1 = [132]$ $\begin{vmatrix} \frac{-1}{2} & \frac{-\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{vmatrix}$	$i_5 = [13]$ $\begin{vmatrix} \frac{-1}{2} & \frac{-\sqrt{3}}{2} \\ \frac{-\sqrt{3}}{2} & \frac{1}{2} \end{vmatrix}$	$r_4 = [234]$ $\begin{vmatrix} \frac{-1}{2} & \frac{-\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{vmatrix}$	$i_6 = [24]$ $\begin{vmatrix} \frac{-1}{2} & \frac{-\sqrt{3}}{2} \\ \frac{-\sqrt{3}}{2} & \frac{1}{2} \end{vmatrix}$
$r_1^2 = [123]$ $\begin{vmatrix} \frac{-1}{2} & \frac{\sqrt{3}}{2} \\ \frac{-\sqrt{3}}{2} & \frac{-1}{2} \end{vmatrix}$	$i_2 = [23]$ $\begin{vmatrix} \frac{-1}{2} & \frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & \frac{1}{2} \end{vmatrix}$	$r_2^2 = [142]$ $\begin{vmatrix} \frac{-1}{2} & \frac{\sqrt{3}}{2} \\ \frac{-\sqrt{3}}{2} & \frac{-1}{2} \end{vmatrix}$	$R_2^3 = [1342]$ $\begin{vmatrix} \frac{-1}{2} & \frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & \frac{1}{2} \end{vmatrix}$
$R_2^2 = [14][23]$ $\begin{vmatrix} 1 & 0 \\ 0 & 1 \end{vmatrix}$	$R_3^3 = [1324]$ $\begin{vmatrix} 1 & 0 \\ 0 & -1 \end{vmatrix}$	$R_3^2 = [12][34]$ $\begin{vmatrix} 1 & 0 \\ 0 & 1 \end{vmatrix}$	$i_3 = [34]$ $\begin{vmatrix} 1 & 0 \\ 0 & -1 \end{vmatrix}$
$r_2 = [124]$ $\begin{vmatrix} \frac{-1}{2} & \frac{-\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & \frac{-1}{2} \end{vmatrix}$	$R_1 = [1234]$ $\begin{vmatrix} \frac{-1}{2} & \frac{-\sqrt{3}}{2} \\ \frac{-\sqrt{3}}{2} & \frac{1}{2} \end{vmatrix}$	$r_3 = [143]$ $\begin{vmatrix} \frac{-1}{2} & \frac{-\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & \frac{-1}{2} \end{vmatrix}$	$R_1^3 = [1432]$ $\begin{vmatrix} \frac{-1}{2} & \frac{-\sqrt{3}}{2} \\ \frac{-\sqrt{3}}{2} & \frac{1}{2} \end{vmatrix}$
$r_3^2 = [134]$ $\begin{vmatrix} \frac{-1}{2} & \frac{\sqrt{3}}{2} \\ \frac{-\sqrt{3}}{2} & \frac{-1}{2} \end{vmatrix}$	$i_1 = [14]$ $\begin{vmatrix} \frac{-1}{2} & \frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & \frac{1}{2} \end{vmatrix}$	$r_4^2 = [243]$ $\begin{vmatrix} \frac{-1}{2} & \frac{\sqrt{3}}{2} \\ \frac{-\sqrt{3}}{2} & \frac{-1}{2} \end{vmatrix}$	$R_2 = [1243]$ $\begin{vmatrix} \frac{-1}{2} & \frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & \frac{1}{2} \end{vmatrix}$

For scalar (A_1) $\left|\begin{matrix} A_1 \\ A_1 \\ A \end{matrix}\right\rangle$ and pseudoscalar (A_2) $\left|\begin{matrix} A_2 \\ A_2 \\ B \end{matrix}\right\rangle$ representations, see the O character table.

TABLE F.2.6 $O \supset D_4 \supset C_4$ **Subgroup Chain Labeled Irreducible Representations (Fourfold Moving-Wave Bases)**

(a) Vector T_1 Representation

$$\mathscr{D}^{T_1}(1) = \left|\begin{matrix} 1 & \cdot & \cdot \\ \cdot & 1 & \cdot \\ \cdot & \cdot & 1 \end{matrix}\right| \qquad R_1^2 = \left|\begin{matrix} \cdot & -1 & \cdot \\ -1 & \cdot & \cdot \\ \cdot & \cdot & -1 \end{matrix}\right|$$

$$r_1 = \left|\begin{matrix} \frac{-i}{2} & \frac{i}{2} & \frac{-1}{\sqrt{2}} \\ \frac{-i}{2} & \frac{i}{2} & \frac{1}{\sqrt{2}} \\ \frac{-i}{\sqrt{2}} & \frac{-i}{\sqrt{2}} & \cdot \end{matrix}\right| \qquad r_2 = \left|\begin{matrix} \frac{-i}{2} & \frac{i}{2} & \frac{1}{\sqrt{2}} \\ \frac{-i}{2} & \frac{i}{2} & \frac{-1}{\sqrt{2}} \\ \frac{i}{\sqrt{2}} & \frac{i}{\sqrt{2}} & \cdot \end{matrix}\right|$$

$$r_1^2 = \left|\begin{matrix} \frac{i}{2} & \frac{i}{2} & \frac{i}{\sqrt{2}} \\ \frac{i}{2} & \frac{i}{2} & \frac{i}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & \cdot \end{matrix}\right| \qquad r_2^2 = \left|\begin{matrix} \frac{i}{2} & \frac{i}{2} & \frac{-i}{\sqrt{2}} \\ \frac{-i}{2} & \frac{-i}{2} & \frac{-i}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{-1}{\sqrt{2}} & \cdot \end{matrix}\right|$$

$$\mathscr{D}^{T_1}(R_3^2) = \left|\begin{matrix} -1 & \cdot & \cdot \\ \cdot & -1 & \cdot \\ \cdot & \cdot & 1 \end{matrix}\right| \qquad R_2^2 = \left|\begin{matrix} \cdot & 1 & \cdot \\ 1 & \cdot & \cdot \\ \cdot & \cdot & -1 \end{matrix}\right|$$

$$r_4 = \left|\begin{matrix} \frac{i}{2} & \frac{-i}{2} & \frac{-1}{\sqrt{2}} \\ \frac{i}{2} & \frac{-i}{2} & \frac{1}{\sqrt{2}} \\ \frac{i}{\sqrt{2}} & \frac{i}{\sqrt{2}} & \cdot \end{matrix}\right| \qquad r_3 = \left|\begin{matrix} \frac{i}{2} & \frac{i}{2} & \frac{1}{\sqrt{2}} \\ \frac{i}{2} & \frac{i}{2} & \frac{1}{\sqrt{2}} \\ \frac{i}{\sqrt{2}} & \frac{i}{\sqrt{2}} & \cdot \end{matrix}\right|$$

$$r_3^2 = \left|\begin{matrix} \frac{i}{2} & \frac{i}{2} & \frac{i}{\sqrt{2}} \\ \frac{i}{2} & \frac{i}{2} & \frac{i}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{-1}{\sqrt{2}} & \cdot \end{matrix}\right| \qquad r_4^2 = \left|\begin{matrix} \frac{-i}{2} & \frac{-i}{2} & \frac{-i}{\sqrt{2}} \\ \frac{i}{2} & \frac{i}{2} & \frac{-i}{\sqrt{2}} \\ \frac{-1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & \cdot \end{matrix}\right|$$

$$\mathscr{D}^{T_1}(R_3) = \left|\begin{matrix} -i & \cdot & \cdot \\ \cdot & i & \cdot \\ \cdot & \cdot & 1 \end{matrix}\right| \qquad i_4 = \left|\begin{matrix} \cdot & -i & \cdot \\ i & \cdot & \cdot \\ \cdot & \cdot & -1 \end{matrix}\right|$$

$$i_1 = \left|\begin{matrix} \frac{-1}{2} & \frac{-1}{2} & \frac{-1}{\sqrt{2}} \\ \frac{-1}{2} & \frac{-1}{2} & \frac{1}{\sqrt{2}} \\ \frac{-1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & \cdot \end{matrix}\right| \qquad i_2 = \left|\begin{matrix} \frac{-1}{2} & \frac{1}{2} & \frac{1}{\sqrt{2}} \\ \frac{-1}{2} & \frac{-1}{2} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{-1}{\sqrt{2}} & \cdot \end{matrix}\right|$$

$$R_1^3 = \left|\begin{matrix} \frac{1}{2} & \frac{-1}{2} & \frac{i}{\sqrt{2}} \\ \frac{1}{2} & \frac{1}{2} & \frac{i}{\sqrt{2}} \\ \frac{i}{\sqrt{2}} & \frac{i}{\sqrt{2}} & \cdot \end{matrix}\right| \qquad R_1 = \left|\begin{matrix} \frac{1}{2} & \frac{-1}{2} & \frac{-i}{\sqrt{2}} \\ \frac{-1}{2} & \frac{1}{2} & \frac{-i}{\sqrt{2}} \\ \frac{-i}{\sqrt{2}} & \frac{-i}{\sqrt{2}} & \cdot \end{matrix}\right|$$

TABLE F.2.6 *(Continued)*

$$\mathscr{D}^{T_1}(R_3^3) = \begin{vmatrix} i & \cdot & \cdot \\ \cdot & -i & \cdot \\ \cdot & \cdot & 1 \end{vmatrix} \quad i_3 = \begin{vmatrix} \cdot & i & \cdot \\ -i & \cdot & \cdot \\ \cdot & \cdot & -1 \end{vmatrix} \quad R_2 = \begin{vmatrix} \frac{1}{2} & \frac{1}{2} & \frac{-1}{\sqrt{2}} \\ \frac{1}{2} & \frac{1}{2} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{-1}{\sqrt{2}} & \cdot \end{vmatrix} \quad R_2^3 = \begin{vmatrix} \frac{1}{2} & \frac{1}{2} & \frac{1}{\sqrt{2}} \\ \frac{1}{2} & \frac{1}{2} & \frac{-1}{\sqrt{2}} \\ \frac{-1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & \cdot \end{vmatrix} \quad i_6 = \begin{vmatrix} \frac{-1}{2} & \frac{1}{2} & \frac{i}{\sqrt{2}} \\ \frac{1}{2} & \frac{-1}{2} & \frac{i}{\sqrt{2}} \\ \frac{-i}{\sqrt{2}} & \frac{-i}{\sqrt{2}} & \cdot \end{vmatrix} \quad i_5 = \begin{vmatrix} \frac{-1}{2} & \frac{1}{2} & \frac{-i}{\sqrt{2}} \\ \frac{1}{2} & \frac{-1}{2} & \frac{-i}{\sqrt{2}} \\ \frac{i}{\sqrt{2}} & \frac{i}{\sqrt{2}} & \cdot \end{vmatrix}$$

$$\text{basis} \begin{matrix} O: \\ D_4: \\ C_4: \end{matrix} \left| \begin{matrix} T_1 \\ E \\ 1_4 \end{matrix} \right\rangle \left| \begin{matrix} T_1 \\ E \\ 3_4 \end{matrix} \right\rangle \left| \begin{matrix} T_1 \\ A_2 \\ 0_4 \end{matrix} \right\rangle$$

(b) Tensor T_2 Representation

$$\mathscr{D}^{T_2}(1) = \begin{vmatrix} 1 & \cdot & \cdot \\ \cdot & 1 & \cdot \\ \cdot & \cdot & 1 \end{vmatrix} \quad R_1^2 = \begin{vmatrix} \cdot & -1 & \cdot \\ -1 & \cdot & \cdot \\ \cdot & \cdot & -1 \end{vmatrix} \quad r_1 = \begin{vmatrix} \frac{i}{2} & \frac{-i}{2} & \frac{-1}{\sqrt{2}} \\ \frac{i}{2} & \frac{-i}{2} & \frac{1}{\sqrt{2}} \\ \frac{i}{\sqrt{2}} & \frac{i}{\sqrt{2}} & \cdot \end{vmatrix} \quad r_2 = \begin{vmatrix} \frac{i}{2} & \frac{-i}{2} & \frac{1}{\sqrt{2}} \\ \frac{i}{2} & \frac{-i}{2} & \frac{-1}{\sqrt{2}} \\ \frac{-i}{\sqrt{2}} & \frac{-i}{\sqrt{2}} & \cdot \end{vmatrix} \quad r_1^2 = \begin{vmatrix} \frac{-i}{2} & \frac{-i}{2} & \frac{-i}{\sqrt{2}} \\ \frac{i}{2} & \frac{i}{2} & \frac{-i}{\sqrt{2}} \\ \frac{-1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & \cdot \end{vmatrix} \quad r_2^2 = \begin{vmatrix} \frac{-i}{2} & \frac{-i}{2} & \frac{i}{\sqrt{2}} \\ \frac{i}{2} & \frac{i}{2} & \frac{i}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{-1}{\sqrt{2}} & \cdot \end{vmatrix}$$

$$\mathscr{D}^{T_2}(R_3^2) = \begin{vmatrix} -1 & \cdot & \cdot \\ \cdot & -1 & \cdot \\ \cdot & \cdot & 1 \end{vmatrix} \quad R_2^2 = \begin{vmatrix} \cdot & 1 & \cdot \\ 1 & \cdot & \cdot \\ \cdot & \cdot & -1 \end{vmatrix} \quad r_4 = \begin{vmatrix} \frac{-i}{2} & \frac{i}{2} & \frac{-1}{\sqrt{2}} \\ \frac{-i}{2} & \frac{i}{2} & \frac{1}{\sqrt{2}} \\ \frac{-i}{\sqrt{2}} & \frac{-i}{\sqrt{2}} & \cdot \end{vmatrix} \quad r_3 = \begin{vmatrix} \frac{-i}{2} & \frac{i}{2} & \frac{1}{\sqrt{2}} \\ \frac{-i}{2} & \frac{i}{2} & \frac{-1}{\sqrt{2}} \\ \frac{i}{\sqrt{2}} & \frac{i}{\sqrt{2}} & \cdot \end{vmatrix} \quad r_3^2 = \begin{vmatrix} \frac{i}{2} & \frac{i}{2} & \frac{-i}{\sqrt{2}} \\ \frac{-i}{2} & \frac{-i}{2} & \frac{-i}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{-1}{\sqrt{2}} & \cdot \end{vmatrix} \quad r_4^2 = \begin{vmatrix} \frac{i}{2} & \frac{i}{2} & \frac{i}{\sqrt{2}} \\ \frac{-i}{2} & \frac{-i}{2} & \frac{i}{\sqrt{2}} \\ \frac{-1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & \cdot \end{vmatrix}$$

$$\mathscr{D}^{T_2}(R_3) = \begin{vmatrix} -i & \cdot & \cdot \\ \cdot & i & \cdot \\ \cdot & \cdot & -1 \end{vmatrix} \quad i_4 = \begin{vmatrix} \cdot & -i & \cdot \\ i & \cdot & \cdot \\ \cdot & \cdot & 1 \end{vmatrix} \quad i_1 = \begin{vmatrix} \frac{1}{2} & \frac{1}{2} & \frac{1}{\sqrt{2}} \\ \frac{1}{2} & \frac{1}{2} & \frac{-1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{-1}{\sqrt{2}} & \cdot \end{vmatrix} \quad i_2 = \begin{vmatrix} \frac{1}{2} & \frac{1}{2} & \frac{-1}{\sqrt{2}} \\ \frac{1}{2} & \frac{1}{2} & \frac{1}{\sqrt{2}} \\ \frac{-1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & \cdot \end{vmatrix} \quad R_1^3 = \begin{vmatrix} \frac{-1}{2} & \frac{1}{2} & \frac{i}{\sqrt{2}} \\ \frac{1}{2} & \frac{-1}{2} & \frac{i}{\sqrt{2}} \\ \frac{i}{\sqrt{2}} & \frac{i}{\sqrt{2}} & \cdot \end{vmatrix} \quad R_1 = \begin{vmatrix} \frac{-1}{2} & \frac{1}{2} & \frac{-i}{\sqrt{2}} \\ \frac{1}{2} & \frac{-1}{2} & \frac{-i}{\sqrt{2}} \\ \frac{-i}{\sqrt{2}} & \frac{-i}{\sqrt{2}} & \cdot \end{vmatrix}$$

$$\mathscr{D}^{T_2}(R_3^3) = \begin{vmatrix} i & \cdot & \cdot \\ \cdot & -i & \cdot \\ \cdot & \cdot & -1 \end{vmatrix} \quad i_3 = \begin{vmatrix} \cdot & i & \cdot \\ -i & \cdot & \cdot \\ \cdot & \cdot & 1 \end{vmatrix} \quad R_2 = \begin{vmatrix} \frac{-1}{2} & \frac{-1}{2} & \frac{1}{\sqrt{2}} \\ \frac{-1}{2} & \frac{-1}{2} & \frac{-1}{\sqrt{2}} \\ \frac{-1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & \cdot \end{vmatrix} \quad R_2^3 = \begin{vmatrix} \frac{-1}{2} & \frac{-1}{2} & \frac{-1}{\sqrt{2}} \\ \frac{-1}{2} & \frac{-1}{2} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{-1}{\sqrt{2}} & \cdot \end{vmatrix} \quad i_6 = \begin{vmatrix} \frac{1}{2} & \frac{-1}{2} & \frac{i}{\sqrt{2}} \\ \frac{-1}{2} & \frac{1}{2} & \frac{i}{\sqrt{2}} \\ \frac{-i}{\sqrt{2}} & \frac{-i}{\sqrt{2}} & \cdot \end{vmatrix} \quad i_5 = \begin{vmatrix} \frac{1}{2} & \frac{-1}{2} & \frac{-i}{\sqrt{2}} \\ \frac{-1}{2} & \frac{1}{2} & \frac{-i}{\sqrt{2}} \\ \frac{i}{\sqrt{2}} & \frac{i}{\sqrt{2}} & \cdot \end{vmatrix}$$

$$\text{basis} \quad \begin{matrix} O: \\ D_4: \\ C_4: \end{matrix} \left|\begin{matrix} T_2 \\ E \\ 1_4 \end{matrix}\right\rangle \left|\begin{matrix} T_2 \\ E \\ 3_4 \end{matrix}\right\rangle \left|\begin{matrix} T_2 \\ B_2 \\ 2_4 \end{matrix}\right\rangle$$

The tensor E representation is identical to that of $D_4 \supset D_2$ standing-wave basis.

