

PG No. 15  $D_{4h}$  4/mmm [ tetragonal ] (polar, internal polar dipole)

\* Harmonics for rank 0

$$\vec{\mathbb{Q}}_0^{(1,1)}[q](A_{1g})$$

\*\* symmetry

1

\*\* expression

$$\frac{\sqrt{3}Q_x x}{3} + \frac{\sqrt{3}Q_y y}{3} + \frac{\sqrt{3}Q_z z}{3}$$

\* Harmonics for rank 1

$$\vec{\mathbb{Q}}_1^{(1,-1)}[q](A_{2u})$$

\*\* symmetry

$z$

\*\* expression

$Q_z$

$$\vec{\mathbb{Q}}_1^{(1,1)}[q](A_{2u})$$

\*\* symmetry

$z$

\*\* expression

$$\frac{3\sqrt{10}Q_x x z}{10} + \frac{3\sqrt{10}Q_y y z}{10} - \frac{\sqrt{10}Q_z (x^2 + y^2 - 2z^2)}{10}$$

$$\vec{\mathbb{Q}}_{1,1}^{(1,-1)}[q](E_u), \vec{\mathbb{Q}}_{1,2}^{(1,-1)}[q](E_u)$$

\*\* symmetry

$x$

$y$

\*\* expression

$Q_x$

$Q_y$

$$\vec{\mathbb{Q}}_{1,1}^{(1,1)}[q](E_u), \vec{\mathbb{Q}}_{1,2}^{(1,1)}[q](E_u)$$

\*\* symmetry

$x$

$y$

\*\* expression

$$\frac{\sqrt{10}Q_x (2x^2 - y^2 - z^2)}{10} + \frac{3\sqrt{10}Q_y x y}{10} + \frac{3\sqrt{10}Q_z x z}{10}$$

$$\frac{3\sqrt{10}Q_x x y}{10} - \frac{\sqrt{10}Q_y (x^2 - 2y^2 + z^2)}{10} + \frac{3\sqrt{10}Q_z y z}{10}$$

\* Harmonics for rank 2

$$\vec{\mathbb{Q}}_2^{(1,-1)}[q](A_{1g})$$

\*\* symmetry

$$-\frac{x^2}{2} - \frac{y^2}{2} + z^2$$

\*\* expression

$$-\frac{\sqrt{6}Q_x x}{6} - \frac{\sqrt{6}Q_y y}{6} + \frac{\sqrt{6}Q_z z}{3}$$

$$\vec{\mathbb{Q}}_2^{(1,1)}[q](A_{1g})$$

\*\* symmetry

$$-\frac{x^2}{2} - \frac{y^2}{2} + z^2$$

\*\* expression

$$-\frac{\sqrt{21}Q_xx(x^2+y^2-4z^2)}{14}-\frac{\sqrt{21}Q_yy(x^2+y^2-4z^2)}{14}-\frac{\sqrt{21}Q_zz(3x^2+3y^2-2z^2)}{14}$$

$\tilde{\mathbb{Q}}_2^{(1,-1)}[q](B_{1g})$

\*\* symmetry

$$\frac{\sqrt{3}(x-y)(x+y)}{2}$$

\*\* expression

$$\frac{\sqrt{2}Q_xx}{2}-\frac{\sqrt{2}Q_yy}{2}$$

$\tilde{\mathbb{Q}}_2^{(1,1)}[q](B_{1g})$

\*\* symmetry

$$\frac{\sqrt{3}(x-y)(x+y)}{2}$$

\*\* expression

$$\frac{\sqrt{7}Q_xx(3x^2-7y^2-2z^2)}{14}+\frac{\sqrt{7}Q_yy(7x^2-3y^2+2z^2)}{14}+\frac{5\sqrt{7}Q_zz(x-y)(x+y)}{14}$$

$\tilde{\mathbb{Q}}_2^{(1,-1)}[q](B_{2g})$

\*\* symmetry

$$\sqrt{3}xy$$

\*\* expression

$$\frac{\sqrt{2}Q_xy}{2}+\frac{\sqrt{2}Q_yx}{2}$$

$\tilde{\mathbb{Q}}_2^{(1,1)}[q](B_{2g})$

\*\* symmetry

$$\sqrt{3}xy$$

\*\* expression

$$\frac{\sqrt{7}Q_xy(4x^2-y^2-z^2)}{7}-\frac{\sqrt{7}Q_yx(x^2-4y^2+z^2)}{7}+\frac{5\sqrt{7}Q_zxyz}{7}$$

$\tilde{\mathbb{Q}}_{2,1}^{(1,-1)}[q](E_g), \tilde{\mathbb{Q}}_{2,2}^{(1,-1)}[q](E_g)$

\*\* symmetry

$$\sqrt{3}yz$$

$$\sqrt{3}xz$$

\*\* expression

$$\frac{\sqrt{2}Q_yz}{2}+\frac{\sqrt{2}Q_zy}{2}$$

$$\frac{\sqrt{2}Q_xz}{2}+\frac{\sqrt{2}Q_zx}{2}$$

$\tilde{\mathbb{Q}}_{2,1}^{(1,1)}[q](E_g), \tilde{\mathbb{Q}}_{2,2}^{(1,1)}[q](E_g)$

\*\* symmetry

$$\sqrt{3}yz$$

$$\sqrt{3}xz$$

\*\* expression

$$\frac{5\sqrt{7}Q_xxyz}{7}-\frac{\sqrt{7}Q_yz(x^2-4y^2+z^2)}{7}-\frac{\sqrt{7}Q_zy(x^2+y^2-4z^2)}{7}$$

$$\frac{\sqrt{7}Q_xz(4x^2-y^2-z^2)}{7}+\frac{5\sqrt{7}Q_yxyz}{7}-\frac{\sqrt{7}Q_zx(x^2+y^2-4z^2)}{7}$$

\* Harmonics for rank 3

$\vec{\mathbb{Q}}_3^{(1,-1)}[q](A_{2u})$

\*\* symmetry

$$-\frac{z(3x^2 + 3y^2 - 2z^2)}{2}$$

\*\* expression

$$-\frac{\sqrt{15}Q_xxz}{5} - \frac{\sqrt{15}Q_yyz}{5} - \frac{\sqrt{15}Q_z(x^2 + y^2 - 2z^2)}{10}$$

$\vec{\mathbb{Q}}_3^{(1,1)}[q](A_{2u})$

\*\* symmetry

$$-\frac{z(3x^2 + 3y^2 - 2z^2)}{2}$$

\*\* expression

$$-\frac{5Q_xxz(3x^2 + 