TABLE F.2.7 $O \supset D_3 \supset C_3$ Subgroup Chain Labeled Irreducible Representations (Threefold Moving-Wave Bases)

(a) Vector T_1 Representation

$\mathcal{D}^{T_1}(1) =$

$$\begin{vmatrix} 1 & \cdot & \cdot \\ \cdot & 1 & \cdot \\ \cdot & \cdot & 1 \end{vmatrix}$$

$i_4 = [12]$

$$\begin{vmatrix} \cdot & -1 & \cdot \\ -1 & \cdot & \cdot \\ \cdot & \cdot & -1 \end{vmatrix}$$

$R_1^2 = [13][24]$

$$\begin{vmatrix} \frac{-1}{3} & \frac{-1}{3} + i\frac{\sqrt{3}}{3} & \frac{i}{3} - \frac{\sqrt{3}}{3} \\ \frac{-1}{3} - i\frac{\sqrt{3}}{3} & \frac{-1}{3} & \frac{i}{3} + \frac{\sqrt{3}}{3} \\ \frac{-i}{3} - \frac{\sqrt{3}}{3} & \frac{-i}{3} + \frac{\sqrt{3}}{3} & \frac{-1}{3} \end{vmatrix}$$

$R_3 = [1423]$

$$\begin{vmatrix} \frac{1}{3} - i\frac{\sqrt{3}}{3} & \frac{1}{3} & \frac{-i}{3} + \frac{\sqrt{3}}{3} \\ \frac{1}{3} & \frac{1}{3} + i\frac{\sqrt{3}}{3} & \frac{-i}{3} - \frac{\sqrt{3}}{3} \\ \frac{i}{3} - \frac{\sqrt{3}}{3} & \frac{i}{3} + \frac{\sqrt{3}}{3} & \frac{1}{3} \end{vmatrix}$$

$r_1 = [132]$

$$\begin{vmatrix} \frac{-1}{2} - i\frac{\sqrt{3}}{2} & \cdot & \cdot \\ \cdot & \frac{-1}{2} + i\frac{\sqrt{3}}{2} & \cdot \\ \cdot & \cdot & 1 \end{vmatrix}$$

$i_5 = [13]$

$$\begin{vmatrix} \cdot & \frac{1}{2} - i\frac{\sqrt{3}}{2} & \cdot \\ \frac{1}{2} + i\frac{\sqrt{3}}{2} & \cdot & \cdot \\ \cdot & \cdot & -1 \end{vmatrix}$$

$r_4 = [234]$

$$\begin{vmatrix} \frac{1}{6} + i\frac{\sqrt{3}}{6} & \frac{-1}{3} - i\frac{\sqrt{3}}{3} & \frac{i}{3} - \frac{\sqrt{3}}{3} \\ \frac{-1}{3} + i\frac{\sqrt{3}}{3} & \frac{1}{6} - i\frac{\sqrt{3}}{6} & \frac{i}{3} + \frac{\sqrt{3}}{3} \\ \frac{2i}{3} & \frac{2i}{3} & \frac{-1}{3} \end{vmatrix}$$

$i_6 = [24]$

$$\begin{vmatrix} \frac{-2}{3} & \frac{1}{6} + i\frac{\sqrt{3}}{6} & \frac{-i}{3} + \frac{\sqrt{3}}{3} \\ \frac{-1}{6} - i\frac{\sqrt{3}}{6} & \frac{2}{3} & \frac{-i}{3} - \frac{\sqrt{3}}{3} \\ \frac{i}{3} + \frac{\sqrt{3}}{3} & \frac{i}{3} - \frac{\sqrt{3}}{3} & \frac{1}{3} \end{vmatrix}$$

$r_1^2 = [123]$

$$\begin{vmatrix} \frac{-1}{2} + i\frac{\sqrt{3}}{2} & \cdot & \cdot \\ \cdot & \frac{-1}{2} - i\frac{\sqrt{3}}{2} & \cdot \\ \cdot & \cdot & 1 \end{vmatrix}$$

$i_2 = [23]$

$$\begin{vmatrix} \cdot & \frac{1}{2} + i\frac{\sqrt{3}}{2} & \cdot \\ \frac{1}{2} - i\frac{\sqrt{3}}{2} & \cdot & \cdot \\ \cdot & \cdot & -1 \end{vmatrix}$$

$r_2^2 = [142]$

$$\begin{vmatrix} \frac{1}{6} - i\frac{\sqrt{3}}{6} & \frac{2}{3} & \frac{i}{3} - \frac{\sqrt{3}}{3} \\ \frac{2}{3} & \frac{1}{6} + i\frac{\sqrt{3}}{6} & \frac{i}{3} + \frac{\sqrt{3}}{3} \\ \frac{-i}{3} + \frac{\sqrt{3}}{3} & \frac{-i}{3} - \frac{\sqrt{3}}{3} & \frac{-1}{3} \end{vmatrix}$$

$R_2^3 = [1342]$

$$\begin{vmatrix} \frac{1}{3} + i\frac{\sqrt{3}}{3} & \frac{-1}{6} - i\frac{\sqrt{3}}{6} & \frac{-i}{3} + \frac{\sqrt{3}}{3} \\ \frac{1}{6} + i\frac{\sqrt{3}}{6} & \frac{1}{3} - i\frac{\sqrt{3}}{3} & \frac{-i}{3} - \frac{\sqrt{3}}{3} \\ \frac{2i}{3} & \frac{-2i}{3} & \frac{1}{3} \end{vmatrix}$$

$R_2^2 = [14][23]$

$$\begin{vmatrix} \frac{-1}{3} & \frac{-1}{3} - i\frac{\sqrt{3}}{3} & \frac{i}{3} + \frac{\sqrt{3}}{3} \\ \frac{-1}{3} + i\frac{\sqrt{3}}{3} & \frac{-1}{3} & \frac{i}{3} - \frac{\sqrt{3}}{3} \\ \frac{-i}{3} + \frac{\sqrt{3}}{3} & \frac{-i}{3} - \frac{\sqrt{3}}{3} & \frac{-1}{3} \end{vmatrix}$$

$R_3^3 = [1324]$

$$\begin{vmatrix} \frac{1}{3} + i\frac{\sqrt{3}}{3} & \frac{1}{3} & \frac{-i}{3} - \frac{\sqrt{3}}{3} \\ \frac{1}{3} & \frac{1}{3} - i\frac{\sqrt{3}}{3} & \frac{-i}{3} + \frac{\sqrt{3}}{3} \\ \frac{i}{3} + \frac{\sqrt{3}}{3} & \frac{i}{3} - \frac{\sqrt{3}}{3} & \frac{1}{3} \end{vmatrix}$$

$R_3^2 = [12][34]$

$$\begin{vmatrix} \frac{-1}{3} & \frac{2}{3} & \frac{-2i}{3} \\ \frac{2}{3} & \frac{-1}{3} & \frac{-2i}{3} \\ \frac{2i}{3} & \frac{2i}{3} & \frac{-1}{3} \end{vmatrix}$$

$i_3 = [34]$

$$\begin{vmatrix} \frac{-2}{3} & \frac{1}{3} & \frac{2i}{3} \\ \frac{1}{3} & \frac{-2}{3} & \frac{2i}{3} \\ \frac{-2i}{3} & \frac{-2i}{3} & \frac{1}{3} \end{vmatrix}$$

$r_2 = [124]$

$$\begin{vmatrix} \frac{1}{6} + i\frac{\sqrt{3}}{6} & \frac{2}{3} & \frac{i}{3} + \frac{\sqrt{3}}{3} \\ \frac{2}{3} & \frac{1}{6} - i\frac{\sqrt{3}}{6} & \frac{i}{3} - \frac{\sqrt{3}}{3} \\ \frac{-i}{3} - \frac{\sqrt{3}}{3} & \frac{-i}{3} + \frac{\sqrt{3}}{3} & \frac{-1}{3} \end{vmatrix}$$

$R_1 = [1234]$

$$\begin{vmatrix} \frac{1}{3} - i\frac{\sqrt{3}}{3} & \frac{-1}{6} + i\frac{\sqrt{3}}{6} & \frac{-i}{3} - \frac{\sqrt{3}}{3} \\ \frac{-1}{6} - i\frac{\sqrt{3}}{6} & \frac{1}{3} + i\frac{\sqrt{3}}{3} & \frac{-i}{3} + \frac{\sqrt{3}}{3} \\ \frac{-2i}{3} & \frac{-2i}{3} & \frac{1}{3} \end{vmatrix}$$

$r_3 = [143]$

$$\begin{vmatrix} \frac{1}{6} + i\frac{\sqrt{3}}{6} & \frac{-1}{3} + i\frac{\sqrt{3}}{3} & \frac{-2i}{3} \\ \frac{-1}{3} - i\frac{\sqrt{3}}{3} & \frac{1}{6} - i\frac{\sqrt{3}}{6} & \frac{2i}{3} \\ \frac{-i}{3} + \frac{\sqrt{3}}{3} & \frac{-i}{3} - \frac{\sqrt{3}}{3} & \frac{-1}{3} \end{vmatrix}$$

$R_1^3 = [1432]$

$$\begin{vmatrix} \frac{1}{3} + i\frac{\sqrt{3}}{3} & \frac{-1}{6} + i\frac{\sqrt{3}}{6} & \frac{2i}{3} \\ \frac{-1}{6} - i\frac{\sqrt{3}}{6} & \frac{1}{3} - i\frac{\sqrt{3}}{3} & \frac{2i}{3} \\ \frac{i}{3} - \frac{\sqrt{3}}{3} & \frac{i}{3} + \frac{\sqrt{3}}{3} & \frac{1}{3} \end{vmatrix}$$

$r_3^2 = [134]$

$$\begin{vmatrix} \frac{1}{6} - i\frac{\sqrt{3}}{6} & \frac{-1}{3} + i\frac{\sqrt{3}}{3} & \frac{i}{3} + \frac{\sqrt{3}}{3} \\ \frac{-1}{3} - i\frac{\sqrt{3}}{3} & \frac{1}{6} + i\frac{\sqrt{3}}{6} & \frac{i}{3} - \frac{\sqrt{3}}{3} \\ \frac{2i}{3} & \frac{2i}{3} & \frac{-1}{3} \end{vmatrix}$$

$i_1 = [14]$

$$\begin{vmatrix} \frac{-2}{3} & \frac{-1}{6} - i\frac{\sqrt{3}}{6} & \frac{-i}{3} - \frac{\sqrt{3}}{3} \\ \frac{-1}{6} + i\frac{\sqrt{3}}{6} & \frac{-2}{3} & \frac{-i}{3} + \frac{\sqrt{3}}{3} \\ \frac{i}{3} - \frac{\sqrt{3}}{3} & \frac{i}{3} + \frac{\sqrt{3}}{3} & \frac{1}{3} \end{vmatrix}$$

$r_4^2 = [243]$

$$\begin{vmatrix} \frac{1}{6} - i\frac{\sqrt{3}}{6} & \frac{-1}{3} - i\frac{\sqrt{3}}{3} & \frac{-2i}{3} \\ \frac{-1}{3} + i\frac{\sqrt{3}}{3} & \frac{1}{6} + i\frac{\sqrt{3}}{6} & \frac{-2i}{3} \\ \frac{-i}{3} - \frac{\sqrt{3}}{3} & \frac{-i}{3} + \frac{\sqrt{3}}{3} & \frac{-1}{3} \end{vmatrix}$$

$R_2 = [1243]$

$$\begin{vmatrix} \frac{1}{3} - i\frac{\sqrt{3}}{3} & \frac{-1}{6} - i\frac{\sqrt{3}}{6} & \frac{2i}{3} \\ \frac{-1}{6} + i\frac{\sqrt{3}}{6} & \frac{1}{3} + i\frac{\sqrt{3}}{3} & \frac{2i}{3} \\ \frac{i}{3} + \frac{\sqrt{3}}{3} & \frac{i}{3} - \frac{\sqrt{3}}{3} & \frac{1}{3} \end{vmatrix}$$

$$\begin{matrix} O: \\ D_3: \\ C_3: \end{matrix} \left|\begin{matrix} T_1 \\ E \\ 1_3 \end{matrix}\right\rangle \left|\begin{matrix} T_1 \\ E \\ 2_3 \end{matrix}\right\rangle \left|\begin{matrix} T_1 \\ A_2 \\ 0_3 \end{matrix}\right\rangle$$

The $O \supset D_3 \supset C_3$ T_1 representation is obtained from that of $O \supset D_4 \supset D_2$ by the following transformation matrix:

	$\|x_1\rangle$	$\|x_2\rangle$	$x_3\rangle$
$\langle 1_3\|$	$\frac{-1}{2} + i\frac{\sqrt{3}}{6}$	$\frac{1}{2} + i\frac{\sqrt{3}}{6}$	$-i\frac{\sqrt{3}}{3}$
$\langle 2_3\|$	$\frac{1}{2} + i\frac{\sqrt{3}}{6}$	$\frac{-1}{2} + i\frac{\sqrt{3}}{6}$	$-i\frac{\sqrt{3}}{3}$
$\langle 0_3\|$	$\frac{\sqrt{3}}{3}$	$\frac{\sqrt{3}}{3}$	$\frac{\sqrt{3}}{3}$

=

	$\|v_1\rangle$	$\|v_2\rangle$	$\|v_3\rangle$
$\langle 1_3\|$	$\frac{-1}{\sqrt{2}}$	$\frac{i}{\sqrt{2}}$	0
$\langle 2_3\|$	$\frac{1}{\sqrt{2}}$	$\frac{i}{\sqrt{2}}$	0
$\langle 0_3\|$	0	0	1

·

	$\|x_1\rangle$	$\|x_2\rangle$	$\|x_3\rangle$
$\langle v_1\|$	$\frac{1}{\sqrt{2}}$	$\frac{-1}{\sqrt{2}}$	0
$\langle v_2\|$	$\frac{1}{\sqrt{6}}$	$\frac{-1}{\sqrt{6}}$	$\frac{-2}{\sqrt{6}}$
$\langle v_3\|$	$\frac{1}{\sqrt{3}}$	$\frac{1}{\sqrt{3}}$	$\frac{1}{\sqrt{3}}$

, where

$$|x_1\rangle = \left|\begin{matrix} T_1 \\ E \\ B_1 \end{matrix}\right\rangle \quad |x_1\rangle = \left|\begin{matrix} T_1 \\ E \\ B_2 \end{matrix}\right\rangle \quad |x_1\rangle = \left|\begin{matrix} T_1 \\ A_2 \\ A_2 \end{matrix}\right\rangle \begin{matrix} :O \\ :D_4 \\ :D_2 \end{matrix}$$

$$|v_1\rangle = \left|\begin{matrix} T_1 \\ E \\ A \end{matrix}\right\rangle \quad |v_2\rangle = \left|\begin{matrix} T_1 \\ E \\ B \end{matrix}\right\rangle \quad |v_3\rangle = \left|\begin{matrix} T_1 \\ A_2 \\ B \end{matrix}\right\rangle \begin{matrix} :O \\ :D_3 \\ :C_2 \end{matrix}$$

$$|1_3\rangle = \left|\begin{matrix} T_1 \\ E \\ 1_3 \end{matrix}\right\rangle \quad |2_3\rangle = \left|\begin{matrix} T_1 \\ E \\ 2_3 \end{matrix}\right\rangle \quad |0_3\rangle = \left|\begin{matrix} T_1 \\ A_2 \\ 0_3 \end{matrix}\right\rangle \begin{matrix} :O \\ :D_3 \\ :C_3 \end{matrix}$$

TABLE F.2.7 *(Continued)*

(b) Tensor Representation T_2

$\mathscr{D}^{T_2}(1) =$

$$\begin{vmatrix} 1 & \cdot & \cdot \\ \cdot & 1 & \cdot \\ \cdot & \cdot & 1 \end{vmatrix}$$

$i_4 = [12]$

$$\begin{vmatrix} 1 & \cdot & \cdot \\ \cdot & \cdot & -1 \\ \cdot & -1 & \cdot \end{vmatrix}$$

$R_1^2 = [13][24]$

$$\begin{vmatrix} \frac{-1}{3} & \frac{1}{3} - i\frac{\sqrt{3}}{3} & \frac{-1}{3} \;\; i\frac{\sqrt{3}}{3} \\ \frac{1}{3} + i\frac{\sqrt{3}}{3} & \frac{-1}{3} & \frac{1}{3} - i\frac{\sqrt{3}}{3} \\ \frac{-1}{3} + i\frac{\sqrt{3}}{3} & \frac{1}{3} + i\frac{\sqrt{3}}{3} & \frac{-1}{3} \end{vmatrix}$$

$R_3 = [1423]$

$$\begin{vmatrix} \frac{-1}{3} & \frac{1}{3} + i\frac{\sqrt{3}}{3} & \frac{-1}{3} + i\frac{\sqrt{3}}{3} \\ \frac{1}{3} + i\frac{\sqrt{3}}{3} & \frac{-1}{3} + i\frac{\sqrt{3}}{3} & \frac{1}{3} \\ \frac{1}{3} + i\frac{\sqrt{3}}{3} & \frac{1}{3} & \frac{-1}{3} - i\frac{\sqrt{3}}{3} \end{vmatrix}$$

$r_1 = [132]$

$$\begin{vmatrix} 1 & \cdot & \cdot \\ \cdot & \frac{-1}{2} - i\frac{\sqrt{3}}{2} & \cdot \\ \cdot & \cdot & \frac{-1}{2} + i\frac{\sqrt{3}}{2} \end{vmatrix}$$

$i_5 = [13]$

$$\begin{vmatrix} 1 & \cdot & \cdot \\ \cdot & \cdot & \frac{1}{2} - i\frac{\sqrt{3}}{2} \\ \cdot & \frac{1}{2} + i\frac{\sqrt{3}}{2} & \cdot \end{vmatrix}$$

$r_4 = [234]$

$$\begin{vmatrix} \frac{-1}{3} & \frac{-2}{3} & \frac{2}{3} \\ \frac{1}{3} + i\frac{\sqrt{3}}{3} & \frac{1}{6} + i\frac{\sqrt{3}}{6} & \frac{1}{3} + i\frac{\sqrt{3}}{3} \\ \frac{-1}{3} + i\frac{\sqrt{3}}{3} & \frac{1}{3} - i\frac{\sqrt{3}}{3} & \frac{1}{6} - i\frac{\sqrt{3}}{6} \end{vmatrix}$$

$i_6 = [24]$

$$\begin{vmatrix} \frac{1}{3} & \frac{1}{3} - i\frac{\sqrt{3}}{3} & \frac{-1}{3} - i\frac{\sqrt{3}}{3} \\ \frac{1}{3} + i\frac{\sqrt{3}}{3} & \frac{2}{3} & \frac{-1}{6} + i\frac{\sqrt{3}}{6} \\ \frac{1}{3} + i\frac{\sqrt{3}}{3} & \frac{-1}{6} - i\frac{\sqrt{3}}{6} & \frac{2}{3} \end{vmatrix}$$

$r_1^2 = [123]$

$$\begin{vmatrix} 1 & \cdot & \cdot \\ \cdot & \frac{-1}{2} + i\frac{\sqrt{3}}{2} & \cdot \\ \cdot & \cdot & \frac{-1}{2} - i\frac{\sqrt{3}}{2} \end{vmatrix}$$

$i_2 = [23]$

$$\begin{vmatrix} 1 & \cdot & \cdot \\ \cdot & \cdot & \frac{1}{2} + i\frac{\sqrt{3}}{2} \\ \cdot & \frac{1}{2} - i\frac{\sqrt{3}}{2} & \cdot \end{vmatrix}$$

$r_2^2 = [142]$

$$\begin{vmatrix} \frac{-1}{3} & \frac{1}{3} + i\frac{\sqrt{3}}{3} & \frac{-1}{3} + i\frac{\sqrt{3}}{3} \\ \frac{1}{3} + i\frac{\sqrt{3}}{3} & \frac{1}{6} - i\frac{\sqrt{3}}{6} & \frac{-2}{3} \\ \frac{-1}{3} + i\frac{\sqrt{3}}{3} & \frac{-2}{3} & \frac{1}{6} + i\frac{\sqrt{3}}{6} \end{vmatrix}$$

$R_3^3 = [1342]$

$$\begin{vmatrix} \frac{1}{3} & \frac{-2}{3} & \frac{2}{3} \\ \frac{1}{3} + i\frac{\sqrt{3}}{3} & \frac{-1}{3} - i\frac{\sqrt{3}}{3} & \frac{-1}{6} - i\frac{\sqrt{3}}{6} \\ \frac{1}{3} + i\frac{\sqrt{3}}{3} & \frac{-1}{6} + i\frac{\sqrt{3}}{6} & \frac{-1}{3} + i\frac{\sqrt{3}}{3} \end{vmatrix}$$

$R_2^2 = [14][23]$

$$\begin{vmatrix} \frac{-1}{3} & \frac{1}{3} + i\frac{\sqrt{3}}{3} & \frac{-1}{3} + i\frac{\sqrt{3}}{3} \\ \frac{1}{3} - i\frac{\sqrt{3}}{3} & \frac{-1}{3} & \frac{1}{3} + i\frac{\sqrt{3}}{3} \\ \frac{-1}{3} - i\frac{\sqrt{3}}{3} & \frac{1}{3} - i\frac{\sqrt{3}}{3} & \frac{-1}{3} \end{vmatrix}$$

$R_3^3 = [1324]$

$$\begin{vmatrix} \frac{-1}{3} & \frac{1}{3} - i\frac{\sqrt{3}}{3} & \frac{-1}{3} + i\frac{\sqrt{3}}{3} \\ \frac{1}{3} - i\frac{\sqrt{3}}{3} & \frac{-1}{3} - i\frac{\sqrt{3}}{3} & \frac{1}{3} \\ \frac{-1}{3} - i\frac{\sqrt{3}}{3} & \frac{1}{3} & \frac{-1}{3} + i\frac{\sqrt{3}}{3} \end{vmatrix}$$

$R_3^2 = [12][34]$

$$\begin{vmatrix} \frac{1}{3} & \frac{-2}{3} & \frac{2}{3} \\ \frac{-2}{3} & \frac{1}{3} & \frac{2}{3} \\ \frac{2}{3} & \frac{2}{3} & \frac{1}{3} \end{vmatrix}$$

$i_3 = [34]$

$$\begin{vmatrix} \frac{-1}{3} & \frac{-2}{3} & \frac{2}{3} \\ \frac{-2}{3} & \frac{2}{3} & \frac{1}{3} \\ \frac{2}{3} & \frac{1}{3} & \frac{2}{3} \end{vmatrix}$$

$r_2 = [124]$

$$\begin{vmatrix} \frac{-1}{3} & \frac{1}{3} - i\frac{\sqrt{3}}{3} & \frac{-1}{3} - i\frac{\sqrt{3}}{3} \\ \frac{1}{3} - i\frac{\sqrt{3}}{3} & \frac{1}{6} + i\frac{\sqrt{3}}{6} & \frac{-2}{3} \\ \frac{-1}{3} - i\frac{\sqrt{3}}{3} & \frac{-2}{3} & \frac{1}{6} - i\frac{\sqrt{3}}{6} \end{vmatrix}$$

$R_1 = [1234]$

$$\begin{vmatrix} \frac{-1}{3} & \frac{-2}{3} & \frac{2}{3} \\ \frac{1}{3} - i\frac{\sqrt{3}}{3} & \frac{-1}{3} + i\frac{\sqrt{3}}{3} & \frac{-1}{6} + i\frac{\sqrt{3}}{6} \\ \frac{-1}{3} - i\frac{\sqrt{3}}{3} & \frac{-1}{6} - i\frac{\sqrt{3}}{6} & \frac{-1}{3} - i\frac{\sqrt{3}}{3} \end{vmatrix}$$

$r_3 = [143]$

$$\begin{vmatrix} \frac{-1}{3} & \frac{1}{3} + i\frac{\sqrt{3}}{3} & \frac{-1}{3} + i\frac{\sqrt{3}}{3} \\ \frac{-2}{3} & \frac{1}{6} + i\frac{\sqrt{3}}{6} & \frac{1}{3} - i\frac{\sqrt{3}}{3} \\ \frac{2}{3} & \frac{1}{3} + i\frac{\sqrt{3}}{3} & \frac{1}{6} - i\frac{\sqrt{3}}{6} \end{vmatrix}$$

$R_1^3 = [1432]$

$$\begin{vmatrix} \frac{-1}{3} & \frac{1}{3} + i\frac{\sqrt{3}}{3} & \frac{-1}{3} + i\frac{\sqrt{3}}{3} \\ \frac{-2}{3} & \frac{-1}{3} - i\frac{\sqrt{3}}{3} & \frac{-1}{6} + i\frac{\sqrt{3}}{6} \\ \frac{2}{3} & \frac{-1}{6} - i\frac{\sqrt{3}}{6} & \frac{-1}{3} + i\frac{\sqrt{3}}{3} \end{vmatrix}$$

$r_3^2 = [134]$

$$\begin{vmatrix} \frac{-1}{3} & \frac{-2}{3} & \frac{2}{3} \\ \frac{1}{3} - i\frac{\sqrt{3}}{3} & \frac{1}{6} - i\frac{\sqrt{3}}{6} & \frac{1}{3} - i\frac{\sqrt{3}}{3} \\ \frac{-1}{3} - i\frac{\sqrt{3}}{3} & \frac{1}{3} + i\frac{\sqrt{3}}{3} & \frac{1}{6} + i\frac{\sqrt{3}}{6} \end{vmatrix}$$

$i_1 = [14]$

$$\begin{vmatrix} \frac{-1}{3} & \frac{1}{3} + i\frac{\sqrt{3}}{3} & \frac{-1}{3} + i\frac{\sqrt{3}}{3} \\ \frac{1}{3} - i\frac{\sqrt{3}}{3} & \frac{2}{3} & \frac{-1}{6} - i\frac{\sqrt{3}}{6} \\ \frac{-1}{3} - i\frac{\sqrt{3}}{3} & \frac{-1}{6} + i\frac{\sqrt{3}}{6} & \frac{2}{3} \end{vmatrix}$$

$r_4^2 = [243]$

$$\begin{vmatrix} \frac{-1}{3} & \frac{1}{3} - i\frac{\sqrt{3}}{3} & \frac{-1}{3} - i\frac{\sqrt{3}}{3} \\ \frac{-2}{3} & \frac{1}{6} - i\frac{\sqrt{3}}{6} & \frac{1}{3} + i\frac{\sqrt{3}}{3} \\ \frac{2}{3} & \frac{1}{3} - i\frac{\sqrt{3}}{3} & \frac{1}{6} + i\frac{\sqrt{3}}{6} \end{vmatrix}$$

$R_2 = [1243]$

$$\begin{vmatrix} \frac{-1}{3} & \frac{1}{3} - i\frac{\sqrt{3}}{3} & \frac{-1}{3} - i\frac{\sqrt{3}}{3} \\ \frac{-2}{3} & \frac{-1}{3} + i\frac{\sqrt{3}}{3} & \frac{-1}{6} - i\frac{\sqrt{3}}{6} \\ \frac{2}{3} & \frac{-1}{6} + i\frac{\sqrt{3}}{6} & \frac{-1}{3} - i\frac{\sqrt{3}}{3} \end{vmatrix}$$

$$\begin{matrix} O: \\ D_3: \\ C_3: \end{matrix} \left|\begin{matrix} T_2 \\ A_1 \\ 0_3 \end{matrix}\right\rangle \left|\begin{matrix} T_2 \\ E \\ 1_3 \end{matrix}\right\rangle \left|\begin{matrix} T_2 \\ E \\ 2_3 \end{matrix}\right\rangle$$

The $O \supset D_3 \supset C_3$ T_2 representation is obtained from that of $O \supset D_4 \supset D_2$ by the following transformation matrix:

$$\begin{array}{c|ccc} & |x_1\rangle & |x_2\rangle & |x_3\rangle \\ \hline \langle 0_3| & \frac{\sqrt{3}}{3} & \frac{-\sqrt{3}}{3} & \frac{\sqrt{3}}{3} \\ \langle 1_3| & \frac{i}{2} + \frac{\sqrt{3}}{6} & \frac{i}{2} - \frac{\sqrt{3}}{6} & \frac{-\sqrt{3}}{3} \\ \langle 2_3| & \frac{i}{2} - \frac{\sqrt{3}}{6} & \frac{i}{2} + \frac{\sqrt{3}}{6} & \frac{\sqrt{3}}{3} \end{array} = \begin{array}{c|ccc} & |v_1\rangle & |v_2\rangle & |v_3\rangle \\ \hline \langle 0_3| & 1 & 0 & 0 \\ \langle 1_3| & 0 & \frac{-1}{\sqrt{2}} & \frac{i}{\sqrt{2}} \\ \langle 2_3| & 0 & \frac{1}{\sqrt{2}} & \frac{i}{\sqrt{2}} \end{array} \cdot \begin{array}{c|ccc} & |x_1\rangle & |x_2\rangle & |x_3\rangle \\ \hline \langle v_1| & \frac{1}{\sqrt{3}} & \frac{-1}{\sqrt{3}} & \frac{1}{\sqrt{3}} \\ \langle v_2| & \frac{-1}{\sqrt{6}} & \frac{1}{\sqrt{6}} & \frac{2}{\sqrt{6}} \\ \langle v_3| & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \end{array},$$

where

$$|x_1\rangle = \left|\begin{matrix} T_2 \\ E \\ B_1 \end{matrix}\right\rangle \quad |x_2\rangle = \left|\begin{matrix} T_2 \\ E \\ B_2 \end{matrix}\right\rangle \quad |x_3\rangle = \left|\begin{matrix} T_2 \\ B_2 \\ A_2 \end{matrix}\right\rangle \begin{matrix} :O \\ :D_4 \\ :D_2 \end{matrix}$$

$$|v_1\rangle = \left|\begin{matrix} T_2 \\ A_1 \\ A \end{matrix}\right\rangle \quad |v_2\rangle = \left|\begin{matrix} T_2 \\ E \\ A \end{matrix}\right\rangle \quad |v_3\rangle = \left|\begin{matrix} T_2 \\ E \\ B \end{matrix}\right\rangle \begin{matrix} :O \\ :D_3 \\ :C_2 \end{matrix}.$$

$$|0_3\rangle = \left|\begin{matrix} T_2 \\ A_1 \\ 0_3 \end{matrix}\right\rangle \quad |1_3\rangle = \left|\begin{matrix} T_2 \\ E \\ 1_3 \end{matrix}\right\rangle \quad |2_3\rangle = \left|\begin{matrix} T_2 \\ E \\ 2_3 \end{matrix}\right\rangle \begin{matrix} :O \\ :D_3 \\ :C_3 \end{matrix}$$

TABLE F.2.7 *(Continued)*

(c) Tensor Representation E

$$\mathcal{D}^{T_2}(1) = \begin{vmatrix} 1 & \cdot \\ \cdot & 1 \end{vmatrix} \qquad i_4 = [12] \quad \begin{vmatrix} \cdot & -1 \\ -1 & \cdot \end{vmatrix} \qquad R_1^2 = [13][24] \quad \begin{vmatrix} 1 & \cdot \\ \cdot & 1 \end{vmatrix} \qquad R_3 = [1423] \quad \begin{vmatrix} \cdot & -1 \\ -1 & \cdot \end{vmatrix}$$

$$r_1 = [132] \quad \begin{vmatrix} \frac{-1}{2} - i\frac{\sqrt{3}}{2} & \cdot \\ \cdot & \frac{-1}{2} + i\frac{\sqrt{3}}{2} \end{vmatrix} \qquad i_5 = [13] \quad \begin{vmatrix} \cdot & \frac{-1}{2} - i\frac{\sqrt{3}}{2} \\ \frac{-1}{2} + i\frac{\sqrt{3}}{2} & \cdot \end{vmatrix}$$

$$r_4 = [234] \quad \begin{vmatrix} \frac{-1}{2} - i\frac{\sqrt{3}}{2} & \cdot \\ \cdot & \frac{-1}{2} + i\frac{\sqrt{3}}{2} \end{vmatrix} \qquad i_6 = [24] \quad \begin{vmatrix} \cdot & \frac{-1}{2} - i\frac{\sqrt{3}}{2} \\ \frac{-1}{2} + i\frac{\sqrt{3}}{2} & \cdot \end{vmatrix}$$

$$r_1^2 = [123] \quad \begin{vmatrix} \frac{-1}{2} + i\frac{\sqrt{3}}{2} & \cdot \\ \cdot & \frac{-1}{2} - i\frac{\sqrt{3}}{2} \end{vmatrix} \qquad i_2 = [23] \quad \begin{vmatrix} \cdot & \frac{-1}{2} + i\frac{\sqrt{3}}{2} \\ \frac{-1}{2} - i\frac{\sqrt{3}}{2} & \cdot \end{vmatrix}$$

$$r_2^2 = [142] \quad \begin{vmatrix} \frac{-1}{2} + i\frac{\sqrt{3}}{2} & \cdot \\ \cdot & \frac{-1}{2} - i\frac{\sqrt{3}}{2} \end{vmatrix} \qquad R_2^3 = [1342] \quad \begin{vmatrix} \cdot & \frac{-1}{2} + i\frac{\sqrt{3}}{2} \\ \frac{-1}{2} - i\frac{\sqrt{3}}{2} & \cdot \end{vmatrix}$$

$R_2^2 = [14][23]$
$$\begin{vmatrix} 1 & \cdot \\ \cdot & 1 \end{vmatrix}$$

$R_3^3 = [1324]$
$$\begin{vmatrix} \cdot & -1 \\ -1 & \cdot \end{vmatrix}$$

$R_3^2 = [12][34]$
$$\begin{vmatrix} 1 & \cdot \\ \cdot & 1 \end{vmatrix}$$

$i_3 = [34]$
$$\begin{vmatrix} \cdot & -1 \\ -1 & \cdot \end{vmatrix}$$

$r_2 = [124]$
$$\begin{vmatrix} \frac{-1}{2} - i\frac{\sqrt{3}}{2} & \cdot \\ \cdot & \frac{-1}{2} + i\frac{\sqrt{3}}{2} \end{vmatrix}$$

$R_1 = [1234]$
$$\begin{vmatrix} \cdot & \frac{-1}{2} - i\frac{\sqrt{3}}{2} \\ \frac{-1}{2} + i\frac{\sqrt{3}}{2} & \cdot \end{vmatrix}$$

$r_3 = [143]$
$$\begin{vmatrix} \frac{-1}{2} - i\frac{\sqrt{3}}{2} & \cdot \\ \cdot & \frac{-1}{2} + i\frac{\sqrt{3}}{2} \end{vmatrix}$$

$R_1^3 = [1432]$
$$\begin{vmatrix} \cdot & \frac{-1}{2} - i\frac{\sqrt{3}}{2} \\ \frac{-1}{2} + i\frac{\sqrt{3}}{2} & \cdot \end{vmatrix}$$

$r_3^2 = [134]$
$$\begin{vmatrix} \frac{-1}{2} + i\frac{\sqrt{3}}{2} & \cdot \\ \cdot & \frac{-1}{2} - i\frac{\sqrt{3}}{2} \end{vmatrix}$$

$i_1 = [14]$
$$\begin{vmatrix} \cdot & \frac{-1}{2} + i\frac{\sqrt{3}}{2} \\ \frac{-1}{2} - i\frac{\sqrt{3}}{2} & \cdot \end{vmatrix}$$

$r_4^2 = [243]$
$$\begin{vmatrix} \frac{-1}{2} + i\frac{\sqrt{3}}{2} & \cdot \\ \cdot & \frac{-1}{2} - i\frac{\sqrt{3}}{2} \end{vmatrix}$$

$R_2 = [1243]$
$$\begin{vmatrix} \cdot & \frac{-1}{2} + i\frac{\sqrt{3}}{2} \\ \frac{-1}{2} - i\frac{\sqrt{3}}{2} & \cdot \end{vmatrix}$$

$$\begin{matrix} O: \\ D_3: \\ C_3: \end{matrix} \left| \begin{matrix} E \\ E \\ 1_3 \end{matrix} \right\rangle \left| \begin{matrix} E \\ E \\ 2_3 \end{matrix} \right\rangle$$

The $O \supset D_3 \supset C_3$ E representation is obtained from that of $O \supset D_4 \supset D_2$ by the following transformation matrix:

$$\begin{array}{c|cc|} & |x_1\rangle & |x_2\rangle \\ \hline \langle 1_3| & \frac{-1}{\sqrt{2}} & \frac{i}{\sqrt{2}} \\ \langle 2_3| & \frac{1}{\sqrt{2}} & \frac{i}{\sqrt{2}} \\ \hline \end{array} = \begin{array}{c|cc|} & |v_1\rangle & |v_2\rangle \\ \hline \langle 1_3| & \frac{-1}{\sqrt{2}} & \frac{i}{\sqrt{2}} \\ \langle 2_3| & \frac{1}{\sqrt{2}} & \frac{i}{\sqrt{2}} \\ \hline \end{array} \cdot \begin{array}{c|cc|} & |x_1\rangle & |x_2\rangle \\ \hline \langle v_1| & 1 & 0 \\ \langle v_2| & 0 & 1 \\ \hline \end{array}, \quad \text{where} \quad \begin{matrix} |x_1\rangle = \left| \begin{matrix} E \\ E \\ B_1 \end{matrix} \right\rangle & |x_2\rangle = \left| \begin{matrix} E \\ E \\ B_2 \end{matrix} \right\rangle \begin{matrix} :O \\ :D_4 \\ :D_2 \end{matrix} \\ |v_1\rangle = \left| \begin{matrix} E \\ E \\ A \end{matrix} \right\rangle & |v_2\rangle = \left| \begin{matrix} E \\ E \\ B \end{matrix} \right\rangle \begin{matrix} :O \\ :D_3 \\ :C_2 \end{matrix} \\ |1_3\rangle = \left| \begin{matrix} E \\ E \\ 1_1 \end{matrix} \right\rangle & |2_3\rangle = \left| \begin{matrix} E \\ E \\ 2_3 \end{matrix} \right\rangle \begin{matrix} :O \\ :D_3 \\ :C_3 \end{matrix} \end{matrix}.$$

F.3. CLEBSCH-GORDAN COEFFICIENTS

These coupling coefficients in Table F.3.1 and F.3.2 belong to the representations and bases listed in Tables F.2.1 and F.2.2. To obtain $O \supset D_4 \supset D_2$ labeled coefficients, change the sign of the second component of T_2. [Compare Tables F.2.1(b) and F.2.3(b).]

TABLE F.3.1 Standard Fourfold Axial Octahedral Clebsch-Gordan Coefficients

(a) $T_1 \otimes T_1$

T_1	T_1	A_1	E 1	2	T_1 1	2	3	T_2 1	2	3
1	1	$\frac{1}{\sqrt{3}}$	$\frac{1}{\sqrt{6}}$	$\frac{-1}{\sqrt{2}}$	·	·	·	·	·	·
1	2	·	·	·	·	·	$\frac{1}{\sqrt{2}}$	·	·	$\frac{1}{\sqrt{2}}$
1	3	·	·	·	·	$\frac{-1}{\sqrt{2}}$	·	·	$\frac{1}{\sqrt{2}}$	·
2	1	·	·	·	·	·	$\frac{-1}{\sqrt{2}}$	·	·	$\frac{1}{\sqrt{2}}$
2	2	$\frac{1}{\sqrt{3}}$	$\frac{1}{\sqrt{6}}$	$\frac{1}{\sqrt{12}}$	·	·	·	·	·	·
2	3	·	·	·	$\frac{1}{\sqrt{2}}$	·	·	$\frac{1}{\sqrt{2}}$	·	·
3	1	·	·	·	·	$\frac{1}{\sqrt{2}}$	·	·	$\frac{1}{\sqrt{2}}$	·
3	2	·	·	·	$\frac{-1}{\sqrt{2}}$	·	·	$\frac{1}{\sqrt{2}}$	·	·
3	3	$\frac{1}{\sqrt{3}}$	$\frac{-2}{\sqrt{6}}$	0	·	·	·	·	·	·

(b) $T_1 \otimes T_2$

T_1	T_2	A_2	E 1	2	T_1 1	2	3	T_2 1	2	3
1	1	$\frac{1}{\sqrt{3}}$	$\frac{1}{\sqrt{2}}$	$\frac{1}{\sqrt{6}}$	·	·	·	·	·	·
1	2	·	·	·	·	·	$\frac{1}{\sqrt{2}}$	·	·	$\frac{1}{\sqrt{2}}$
1	3	·	·	·	·	$\frac{1}{\sqrt{2}}$	·	·	$\frac{-1}{\sqrt{2}}$	·
2	1	·	·	·	·	·	$\frac{1}{\sqrt{2}}$	·	·	$\frac{-1}{\sqrt{2}}$
2	2	$\frac{1}{\sqrt{3}}$	$\frac{-1}{\sqrt{2}}$	$\frac{1}{\sqrt{6}}$	·	·	·	·	·	·
2	3	·	·	·	$\frac{1}{\sqrt{2}}$	·	·	$\frac{1}{\sqrt{2}}$	·	·
3	1	·	·	·	·	$\frac{1}{\sqrt{2}}$	·	·	$\frac{1}{\sqrt{2}}$	·
3	2	·	·	·	$\frac{1}{\sqrt{2}}$	·	·	$\frac{-1}{\sqrt{2}}$	·	·
3	3	$\frac{1}{\sqrt{3}}$	0	$\frac{-2}{\sqrt{6}}$	·	·	·	·	·	·

(c) $T_2 \otimes T_2$

T_2	T_2	A_1	E 1	2	T_1 1	2	3	T_2 1	2	3
1	1	$\frac{1}{\sqrt{3}}$	$\frac{1}{\sqrt{6}}$	$\frac{-1}{\sqrt{2}}$	·	·	·	·	·	·
1	2	·	·	·	·	·	$\frac{1}{\sqrt{2}}$	·	·	$\frac{1}{\sqrt{2}}$
1	3	·	·	·	·	$\frac{-1}{\sqrt{2}}$	·	·	$\frac{1}{\sqrt{2}}$	·
2	1	·	·	·	·	·	$\frac{-1}{\sqrt{2}}$	·	·	$\frac{1}{\sqrt{2}}$
2	2	$\frac{1}{\sqrt{3}}$	$\frac{1}{\sqrt{6}}$	$\frac{1}{\sqrt{2}}$	·	·	·	·	·	·
2	3	·	·	·	$\frac{1}{\sqrt{2}}$	·	·	$\frac{1}{\sqrt{2}}$	·	·
3	1	·	·	·	·	$\frac{1}{\sqrt{2}}$	·	·	$\frac{1}{\sqrt{2}}$	·
3	2	·	·	·	$\frac{-1}{\sqrt{2}}$	·	·	$\frac{1}{\sqrt{2}}$	·	·
3	3	$\frac{1}{\sqrt{3}}$	$\frac{-2}{\sqrt{6}}$	0	·	·	·	·	·	·

TABLE F.3.1 *(Continued)*

(d) $T_1 \otimes E$

T_1	E	T_1 1	2	3	T_2 1	2	3
1	1	$\frac{-1}{2}$	·	·	$\frac{\sqrt{3}}{2}$	·	·
1	2	$\frac{\sqrt{3}}{2}$	·	·	$\frac{1}{2}$	·	·
2	1	·	$\frac{-1}{2}$	·	·	$\frac{-\sqrt{3}}{2}$	·
2	2	·	$\frac{-\sqrt{3}}{2}$	·	·	$\frac{1}{2}$	·
3	1	·	·	1	·	·	·
3	2	·	·	·	·	·	−1

(e) $T_2 \otimes E$

T_2	E	T_1 1	2	3	T_2 1	2	3
1	1	$\frac{\sqrt{3}}{2}$	·	·	$\frac{-1}{2}$	·	·
1	2	$\frac{1}{2}$	·	·	$\frac{\sqrt{3}}{2}$	·	·
2	1	·	$\frac{-\sqrt{3}}{2}$	·	·	$\frac{-1}{2}$	·
2	2	·	$\frac{1}{2}$	·	·	$\frac{-\sqrt{3}}{2}$	·
3	1	·	·	·	·	·	1
3	2	·	·	−1	·	·	·

(f) $T_1 \otimes A_2$

T_1	A_2	T_2 1	2	3
1		1	·	·
2		·	1	·
3		·	·	1

(g) $T_2 \otimes A_2$

T_2	A_2	T_1 1	2	3
1		1	·	·
2		·	1	·
3		·	·	1

(h) $E \otimes E$

E	E	A_1	A_2	E 1	2
1	1	$\frac{1}{\sqrt{2}}$	·	$\frac{1}{\sqrt{2}}$	·
1	2	·	$\frac{1}{\sqrt{2}}$	·	$\frac{-1}{\sqrt{2}}$
2	1	·	$\frac{-1}{\sqrt{2}}$	·	$\frac{-1}{\sqrt{2}}$
2	2	$\frac{1}{\sqrt{2}}$	·	$\frac{-1}{\sqrt{2}}$	·

(i) $E \otimes E$ and $A_2 \otimes A_2$

E	A_2	E 1	2
1		·	1
2		1	·

A_2	A_2	A_1
		1

TABLE F.3.2 $O \supset D_3 \supset C_3$ Subgroup Labeled Clebsch-Gordan Coefficients

(a) $T_1 \otimes T_1$

T_1	T_1	A_1	E		T_1			T_2		
			1	2	1	2	3	1	2	3
1	1	$\frac{1}{\sqrt{3}}$	$\frac{1}{\sqrt{6}}$	·	·	·	·	$\frac{1}{\sqrt{6}}$	$\frac{1}{\sqrt{3}}$	·
1	2	·	·	$\frac{-1}{\sqrt{6}}$	·	·	$\frac{1}{\sqrt{2}}$	·	·	$\frac{-1}{\sqrt{3}}$
1	3	·	·	$\frac{-1}{\sqrt{3}}$	·	$\frac{-1}{\sqrt{2}}$	·	·	·	$\frac{1}{\sqrt{6}}$
2	1	·	·	$\frac{-1}{\sqrt{6}}$	·	·	$\frac{-1}{\sqrt{2}}$	·	·	$\frac{-1}{\sqrt{3}}$
2	2	$\frac{1}{\sqrt{3}}$	$\frac{-1}{\sqrt{6}}$	·	·	·	·	$\frac{1}{\sqrt{6}}$	$\frac{-1}{\sqrt{3}}$	·
2	3	·	$\frac{1}{\sqrt{3}}$	·	$\frac{1}{\sqrt{2}}$	·	·	·	$\frac{-1}{\sqrt{6}}$	·
3	1	·	·	$\frac{-1}{\sqrt{3}}$	·	$\frac{1}{\sqrt{2}}$	·	·	·	$\frac{1}{\sqrt{6}}$
3	2	·	$\frac{1}{\sqrt{3}}$	·	$\frac{-1}{\sqrt{2}}$	·	·	·	$\frac{-1}{\sqrt{6}}$	·
3	3	$\frac{1}{\sqrt{3}}$	·	·	·	·	·	$\frac{-2}{\sqrt{6}}$	·	·

(b) $T_1 \otimes T_2$

T_2	T_1	A_2	E		T_2			T_1		
			1	2	1	2	3	1	2	3
1	1	·	$\frac{1}{\sqrt{3}}$	·	·	$\frac{-1}{\sqrt{2}}$	·	$\frac{1}{\sqrt{6}}$	·	·
1	2	·	·	$\frac{1}{\sqrt{3}}$	·	·	$\frac{-1}{\sqrt{2}}$	·	$\frac{1}{\sqrt{6}}$	·
1	3	$\frac{1}{\sqrt{3}}$	·	·	·	·	·	·	·	$\frac{-2}{\sqrt{6}}$
2	1	·	$\frac{-1}{\sqrt{6}}$	·	$\frac{1}{\sqrt{2}}$	·	·	$\frac{1}{\sqrt{3}}$	·	·
2	2	$\frac{-1}{\sqrt{3}}$	·	$\frac{1}{\sqrt{6}}$	·	·	·	·	$\frac{-1}{\sqrt{3}}$	$\frac{-1}{\sqrt{6}}$
2	3	·	·	$\frac{-1}{\sqrt{3}}$	·	·	$\frac{-1}{\sqrt{2}}$	·	$\frac{-1}{\sqrt{6}}$	·
3	1	$\frac{1}{\sqrt{3}}$	·	$\frac{1}{\sqrt{6}}$	·	·	·	·	$\frac{-1}{\sqrt{3}}$	$\frac{1}{\sqrt{6}}$
3	2	·	$\frac{1}{\sqrt{6}}$	·	$\frac{1}{\sqrt{2}}$	·	·	$\frac{-1}{\sqrt{3}}$	·	·
3	3	·	$\frac{1}{\sqrt{3}}$	·	·	$\frac{1}{\sqrt{2}}$	·	$\frac{1}{\sqrt{6}}$	·	·

(c) $T_2 \otimes T_2$

T_2	T_2	A_1	E		T_1			T_2		
			1	2	1	2	3	1	2	3
1	1	$\frac{1}{\sqrt{3}}$	·	·	·	·	·	$\frac{2}{\sqrt{6}}$	·	·
1	2	·	$\frac{1}{\sqrt{3}}$	·	$\frac{1}{\sqrt{2}}$	·	·	·	$\frac{-1}{\sqrt{6}}$	·
1	3	·	·	$\frac{1}{\sqrt{3}}$	·	$\frac{1}{\sqrt{2}}$	·	·	·	$\frac{-1}{\sqrt{6}}$
2	1	·	$\frac{1}{\sqrt{3}}$	·	$\frac{-1}{\sqrt{2}}$	·	·	·	$\frac{-1}{\sqrt{6}}$	·
2	2	$\frac{1}{\sqrt{3}}$	$\frac{1}{\sqrt{6}}$	·	·	·	·	$\frac{-1}{\sqrt{6}}$	$\frac{1}{\sqrt{3}}$	·
2	3	·	·	$\frac{-1}{\sqrt{6}}$	·	·	$\frac{1}{\sqrt{2}}$	·	·	$\frac{-1}{\sqrt{3}}$
3	1	·	·	$\frac{1}{\sqrt{3}}$	·	$\frac{-1}{\sqrt{2}}$	·	·	·	$\frac{-1}{\sqrt{6}}$
3	2	·	·	$\frac{-1}{\sqrt{6}}$	·	·	$\frac{-1}{\sqrt{2}}$	·	·	$\frac{-1}{\sqrt{3}}$
3	3	$\frac{1}{\sqrt{3}}$	$\frac{-1}{\sqrt{6}}$	·	·	·	·	$\frac{-1}{\sqrt{6}}$	$\frac{-1}{\sqrt{3}}$	·

TABLE F.3.2 *(Continued)*

(d) $T_1 \otimes E$

T_1	E	T_2 1	2	3	T_1 1	2	3
1	1	$\frac{1}{\sqrt{2}}$	$\frac{-1}{2}$	·	$\frac{1}{2}$	·	·
1	2	·	·	$\frac{1}{2}$	·	$\frac{-1}{2}$	$\frac{-1}{\sqrt{2}}$
2	1	·	·	$\frac{1}{2}$	·	$\frac{-1}{2}$	$\frac{1}{\sqrt{2}}$
2	2	$\frac{1}{\sqrt{2}}$	$\frac{1}{2}$	·	$\frac{-1}{2}$	·	·
3	1	·	·	$\frac{1}{\sqrt{2}}$	·	$\frac{1}{\sqrt{2}}$	·
3	2	·	$\frac{-1}{\sqrt{2}}$	·	$\frac{-1}{\sqrt{2}}$	·	·

(e) $T_2 \otimes E$

T_2	E	T_2 1	2	3	T_1 1	2	3
1	1	·	$\frac{1}{\sqrt{2}}$	·	$\frac{1}{\sqrt{2}}$	·	·
1	2	·	·	$\frac{1}{\sqrt{2}}$	·	$\frac{1}{\sqrt{2}}$	·
2	1	$\frac{1}{\sqrt{2}}$	$\frac{1}{2}$	·	$\frac{-1}{2}$	·	·
2	2	·	·	$\frac{-1}{2}$	·	$\frac{1}{2}$	$\frac{-1}{\sqrt{2}}$
3	1	·	·	$\frac{-1}{2}$	·	$\frac{1}{2}$	$\frac{1}{\sqrt{2}}$
3	2	$\frac{1}{\sqrt{2}}$	$\frac{-1}{2}$	·	$\frac{1}{2}$	·	·

(f) $T_1 \otimes A_2$

T_1	A_2	T_2 1	2	3
1		·	·	1
2		·	-1	·
3		1	·	·

(g) $T_2 \otimes A_2$

T_2	A_2	T_1 1	2	3
1		·	·	1
2		·	-1	·
3		1	·	·

(h) $E \otimes E$

E	E	A_1	A_2	E 1	2
1	1	$\frac{1}{\sqrt{2}}$	·	$\frac{1}{\sqrt{2}}$	·
1	2	·	$\frac{1}{\sqrt{2}}$	·	$\frac{-1}{\sqrt{2}}$
2	1	·	$\frac{-1}{\sqrt{2}}$	·	$\frac{-1}{\sqrt{2}}$
2	2	$\frac{1}{\sqrt{2}}$	·	$\frac{-1}{\sqrt{2}}$	·

(i) $E \otimes E$ and $A_2 \otimes A_2$

E	A_2	E 1	2
1		·	1
2		1	·

A_2	A_2	A_1
		1

F.4. CHARACTER TABLES FOR OCTAHEDRAL SUBGROUPS

Tables F.4.1 through F.4.7 list the characters of the important types of subgroups of octahedral O and O_h symmetry. The characters of O and O_h are given first and then subgroups are listed.

TABLE F.4.1 Octahedral Characters for Groups O and $O_h = O \times C_i$

O_h	$\mathbf{1}$	$\mathbf{r}, \mathbf{r}^2$	$\mathbf{R}^2$	$\mathbf{R}, \mathbf{R}^3$	$\mathbf{i}$	$\mathbf{I}$	$\mathbf{Ir}, \mathbf{Ir}^2$	$\mathbf{IR}^2$	$\mathbf{IR}, \mathbf{IR}^3$	$\mathbf{Ii}$
A_{1g}	1	1	1	1	1	1	1	1	1	1
A_{2g}	1	1	1	−1	−1	1	1	1	−1	−1
E_g	2	−1	2	0	0	2	−1	2	0	0
T_{1g}	3	0	−1	1	−1	3	0	−1	1	−1
T_{2g}	3	0	−1	−1	1	3	0	−1	−1	1
A_{1u}	1	1	1	1	1	−1	−1	−1	−1	−1
A_{2u}	1	1	1	−1	−1	−1	−1	−1	1	1
E_u	2	−1	2	0	0	−2	1	−2	0	0
T_{1u}	3	0	−1	1	−1	−3	0	1	−1	1
T_{2u}	3	0	−1	−1	1	−3	0	1	1	−1

TABLE F.4.2 Characters for Dihedral Groups D_4, D_3, and Two Kinds of D_2.

D_4	$\mathbf{1}$	$\mathbf{R}_3^2$	$\mathbf{R}_3, \mathbf{R}_3^3$	$\mathbf{R}_1^2, \mathbf{R}_2^2$	$\mathbf{i}_3, \mathbf{i}_4$
A_1	1	1	1	1	1
B_1	1	1	−1	1	−1
A_2	1	1	1	−1	−1
B_2	1	1	−1	−1	1
E	2	−2	0	0	0

D_3	$\mathbf{1}$	$\mathbf{r}_1, \mathbf{r}_1^2$	$\mathbf{i}_2, \mathbf{i}_4, \mathbf{i}_5$
A_1	1	1	1
A_2	1	1	−1
E	2	−1	0

D_2'	$\mathbf{1}$	$\mathbf{R}_3^2$	$\mathbf{R}_1^2$	$\mathbf{R}_2^2$
D_2	$\mathbf{1}$	$\mathbf{R}_3^2$	$\mathbf{i}_3$	$\mathbf{i}_4$
A_1	1	1	1	1
B_1	1	−1	1	−1
A_2	1	1	−1	−1
B_2	1	−1	−1	1

TABLE F.4.3 Characters for Cyclic Groups $C_4 \cong C_{2s}$, C_3, and Two Kinds of C_2.

C_{2s}	$\mathbf{1}$	$\mathbf{IR}_3$	$\mathbf{R}_3^2$	$\mathbf{IR}_3^3$
C_4	$\mathbf{1}$	$\mathbf{R}_3$	$\mathbf{R}_3^2$	$\mathbf{R}_3^3$
0_4	1	1	1	1
1_4	1	$-i$	−1	i
2_4	1	−1	1	−1
3_4	1	i	−1	$-i$

C_3	$\mathbf{1}$	$\mathbf{r}_1$	$\mathbf{r}_1^2$
0_3	1	1	1
1_3	1	$e^{\frac{-2\pi i}{3}}$	$e^{\frac{2\pi i}{3}}$
2_3	1	$e^{\frac{2\pi i}{3}}$	$e^{\frac{-2\pi i}{3}}$

C_2'	$\mathbf{1}$	$\mathbf{R}_3^2$
C_2	$\mathbf{1}$	$\mathbf{i}_3$
0_2	1	1
1_2	1	−1

TABLE F.4.4 Characters for C_{4v}, C_{3v}, and Two C_{2v} Groups That Are Isomorphic to D_4, D_3, and D_2, Respectively.

C_{4v}	$\mathbf{1}$	$\mathbf{R}_3^2$	$\mathbf{R}_3, \mathbf{R}_3^3$	$\mathbf{IR}_1^2, \mathbf{IR}_2^2$	$\mathbf{Ii}_3, \mathbf{Ii}_4$
A'	1	1	1	1	1
B'	1	1	−1	1	−1
A''	1	1	1	−1	−1
B''	1	1	−1	−1	1
E	2	−2	0	0	0

C_{3v}	$\mathbf{1}$	$\mathbf{r}_1, \mathbf{r}_1^2$	$\mathbf{Ii}_2, \mathbf{Ii}_4, \mathbf{Ii}_5$
A'	1	1	1
A''	1	1	−1
E	2	−1	0

C_{2v}'	$\mathbf{1}$	$\mathbf{R}_3^2$	$\mathbf{IR}_2^2$	$\mathbf{IR}_1^2$
C_{2v}	$\mathbf{1}$	$\mathbf{i}_4$	$\mathbf{IR}_3^2$	$\mathbf{Ii}_3$
A'	1	1	1	1
B'	1	−1	1	−1
A''	1	1	−1	−1
B''	1	−1	−1	1

TABLE F.4.5 Characters for D_{2d} and D_{3d} Groups That Are Isomorphic to D_4 and $D_3 \times C_i$, Respectively.

D_{2d}	**1**	$\mathbf{R}_3^2$	$\mathbf{IR}_3, \mathbf{IR}_3^3$	$\mathbf{R}_1^2, \mathbf{R}_2^2$	$\mathbf{Ii}_3, \mathbf{Ii}_4$
A_1	1	1	1	1	1
B_1	1	1	−1	1	−1
A_2	1	1	1	−1	−1
B_2	1	1	−1	−1	1
E	2	−2	0	0	0

D_{3d}	**1**	$\mathbf{r}_1, \mathbf{r}_1^2$	$\mathbf{i}_2, \mathbf{i}_4, \mathbf{i}_5$	**I**	$\mathbf{Ir}_1, \mathbf{Ir}_1^2$	$\mathbf{Ii}_2, \mathbf{Ii}_4, \mathbf{Ii}_5$
A_{1g}	1	1	1	1	1	1
A_{2g}	1	1	−1	1	1	−1
E_g	2	−1	0	2	−1	0
A_{1u}	1	1	1	−1	−1	−1
A_{2u}	1	1	−1	−1	−1	1
E_u	2	−1	0	−2	1	0

D_{4d} is isomorphic to D_8, is not contained in O_h, and is not an allowed crystal point symmetry.

TABLE F.4.6 Characters for $D_{4h} = D_4 \times C_i$ and $D_{2h} = D_2 \times C_i$ ($D_{3h} = D_3 \times C_h \cong D_6$ is not contained in O_h.)

D_{4h}	**1**	$\mathbf{R}_3^2$	$\mathbf{R}_3, \mathbf{R}_3^3$	$\mathbf{R}_1^2, \mathbf{R}_2^2$	$\mathbf{i}_3, \mathbf{i}_4$	**I**	$\mathbf{IR}_3^2$	$\mathbf{IR}_3, \mathbf{IR}_3^3$	$\mathbf{IR}_1^2, \mathbf{IR}_2^2$	$\mathbf{Ii}_3, \mathbf{Ii}_4$
A_{1g}	1	1	1	1	1	1	1	1	1	1
B_{1g}	1	1	−1	1	−1	1	1	−1	1	−1
A_{2g}	1	1	1	−1	−1	1	1	1	−1	−1
B_{2g}	1	1	−1	−1	1	1	1	−1	−1	1
E_g	2	−2	0	0	0	2	−2	0	0	0
A_{1u}	1	1	1	1	1	−1	−1	−1	−1	−1
B_{1u}	1	1	−1	1	−1	−1	−1	1	−1	1
A_{2u}	1	1	1	−1	−1	−1	−1	−1	1	1
B_{2u}	1	1	−1	−1	1	−1	−1	1	1	−1
E_u	2	−2	0	0	0	−2	2	0	0	0

D'_{2h}	**1**	$\mathbf{R}_3^2$	$\mathbf{R}_1^2$	$\mathbf{R}_2^2$	**I**	$\mathbf{IR}_3^2$	$\mathbf{IR}_1^2$	$\mathbf{IR}_2^2$
D_{2h}	**1**	$\mathbf{R}_3^2$	$\mathbf{i}_3$	$\mathbf{i}_4$	**I**	$\mathbf{IR}_3^2$	$\mathbf{Ii}_3$	$\mathbf{Ii}_4$
A_{1g}	1	1	1	1	1	1	1	1
B_{1g}	1	−1	1	−1	1	−1	1	−1
A_{2g}	1	1	−1	−1	1	1	−1	−1
B_{2g}	1	−1	−1	1	1	−1	−1	1
A_{1u}	1	1	1	1	−1	−1	−1	−1
B_{1u}	1	−1	1	−1	−1	1	−1	1
A_{2u}	1	1	−1	−1	−1	−1	1	1
B_{2u}	1	−1	−1	1	−1	1	1	−1

TABLE F.4.7 Characters for $C_{4h} = C_{4i} = C_4 \times C_i$, $C_{3i} = C_3 \times C_i$, and $C_{2h} = C_{2i} = C_2 \times C_i$.

C_{4h}	$\mathbf{1}$	$\mathbf{R}_3$	$\mathbf{R}_3^2$	$\mathbf{R}_3^3$	$\mathbf{I}$	$\mathbf{IR}_3$	$\mathbf{IR}_3^2$	$\mathbf{IR}_3^3$
0_{4g}	1	1	1	1	1	1	1	1
1_{4g}	1	$-i$	-1	i	1	$-i$	-1	i
2_{4g}	1	-1	1	-1	1	-1	1	-1
3_{4g}	1	i	-1	$-i$	1	i	-1	$-i$
0_{4u}	1	1	1	1	-1	-1	-1	-1
1_{4u}	1	$-i$	-1	i	-1	i	1	$-i$
2_{4u}	1	-1	1	-1	-1	1	-1	1
3_{4u}	1	i	-1	$-i$	-1	$-i$	1	i

C_{3i}	$\mathbf{1}$	$\mathbf{r}_1$	$\mathbf{r}_1^2$	$\mathbf{I}$	$\mathbf{Ir}_1$	$\mathbf{Ir}_1^2$
0_{3g}	1	1	1	1	1	1
1_{3g}	1	ε^*	ε^*	1	ε^*	ε
2_{3g}	1	ε	ε^*	1	ε	ε^*
0_{3u}	1	1	1	-1	-1	-1
1_{3u}	1	ε^*	ε	-1	$-\varepsilon^*$	$-\varepsilon$
2_{3u}	1	ε	ε^*	-1	$-\varepsilon$	$-\varepsilon^*$

where $\varepsilon = e^{2\pi i/3}$

C'_{2h}	$\mathbf{1}$	$\mathbf{R}_3^2$	$\mathbf{I}$	$\mathbf{IR}_3^2$
C_{2h}	$\mathbf{1}$	$\mathbf{i}_4$	$\mathbf{I}$	$\mathbf{Ii}_4$
0_{2g}	1	1	1	1
1_{2g}	1	-1	1	-1
0_{2u}	1	1	-1	-1
1_{2u}	1	-1	-1	1

The symmetry $C_{3h} = C_3 \times C_h$ is distinct from $C_{3i} = C_3 \times C_i$ but isomorphic to it:

C_{3h}	$\mathbf{1}$	$\mathbf{r}_1$	$\mathbf{r}_1^2$	σ	$\sigma\mathbf{r}_1$	$\sigma\mathbf{r}_1^2$
$0'_3$	1	1	1	1	1	1
$1'_3$	1	ε^*	ε	1	ε^*	ε
$2'_3$	1	ε	ε^*	1	ε	ε^*
$0''_3$	1	1	1	-1	-1	-1
$1''_3$	1	ε^*	ε	-1	$-\varepsilon^*$	$-\varepsilon$
$2''_3$	1	ε	ε^*	-1	$-\varepsilon$	$-\varepsilon^*$

σ = reflection through a mirror plane normal to $\mathbf{r}_1$ axis

where $\varepsilon = e^{2\pi i/3}$

TABLE F.4.8 Characters for $C_h = C_v \cong C_i \cong C_2$

C_i	$\mathbf{1}$	$\mathbf{I}$
C_h	$\mathbf{1}$	σ
C_2	$\mathbf{1}$	$\mathbf{R}_3^2$
0_2	1	1
1_2	1	-1

$\sigma = \mathbf{IR}_1^2$ = reflection through a mirror-plane normal to $\mathbf{R}_1$ axis
$\mathbf{R}_1^2 = 180°$ x-axis rotation.

F.5. CORRELATION TABLES FOR OCTAHEDRAL SUBGROUPS

Tables F.5.1 through F.5.5 list the correlations of representations of select subgroups of octahedral O and O_h symmetry. Rows have subduced representations $\Gamma \downarrow H$. Columns have induced representations $\gamma(H) \uparrow O$. Details and applications of tables are described in Chapter 4.

TABLE F.5.1 Correlations of O with Dihedral Groups D_4, D_3, $D_2 = \{1, R_3^2, i_3, i_4\}$, and $D_2' = \{1, R_3^2, R_1^2, R_2^2\}$.

$O \supset D_4$	A_1	A_2	B_1	B_2	E
$A_1 \downarrow D_4$	1	·	·	·	·
$A_2 \downarrow D_4$	·	·	1	·	·
$E \downarrow D_4$	1	·	1	·	·
$T_1 \downarrow D_4$	·	1	·	·	1
$T_2 \downarrow D_4$	·	·	·	1	1

$O \supset D_3$	A_1	A_2	E
$A_1 \downarrow D_3$	1	·	·
$A_2 \downarrow D_3$	·	1	·
$E \downarrow D_3$	·	·	1
$T_1 \downarrow D_3$	·	1	1
$T_2 \downarrow D_3$	1	·	1

$O \supset D_2$	A_1	B_1	A_2	B_2
$A_1 \downarrow D_2$	1	·	·	·
$A_2 \downarrow D_2$	·	·	1	·
$E \downarrow D_2$	1	·	1	·
$T_1 \downarrow D_2$	·	1	1	1
$T_2 \downarrow D_2$	1	1	·	1

$O \supset D_2'$	A_1	B_1	A_2	B_2
$A_1 \downarrow D_2'$	1	·	·	·
$A_2 \downarrow D_2'$	1	·	·	·
$E \downarrow D_2'$	2	·	·	·
$T_1 \downarrow D_2'$	·	1	1	1
$T_2 \downarrow D_2'$	·	1	1	1

TABLE F.5.2 Correlations of O with Cyclic Groups C_4, C_3, $C_2 = \{1, i_3\}$, and $C_2' = \{1, R_3^2\}$.

$O \supset C_4$	0_4	1_4	2_4	3_4
$A_1 \downarrow C_4$	1	·	·	·
$A_2 \downarrow C_4$	·	·	1	·
$E \downarrow C_4$	1	·	1	·
$T_1 \downarrow C_4$	1	1	·	1
$T_2 \downarrow C_4$	·	1	1	1

$O \supset C_3$	0_3	1_3	2_3
$A_1 \downarrow C_3$	1	·	·
$A_2 \downarrow C_3$	1	·	·
$E \downarrow C_3$	·	1	1
$T_1 \downarrow C_3$	1	1	1
$T_2 \downarrow C_3$	1	1	1

$O \supset C_2$	0_2	1_2
$A_1 \downarrow C_2$	1	·
$A_2 \downarrow C_2$	·	1
$E \downarrow C_2$	1	1
$T_1 \downarrow C_2$	1	2
$T_2 \downarrow C_2$	2	1

$O \supset C_2'$	0_2	1_2
$A_1 \downarrow C_2'$	1	·
$A_2 \downarrow C_2'$	1	·
$E \downarrow C_2'$	2	·
$T_1 \downarrow C_2'$	1	2
$T_2 \downarrow C_2'$	1	2

TABLE F.5.3 Correlations of D_4 with Subgroups C_4, $D_2 = \{1, R_3^2, i_3, i_4\}$, and $D_2' = \{1, R_3^2, R_1^2, R_2^2\}$

$D_4 \supset C_4$	0_4	1_4	2_4	3_4
$A_1 \downarrow C_4$	1	·	·	·
$B_1 \downarrow C_4$	·	·	1	·
$A_2 \downarrow C_4$	1	·	·	·
$B_2 \downarrow C_4$	·	·	1	·
$E \downarrow C_4$	·	1	·	1

$D_4 \supset D_2$	A_1	B_1	A_2	B_2
$A_1 \downarrow D_2$	1	·	·	·
$B_1 \downarrow D_2$	·	·	1	·
$A_2 \downarrow D_2$	·	·	1	·
$B_2 \downarrow D_2$	1	·	·	·
$E \downarrow D_2$	·	1	·	1

$D_4 \supset D_2'$	A_1	B_1	A_2	B_2
$A_1 \downarrow D_2'$	1	·	·	·
$B_1 \downarrow D_2'$	1	·	·	·
$A_2 \downarrow D_2'$	·	·	1	·
$B_2 \downarrow D_2'$	·	·	1	·
$E \downarrow D_2'$	·	1	·	1

TABLE F.5.4 Correlations of D_3 with Subgroups C_3 and C_2.

$D_3 \supset C_3$	0_3	1_3	2_3
$A_1 \downarrow C_3$	1	·	·
$A_2 \downarrow C_3$	1	·	·
$E \downarrow C_3$	·	1	1

$D_3 \supset C_2$	0_2	1_2
$A_1 \downarrow C_2$	1	·
$A_2 \downarrow C_2$	·	1
$E \downarrow C_2$	1	1

TABLE F.5.5 Correlations of O_h with Groups C_{4v}, C_{3v}, $C_{2v} = \{1, i_4, IR_3^2, Ii_3\}$, and $C'_{2v} = \{1, R_3^2, IR_1^2, IR_2^2\}$.

$O_h \supset C_{4v}$	A'	B'	A''	B''	E
$A_{1g} \downarrow C_{4v}$	1	·	·	·	·
$A_{2g} \downarrow C_{4v}$	·	1	·	·	·
$E_g \downarrow C_{4v}$	1	1	·	·	·
$T_{1g} \downarrow C_{4v}$	·	·	1	·	1
$T_{2g} \downarrow C_{4v}$	·	·	·	1	1
$A_{1u} \downarrow C_{4v}$	·	·	1	·	·
$A_{2u} \downarrow C_{4v}$	·	·	·	1	·
$E_u \downarrow C_{4v}$	·	·	1	1	·
$T_{1u} \downarrow C_{4v}$	1	·	·	·	1
$T_{2u} \downarrow C_{4v}$	·	1	·	·	1

$O_h \supset C_{3v}$	A'	A''	E
$A_{1g} \downarrow C_{3v}$	1	·	·
$A_{2g} \downarrow C_{3v}$	·	1	·
$E_g \downarrow C_{3v}$	·	·	1
$T_{1g} \downarrow C_{3v}$	·	1	1
$T_{2g} \downarrow C_{3v}$	1	·	1
$A_{1u} \downarrow C_{3v}$	·	1	·
$A_{2u} \downarrow C_{3v}$	1	·	·
$E_u \downarrow C_{3v}$	·	·	1
$T_{1u} \downarrow C_{3v}$	1	·	1
$T_{2u} \downarrow C_{3v}$	·	1	1

$O_h \supset C_{2v}$	A'	B'	A''	B''
$A_{1g} \downarrow C_{2v}$	1	·	·	·
$A_{2g} \downarrow C_{2v}$	·	1	·	·
$E_g \downarrow C_{2v}$	1	1	·	·
$T_{1g} \downarrow C_{2v}$	·	1	1	1
$T_{2g} \downarrow C_{2v}$	1	·	1	1
$A_{1u} \downarrow C_{2v}$	·	·	1	·
$A_{2u} \downarrow C_{2v}$	·	·	·	1
$E_u \downarrow C_{2v}$	·	·	1	1
$T_{1u} \downarrow C_{2v}$	1	1	·	1
$T_{2u} \downarrow C_{2v}$	1	1	1	·

$O_h \supset C'_{2v}$	A'	B'	A''	B''
$A_{1g} \downarrow C'_{2v}$	1	·	·	·
$A_{2g} \downarrow C'_{2v}$	1	·	·	·
$E_g \downarrow C'_{2v}$	2	·	·	·
$T_{1g} \downarrow C'_{2v}$	·	1	1	1
$T_{2g} \downarrow C'_{2v}$	·	1	1	1
$A_{1u} \downarrow C'_{2v}$	·	·	1	·
$A_{2u} \downarrow C'_{2v}$	·	·	1	·
$E_u \downarrow C'_{2v}$	·	·	2	·
$T_{1u} \downarrow C'_{2v}$	1	1	·	1
$T_{2u} \downarrow C'_{2v}$	1	1	·	1

F.6. HEXAGONAL SYMMETRIES

All hexagonal and trigonal symmetry groups are subgroups of D_{6h} (Table (F.6.1). They are all isomorphic to outer products involving only C_2, C_3, and D_3. D_{6h} itself is isomorphic to $D_3 \times C_2 \times C_2$. See Chapter 3.

TABLE F.6.1 Characters of D_{6h}.

D_{6h}	1	$\mathbf{h}, \mathbf{h}^5$	ρ_1, ρ_2, ρ_3	$\mathbf{h}^3$	$\mathbf{h}^2, \mathbf{h}^4$	$\rho'_1, \rho'_2, \rho'_3$	I	$\mathbf{Ih}, \mathbf{Ih}^5$	$\sigma_1, \sigma_2, \sigma_3$	σ	$\mathbf{Ih}^2, \mathbf{Ih}^4$	$\sigma'_1, \sigma'_2, \sigma'_3$
A_{1g}	1	1	1	1	1	1	1	1	1	1	1	1
A_{2g}	1	1	−1	1	1	−1	1	1	−1	1	1	−1
E_{2g}	2	−1	0	2	−1	0	2	−1	0	2	−1	0
B_{1g}	1	1	1	−1	−1	−1	1	1	1	−1	−1	−1
B_{2g}	1	1	−1	−1	−1	1	1	1	−1	−1	−1	1
E_{1g}	2	−1	0	−2	1	0	2	−1	0	−2	1	0
A_{1u}	1	1	1	1	1	1	−1	−1	−1	−1	−1	−1
A_{2u}	1	1	−1	1	1	−1	−1	−1	1	−1	−1	1
E_{2u}	2	−1	0	2	−1	0	−2	1	0	−2	1	0
B_{1u}	1	1	1	−1	−1	−1	−1	−1	−1	1	1	1
B_{2u}	1	1	−1	−1	−1	1	−1	−1	1	1	1	−1
E_{1u}	2	−1	0	−2	1	0	−2	1	0	2	−1	0

F.7. ICOSAHEDRAL AND PENTAGONAL SYMMETRIES

The rotational symmetry Y of the icosahedron was mentioned after Figure 4.1.6. It has 60 elements in 5 classes of rotations: one of 0°, 12 each of 72° and 144°, 20 of 120°, and 15 of 180°. These are listed at the top of its character table (Table F.7.1). The largest subgroup is the pentagonal dihedral group D_5. The D_5 characters are given in Table F.7.2.

Representations and correlation tables involving these symmetries as well as applications to the C_{60} rotation and vibration problem can be found in the sequel to this text and in the references [1]–[5] listed below. Reference [4] contains the entire Y-group table.

TABLE F.7.1 Icosahedral (Y) Group Characters

Y classes	0°	72°	144°	120°	180°
$^{\circ}c_g$	1	12	12	20	15
A	1	1	1		1
T_1	3	$\frac{1+\sqrt{5}}{2}$	$\frac{1-\sqrt{5}}{2}$	0	−1
T_3	3	$\frac{1-\sqrt{5}}{2}$	$\frac{1+\sqrt{5}}{2}$	0	−1
G	4	−1	−1	1	0
H	5	0	0	−1	1

TABLE F.7.2 Pentagonal Dihedral (D_5) Group Characters

D_5 classes	0°	72°	144°	180°
$^\circ c_g$	1	2	2	5
A_1	1	1	1	1
A_2	1	1	1	-1
E_1	2	$\frac{-1+\sqrt{5}}{2}$	$\frac{-1-\sqrt{5}}{2}$	0
E_2	2	$\frac{-1-\sqrt{5}}{2}$	$\frac{-1+\sqrt{5}}{2}$	0

REFERENCES

1. W. G. Harter and D. E. Weeks, *Chem. Phys. Lett.* **132**, 387 (1986).
2. D. E. Weeks and W. G. Harter, *Chem. Phys. Lett.* **144**, 366 (1988).
3. W. G. Harter and D. E. Weeks, *J. Chem. Phys.* **90**, 4727 (1989).
4. D. E. Weeks and W. G. Harter, *J. Chem. Phys.* **90**, 4744 (1989).
5. W. G. Harter and T. C. Reimer, *Chem. Phys. Lett.* **194**, 230 (1992).

TABLE 7.1 (j) Subshell Tensors

(a) $j = \frac{1}{2}$

$v_q^1 =$ ($q = 0, 1$)

1	−1	1
1	−1	
		$\sqrt{2}$

(b) $j = \frac{3}{2}$

$v_q^1 =$ ($q = 0, 1, 2, 3$)

3	$-\sqrt{3}$	·	·	
$\sqrt{3}$	1	−2	·	
·	2	−1	$-\sqrt{3}$	
·	·	$\sqrt{3}$	−3	$\sqrt{10}$
				$\sqrt{20}$

$v_q^2 =$

1	−1	1	·	
1	−1	0	1	
1	0	−1	1	$\sqrt{2}$
·	1	−1	1	$\sqrt{2}$
				$\sqrt{4}$

$v_q^3 =$

1	−1	1	−1	1
1	−3	$\sqrt{3}$	−1	$\sqrt{2}$
1	$-\sqrt{3}$	3	−1	$\sqrt{5}$
1	−1	1	−1	$\sqrt{20}$

(c) $j = \frac{5}{2}$

$v_q^1 =$ ($q = 0, 1, 2, 3, 4, 5$)

5	$-\sqrt{5}$	·	·	·	·	
$\sqrt{5}$	3	$-\sqrt{8}$	·	·	·	
·	$\sqrt{8}$	1	−3	·	·	
·	·	3	−1	$-\sqrt{8}$	·	
·	·	·	$\sqrt{8}$	−3	$-\sqrt{5}$	$\sqrt{35}$
·	·	·	·	$\sqrt{5}$	−5	$\sqrt{70}$

$v_q^2 =$

5	$-\sqrt{5}$	$\sqrt{5}$	·	·	·	
$\sqrt{5}$	−1	$-\sqrt{2}$	3	·	·	
$\sqrt{5}$	$\sqrt{2}$	−4	0	3	·	
·	3	0	−4	$\sqrt{2}$	$\sqrt{5}$	$\sqrt{28}$
·	·	3	$-\sqrt{2}$	−1	$\sqrt{5}$	$\sqrt{14}$
·	·	·	$\sqrt{5}$	$-\sqrt{5}$	5	$\sqrt{84}$

$v_q^3 =$

5	$-\sqrt{10}$	$\sqrt{5}$	$-\sqrt{5}$	·	·	
$\sqrt{10}$	−7	1	1	$-\sqrt{8}$	·	
$\sqrt{5}$	−1	−4	$\sqrt{8}$	−1	$-\sqrt{5}$	$\sqrt{18}$
$\sqrt{5}$	1	$-\sqrt{8}$	4	1	$-\sqrt{5}$	$\sqrt{12}$
·	$\sqrt{8}$	−1	−1	7	$-\sqrt{10}$	$\sqrt{30}$
·	·	$\sqrt{5}$	$-\sqrt{5}$	$\sqrt{10}$	−5	$\sqrt{180}$

$v_q^4 =$

1	$-\sqrt{2}$	3	−1	1	·	
$\sqrt{2}$	−3	$\sqrt{5}$	$-\sqrt{5}$	0	1	$\sqrt{2}$
3	$-\sqrt{5}$	2	0	$-\sqrt{5}$	1	$\sqrt{2}$
1	$-\sqrt{5}$	0	2	$-\sqrt{5}$	3	$\sqrt{28}$
1	0	$-\sqrt{5}$	$\sqrt{5}$	−3	$\sqrt{2}$	$\sqrt{14}$
·	1	−1	3	$-\sqrt{2}$	1	$\sqrt{28}$

$v_q^5 =$

1	−1	1	$-\sqrt{2}$	1	−1	1
1	−5	$\sqrt{10}$	$-\sqrt{5}$	$\sqrt{5}$	−1	$\sqrt{2}$
1	$-\sqrt{10}$	10	$-\sqrt{20}$	$\sqrt{5}$	$-\sqrt{2}$	$\sqrt{9}$
$\sqrt{2}$	$-\sqrt{5}$	$\sqrt{20}$	−10	$\sqrt{10}$	−1	$\sqrt{12}$
1	$-\sqrt{5}$	$\sqrt{5}$	$-\sqrt{10}$	5	−1	$\sqrt{42}$
1	−1	$\sqrt{2}$	−1	1	−1	$\sqrt{252}$

Linear relations between the irreducible tensor operators v_q^k and the elementary unitary operators $E_{m,m+q}$ will be used in later chapters. A simple example of such a relation involves the $q = 0$ operators for ($j = 1$). From Eq. (7.3.12) [or the diagonals of Table 7.2(p)] one may write

$$v_0^2 = (E_{11} - 2E_{22} + E_{33})/\sqrt{6},$$
$$v_0^1 = (E_{11} - E_{33})/\sqrt{2},$$
$$v_0^0 = (E_{11} + E_{22} + E_{33})/\sqrt{3}. \qquad (7.3.16)$$

TABLE 7.2 (*l*) Subshell Tensors

(f) $l = 3$

	$q=0$	1	2	3	4	5	6	
-1	1	$-\sqrt{2}$	1	$-\sqrt{2}$	$\sqrt{5}$	-1	1	1
	$\sqrt{2}$	-6	$\sqrt{30}$	$-\sqrt{8}$	3	$-\sqrt{12}$	1	$\sqrt{2}$
	1	$-\sqrt{30}$	15	-10	$\sqrt{15}$	-3	$\sqrt{5}$	$\sqrt{22}$
$v_q^6 =$	$\sqrt{2}$	$-\sqrt{8}$	10	-20	10	$-\sqrt{8}$	$\sqrt{2}$	$\sqrt{22}$
	$\sqrt{5}$	-3	$\sqrt{15}$	-10	15	$-\sqrt{30}$	1	$\sqrt{33}$
	1	$-\sqrt{12}$	3	$-\sqrt{8}$	$\sqrt{30}$	-6	$\sqrt{2}$	$\sqrt{264}$
	1	-1	$\sqrt{5}$	$-\sqrt{2}$	1	$-\sqrt{2}$	1	$\sqrt{924}$
	1	$-\sqrt{5}$	1	$-\sqrt{2}$	1	-1	·	
	$\sqrt{5}$	-4	$\sqrt{27}$	$-\sqrt{2}$	1	0	-1	$\sqrt{2}$
	1	$-\sqrt{27}$	5	$-\sqrt{10}$	0	1	-1	$\sqrt{2}$
$v_q^5 =$	$\sqrt{2}$	$-\sqrt{2}$	$\sqrt{10}$	0	$-\sqrt{10}$	$\sqrt{2}$	$-\sqrt{2}$	$\sqrt{6}$
	1	-1	0	$\sqrt{10}$	-5	$\sqrt{27}$	-1	$\sqrt{6}$
	1	0	-1	$\sqrt{2}$	$-\sqrt{27}$	4	$-\sqrt{5}$	$\sqrt{84}$
	·	1	-1	$\sqrt{2}$	-1	$\sqrt{5}$	-1	$\sqrt{84}$
	3	$-\sqrt{30}$	$\sqrt{54}$	-3	$\sqrt{3}$	·	·	
	$\sqrt{30}$	-7	$\sqrt{32}$	$-\sqrt{3}$	$-\sqrt{2}$	$\sqrt{5}$	·	
	$\sqrt{54}$	$-\sqrt{32}$	1	$\sqrt{15}$	$-\sqrt{40}$	$\sqrt{2}$	$\sqrt{3}$	$\sqrt{11}$
$v_q^4 =$	3	$-\sqrt{3}$	$-\sqrt{15}$	6	$-\sqrt{15}$	$-\sqrt{3}$	3	$\sqrt{22}$
	$\sqrt{3}$	$\sqrt{2}$	$-\sqrt{40}$	$\sqrt{15}$	1	$-\sqrt{32}$	$\sqrt{54}$	$\sqrt{154}$
	·	$\sqrt{5}$	$-\sqrt{2}$	$-\sqrt{3}$	$\sqrt{32}$	-7	$\sqrt{30}$	$\sqrt{154}$
	·	·	$\sqrt{3}$	-3	$\sqrt{54}$	$-\sqrt{30}$	3	$\sqrt{154}$
	1	$-\sqrt{2}$	$\sqrt{2}$	-1	·	·	·	
	$\sqrt{2}$	-1	0	1	$-\sqrt{2}$	·	·	
	$\sqrt{2}$	0	-1	1	0	$-\sqrt{2}$	·	
$v_q^3 =$	1	1	-1	0	1	-1	-1	$\sqrt{6}$
	·	$\sqrt{2}$	0	-1	1	0	$-\sqrt{2}$	$\sqrt{6}$
	·	·	$\sqrt{2}$	-1	0	1	$-\sqrt{2}$	$\sqrt{6}$
	·	·	·	1	$-\sqrt{2}$	$\sqrt{2}$	-1	$\sqrt{6}$
	5	-5	$\sqrt{5}$	·	·	·	·	
	5	0	$-\sqrt{15}$	$\sqrt{10}$	·	·	·	
	$\sqrt{5}$	$\sqrt{15}$	-3	$-\sqrt{2}$	$\sqrt{12}$	·	·	
$v_q^2 =$	·	$\sqrt{10}$	$\sqrt{2}$	-4	$\sqrt{2}$	$\sqrt{10}$	·	
	·	·	$\sqrt{12}$	$-\sqrt{2}$	-3	$\sqrt{15}$	$\sqrt{5}$	$\sqrt{42}$
	·	·	·	$\sqrt{10}$	$-\sqrt{15}$	0	5	$\sqrt{84}$
	·	·	·	·	$\sqrt{5}$	-5	5	$\sqrt{84}$
	3	$-\sqrt{3}$	·	·	·	·	·	
	$\sqrt{3}$	2	$-\sqrt{5}$	·	·	·	·	
	·	$\sqrt{5}$	1	$-\sqrt{6}$	·	·	·	
$v_q^1 =$	·	·	$\sqrt{6}$	0	$-\sqrt{6}$	·	·	
	·	·	·	$\sqrt{6}$	-1	$-\sqrt{5}$	·	
	·	·	·	·	$\sqrt{5}$	-2	$-\sqrt{3}$	$\sqrt{28}$
	·	·	·	·	·	$\sqrt{3}$	-3	$\sqrt{28}$

(d) $l = 2$

$q=0$	1	2	3	4	
1	-1	$\sqrt{3}$	-1	1	1
1	-4	$\sqrt{6}$	$-\sqrt{8}$	1	$\sqrt{2}$
$\sqrt{3}$	$-\sqrt{6}$	6	$-\sqrt{6}$	$\sqrt{3}$	$\sqrt{14}$
1	$-\sqrt{8}$	$\sqrt{6}$	-4	1	$\sqrt{14}$
1	-1	$\sqrt{3}$	-1	1	$\sqrt{70}$
1	$-\sqrt{3}$	1	-1	·	
$\sqrt{3}$	-2	$\sqrt{2}$	0	-1	$\sqrt{2}$
1	$-\sqrt{2}$	0	$\sqrt{2}$	-1	$\sqrt{2}$
1	0	$-\sqrt{2}$	2	$-\sqrt{3}$	$\sqrt{10}$
·	1	-1	$\sqrt{3}$	-1	$\sqrt{10}$
2	$-\sqrt{6}$	$\sqrt{2}$	·	·	
$\sqrt{6}$	-1	-1	$\sqrt{3}$	·	
$\sqrt{2}$	1	-2	1	$\sqrt{2}$	$\sqrt{7}$
·	$\sqrt{3}$	-1	-1	$\sqrt{6}$	$\sqrt{14}$
·	·	$\sqrt{2}$	$-\sqrt{6}$	2	$\sqrt{14}$
2	$-\sqrt{2}$	·	·	·	
$\sqrt{2}$	1	$-\sqrt{3}$	·	·	
·	$\sqrt{3}$	0	$-\sqrt{3}$	·	
·	·	$\sqrt{3}$	-1	$-\sqrt{2}$	$\sqrt{10}$
·	·	·	$\sqrt{2}$	-2	$\sqrt{10}$

(p) $l = 1$

$q=0$	1	2	
1	-1	1	1
1	-2	1	$\sqrt{2}$
1	-1	+1	$\sqrt{6}$
1	-1	·	
1	0	-1	$\sqrt{2}$
·	1	-1	$\sqrt{2}$

TABLE 7.3 (g) $l = 4$

	$q=0$	1	2	3	4	5	6	7	8	
$V_q^8 =$	1	-1	1	-1	$\sqrt{5}$	-1	$\sqrt{7}$	-1	1	1
	1	-8	$\sqrt{28}$	-4	$\sqrt{10}$	$-\sqrt{32}$	2	-4	1	$\sqrt{2}$
	1	$-\sqrt{28}$	28	-14	$\sqrt{70}$	$-\sqrt{28}$	$\sqrt{56}$	-2	$\sqrt{7}$	$\sqrt{30}$
	1	-4	14	-56	$\sqrt{490}$	$-\sqrt{112}$	$\sqrt{28}$	$-\sqrt{32}$	1	$\sqrt{10}$
	$\sqrt{5}$	$-\sqrt{10}$	$\sqrt{70}$	$-\sqrt{490}$	70	$-\sqrt{490}$	$\sqrt{70}$	$-\sqrt{10}$	$\sqrt{5}$	$\sqrt{130}$
	1	$-\sqrt{32}$	$\sqrt{28}$	$-\sqrt{112}$	$\sqrt{490}$	-56	14	-4	1	$\sqrt{78}$
	$\sqrt{7}$	-2	$\sqrt{56}$	$-\sqrt{28}$	$\sqrt{70}$	-14	28	$-\sqrt{28}$	1	$\sqrt{286}$
	1	-4	2	$-\sqrt{32}$	$\sqrt{10}$	-4	$\sqrt{28}$	-8	1	$\sqrt{1430}$
	1	-1	$\sqrt{7}$	-1	$\sqrt{5}$	-1	1	-1	1	$\sqrt{12870}$
$V_q^7 =$	1	$-\sqrt{7}$	3	-5	$\sqrt{5}$	-3	1	-1	·	
	$\sqrt{7}$	-6	10	-8	$\sqrt{90}$	$-\sqrt{8}$	2	0	-1	$\sqrt{2}$
	3	-10	14	$-\sqrt{252}$	$\sqrt{70}$	$-\sqrt{28}$	0	2	-1	$\sqrt{2}$
	5	-8	$\sqrt{252}$	-14	$\sqrt{70}$	0	$-\sqrt{28}$	$\sqrt{8}$	-3	$\sqrt{26}$
	$\sqrt{5}$	$-\sqrt{90}$	$\sqrt{70}$	$-\sqrt{70}$	0	$\sqrt{70}$	$-\sqrt{70}$	$\sqrt{90}$	$-\sqrt{5}$	$\sqrt{26}$
	3	$-\sqrt{8}$	$\sqrt{28}$	0	$-\sqrt{70}$	14	$-\sqrt{252}$	8	-5	$\sqrt{286}$
	1	-2	0	$\sqrt{28}$	$-\sqrt{70}$	$\sqrt{252}$	-14	10	-3	$\sqrt{286}$
	1	0	-2	$\sqrt{8}$	$-\sqrt{90}$	8	-10	6	$-\sqrt{7}$	$\sqrt{858}$
	·	1	-1	3	$-\sqrt{5}$	5	-3	$\sqrt{7}$	-1	$\sqrt{858}$
$V_q^6 =$	4	$-\sqrt{28}$	2	-4	$\sqrt{40}$	-2	2	·	·	
	$\sqrt{28}$	-17	13	-3	$\sqrt{10}$	-1	-1	$\sqrt{7}$	·	
	2	-13	22	$-\sqrt{63}$	0	$\sqrt{7}$	$-\sqrt{28}$	1	2	$\sqrt{15}$
	4	-3	$\sqrt{63}$	1	$-\sqrt{70}$	$\sqrt{7}$	$-\sqrt{7}$	-1	2	$\sqrt{10}$
	$\sqrt{40}$	$-\sqrt{10}$	0	$\sqrt{70}$	-20	$\sqrt{70}$	0	$-\sqrt{10}$	$\sqrt{40}$	$\sqrt{110}$
	2	-1	$-\sqrt{7}$	$\sqrt{7}$	$-\sqrt{70}$	1	$\sqrt{63}$	-3	4	$\sqrt{66}$
	2	1	$-\sqrt{28}$	$\sqrt{7}$	0	$-\sqrt{63}$	22	-13	2	$\sqrt{33}$
	·	$\sqrt{7}$	-1	-1	$\sqrt{10}$	-3	13	-17	$\sqrt{28}$	$\sqrt{660}$
	·	·	2	-2	$\sqrt{40}$	-4	2	$-\sqrt{28}$	4	$\sqrt{1980}$
$V_q^5 =$	4	$-\sqrt{20}$	$\sqrt{20}$	$-\sqrt{80}$	$\sqrt{8}$	-2	·	·	·	
	$\sqrt{20}$	-11	$\sqrt{35}$	$-\sqrt{5}$	$-\sqrt{2}$	$\sqrt{5}$	-3	·	·	
	$\sqrt{20}$	$-\sqrt{35}$	4	$\sqrt{5}$	$-\sqrt{14}$	$\sqrt{35}$	0	-3	·	
	$\sqrt{80}$	$-\sqrt{5}$	$-\sqrt{5}$	9	$-\sqrt{18}$	0	$\sqrt{35}$	$-\sqrt{5}$	-2	$\sqrt{26}$
	$\sqrt{8}$	$\sqrt{2}$	$-\sqrt{14}$	$\sqrt{18}$	0	$-\sqrt{18}$	$\sqrt{14}$	$-\sqrt{2}$	$-\sqrt{8}$	$\sqrt{26}$
	2	$\sqrt{5}$	$-\sqrt{35}$	0	$\sqrt{18}$	-9	$\sqrt{5}$	$\sqrt{5}$	$-\sqrt{80}$	$\sqrt{234}$
	·	3	0	$-\sqrt{35}$	$\sqrt{14}$	$-\sqrt{5}$	-4	$\sqrt{35}$	$-\sqrt{20}$	$\sqrt{78}$
	·	·	3	$-\sqrt{5}$	$\sqrt{2}$	$\sqrt{5}$	$-\sqrt{35}$	11	$-\sqrt{20}$	$\sqrt{156}$
	·	·	·	2	$-\sqrt{8}$	$\sqrt{80}$	$-\sqrt{20}$	$\sqrt{20}$	-4	$\sqrt{468}$

$q = 0 \quad 1 \quad 2 \quad 3 \quad 4 \quad 5 \quad 6 \quad 7 \quad 8$

$$V_q^4 = \left|\begin{array}{ccccccccc}
14 & -\sqrt{490} & \sqrt{630} & -\sqrt{70} & \sqrt{14} & \cdot & \cdot & \cdot & \cdot \\
\sqrt{490} & -21 & \sqrt{70} & \sqrt{70} & -\sqrt{63} & \sqrt{35} & \cdot & \cdot & \cdot \\
\sqrt{630} & -\sqrt{70} & -11 & \sqrt{360} & -11 & -\sqrt{10} & \sqrt{45} & \cdot & \cdot \\
\sqrt{70} & \sqrt{70} & -\sqrt{360} & 9 & 9 & -\sqrt{360} & \sqrt{10} & \sqrt{35} & \cdot \\
\sqrt{14} & \sqrt{63} & -11 & -9 & 18 & -9 & -11 & \sqrt{63} & \sqrt{14} \\
\cdot & \sqrt{35} & \sqrt{10} & -\sqrt{360} & 9 & 9 & -\sqrt{360} & \sqrt{70} & \sqrt{70} \\
\cdot & \cdot & \sqrt{45} & -\sqrt{10} & -11 & \sqrt{360} & -11 & -\sqrt{70} & \sqrt{630} \\
\cdot & \cdot & \cdot & \sqrt{35} & -\sqrt{63} & \sqrt{70} & \sqrt{70} & -21 & \sqrt{490} \\
\cdot & \cdot & \cdot & \cdot & \sqrt{14} & -\sqrt{70} & \sqrt{630} & -\sqrt{490} & 14
\end{array}\right|$$

$\sqrt{143}$, $\sqrt{286}$, $\sqrt{2002}$, $\sqrt{2002}$, $\sqrt{2002}$

$$V_q^3 = \left|\begin{array}{ccccccccc}
14 & -\sqrt{98} & \sqrt{14} & -\sqrt{14} & \cdot & \cdot & \cdot & \cdot & \cdot \\
\sqrt{98} & -7 & -\sqrt{14} & \sqrt{14} & -\sqrt{35} & \cdot & \cdot & \cdot & \cdot \\
\sqrt{14} & \sqrt{14} & -13 & \sqrt{8} & \sqrt{5} & -\sqrt{50} & \cdot & \cdot & \cdot \\
\sqrt{14} & \sqrt{14} & -\sqrt{8} & -9 & \sqrt{45} & 0 & -\sqrt{50} & \cdot & \cdot \\
\cdot & \sqrt{35} & \sqrt{5} & -\sqrt{45} & 0 & \sqrt{45} & -\sqrt{5} & -\sqrt{35} & \cdot \\
\cdot & \cdot & \sqrt{50} & 0 & -\sqrt{45} & 9 & \sqrt{8} & -\sqrt{14} & -\sqrt{14} \\
\cdot & \cdot & \cdot & \sqrt{50} & -\sqrt{5} & -\sqrt{8} & 13 & -\sqrt{14} & -\sqrt{14} \\
\cdot & \cdot & \cdot & \cdot & \sqrt{35} & -\sqrt{14} & \sqrt{14} & 7 & -\sqrt{98} \\
\cdot & \cdot & \cdot & \cdot & \cdot & \sqrt{14} & -\sqrt{14} & \sqrt{98} & -14
\end{array}\right|$$

$\sqrt{198}$, $\sqrt{66}$, $\sqrt{330}$, $\sqrt{990}$

$$V_q^2 = \left|\begin{array}{ccccccccc}
28 & -14 & \sqrt{28} & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
14 & 7 & -\sqrt{175} & \sqrt{63} & \cdot & \cdot & \cdot & \cdot & \cdot \\
\sqrt{28} & \sqrt{175} & -8 & -9 & \sqrt{90} & \cdot & \cdot & \cdot & \cdot \\
\cdot & \sqrt{63} & 9 & -17 & -\sqrt{10} & 10 & \cdot & \cdot & \cdot \\
\cdot & \cdot & \sqrt{90} & \sqrt{10} & -20 & \sqrt{10} & \sqrt{90} & \cdot & \cdot \\
\cdot & \cdot & \cdot & 10 & -\sqrt{10} & -17 & 9 & \sqrt{63} & \cdot \\
\cdot & \cdot & \cdot & \cdot & \sqrt{90} & -9 & -8 & \sqrt{175} & \sqrt{28} \\
\cdot & \cdot & \cdot & \cdot & \cdot & \sqrt{63} & -\sqrt{175} & 7 & 14 \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \sqrt{28} & -14 & 28
\end{array}\right|$$

$\sqrt{462}$, $\sqrt{924}$, $\sqrt{2772}$

$$V_q^1 = \left|\begin{array}{ccccccccc}
4 & -2 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
2 & 3 & -\sqrt{7} & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & \sqrt{7} & 2 & -3 & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & 3 & 1 & -\sqrt{10} & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \sqrt{10} & 0 & -\sqrt{10} & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \sqrt{10} & -1 & -3 & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & 3 & -2 & -\sqrt{7} & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \sqrt{7} & -3 & -2 \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & 2 & -4
\end{array}\right|$$

$\sqrt{60}$, $\sqrt{60}$

TABLE 7.4 Mixed Subshell Tensonrs

(*f*) (*d*)

q = 1	2	3	4	5	
q = 0					
	1	−1	$\sqrt{2}$	$-\sqrt{2}$	1	
	1	$-\sqrt{24}$	3	$-\sqrt{8}$	$\sqrt{3}$	1
	$\sqrt{15}$	$-\sqrt{10}$	$\sqrt{90}$	$-\sqrt{15}$	$\sqrt{5}$	$\sqrt{5}$
$V_q^5 =$	$\sqrt{5}$	$-\sqrt{80}$	$\sqrt{20}$	$-\sqrt{80}$	$\sqrt{5}$	$\sqrt{15}$
	$\sqrt{5}$	$-\sqrt{15}$	$\sqrt{90}$	$-\sqrt{10}$	$\sqrt{15}$	$\sqrt{30}$
	$\sqrt{3}$	$-\sqrt{8}$	3	$-\sqrt{24}$	1	$\sqrt{210}$
	1	$-\sqrt{2}$	$\sqrt{2}$	−1	1	$\sqrt{42}$
	$\sqrt{6}$	$-\sqrt{27}$	3	$-\sqrt{3}$	·	
	$\sqrt{2}$	−7	$\sqrt{48}$	−1	$-\sqrt{2}$	
	$\sqrt{40}$	$-\sqrt{5}$	$\sqrt{15}$	$\sqrt{5}$	$-\sqrt{10}$	$\sqrt{5}$
$V_q^4 =$	$\sqrt{60}$	$-\sqrt{30}$	0	$\sqrt{30}$	$-\sqrt{60}$	$\sqrt{20}$
	$\sqrt{10}$	$-\sqrt{5}$	$-\sqrt{15}$	$\sqrt{5}$	$-\sqrt{40}$	$\sqrt{140}$
	$\sqrt{2}$	1	$-\sqrt{48}$	7	$-\sqrt{2}$	$\sqrt{140}$
	·	$\sqrt{3}$	−3	$\sqrt{27}$	$-\sqrt{6}$	$\sqrt{14}$
	$\sqrt{10}$	$-\sqrt{5}$	$\sqrt{5}$	·	·	
	$\sqrt{10}$	$-\sqrt{15}$	0	$\sqrt{5}$	·	
	$\sqrt{24}$	−1	−3	$\sqrt{3}$	$\sqrt{2}$	
$V_q^3 =$	2	$\sqrt{2}$	$-\sqrt{8}$	$\sqrt{2}$	2	$\sqrt{12}$
	$\sqrt{2}$	$\sqrt{3}$	−3	−1	$\sqrt{24}$	$\sqrt{12}$
	·	$\sqrt{5}$	0	$-\sqrt{15}$	$\sqrt{10}$	$\sqrt{60}$
	·	·	$\sqrt{5}$	$-\sqrt{5}$	$\sqrt{10}$	$\sqrt{30}$
	$\sqrt{5}$	$-\sqrt{5}$	·	·	·	
	$\sqrt{5}$	0	$-\sqrt{5}$	·	·	
	$\sqrt{3}$	$\sqrt{2}$	$-\sqrt{2}$	$-\sqrt{3}$	·	
$V_q^2 =$	1	2	0	−2	−1	
	·	$\sqrt{3}$	$\sqrt{2}$	$-\sqrt{2}$	$-\sqrt{3}$	$\sqrt{14}$
	·	·	$\sqrt{5}$	0	$-\sqrt{5}$	$\sqrt{14}$
	·	·	·	$\sqrt{5}$	$-\sqrt{5}$	$\sqrt{14}$
	$\sqrt{15}$	·	·	·	·	
	$\sqrt{5}$	$\sqrt{10}$	·	·	·	
	1	$\sqrt{8}$	$\sqrt{6}$	·	·	
$V_q^1 =$	·	$\sqrt{3}$	3	$\sqrt{3}$	·	
	·	·	$\sqrt{6}$	$\sqrt{8}$	1	
	·	·	·	$\sqrt{10}$	$\sqrt{5}$	$\sqrt{35}$
	·	·	·	·	$\sqrt{15}$	$\sqrt{35}$

(*f*) (*p*)

q = 2	3	4	
q = 1			
q = 0			
1	−1	1	
$\sqrt{3}$	$-\sqrt{12}$	$\sqrt{3}$	1
$\sqrt{3}$	$-\sqrt{15}$	$\sqrt{15}$	2
$\sqrt{10}$	$-\sqrt{8}$	$\sqrt{10}$	$\sqrt{28}$
$\sqrt{15}$	$-\sqrt{15}$	$\sqrt{3}$	$\sqrt{28}$
$\sqrt{3}$	$-\sqrt{12}$	$\sqrt{3}$	$\sqrt{14}$
1	−1	1	
$\sqrt{3}$	$-\sqrt{3}$	·	
$\sqrt{5}$	−2	−1	
1	−1	$-\sqrt{5}$	2
$\sqrt{6}$	0	$-\sqrt{6}$	$\sqrt{12}$
$\sqrt{5}$	1	−1	$\sqrt{12}$
1	2	$-\sqrt{5}$	$\sqrt{2}$
·	$\sqrt{3}$	$-\sqrt{3}$	
$\sqrt{15}$	·	·	
$\sqrt{10}$	$\sqrt{5}$	·	
$\sqrt{2}$	$\sqrt{8}$	1	
$\sqrt{3}$	$\sqrt{3}$	$\sqrt{3}$	$\sqrt{21}$
1	$\sqrt{8}$	$\sqrt{2}$	$\sqrt{21}$
·	$\sqrt{5}$	$\sqrt{10}$	$\sqrt{7}$
·	·	$\sqrt{15}$	

(*d*) (*p*)

q = 1	2	3	
q = 0			
1	−1	1	
1	$-\sqrt{8}$	$\sqrt{2}$	1
$\sqrt{6}$	$-\sqrt{3}$	$\sqrt{6}$	$\sqrt{3}$
$\sqrt{2}$	$-\sqrt{8}$	1	$\sqrt{15}$
1	−1	1	$\sqrt{5}$
$\sqrt{2}$	$-\sqrt{2}$	·	
1	−1	−1	
$\sqrt{3}$	0	$-\sqrt{3}$	$\sqrt{3}$
1	1	−1	$\sqrt{6}$
·	$\sqrt{2}$	$-\sqrt{2}$	$\sqrt{2}$
$\sqrt{6}$	·	·	
$\sqrt{3}$	$\sqrt{3}$	·	
1	2	1	
·	$\sqrt{3}$	$\sqrt{3}$	$\sqrt{10}$
·	·	$\sqrt{6}$	$\sqrt{10}$

The numbering for E_{ij} reflects the choice of numbers 1 to 5 for d states ($|1\rangle = |^2_2\rangle, |2\rangle = |^2_1\rangle, \ldots, |5\rangle = |^{\,2}_{-2}\rangle$) and 6 to 8 for the p states ($|6\rangle = |^1_1\rangle, |7\rangle = |^1_0\rangle, |8\rangle = |^{\,1}_{-1}\rangle$. The tables exhibit the $v_q^k(l_1 l_2)$ matrices for $l_1 - l_2 \equiv \Delta > 0$, and the transpose is found using the symmetry relation

$$v_q^k(l_2 l_1) = (-1)^{l+q}\tilde{v}^k_{-q}(l_1 l_2). \qquad (7.3.19)$$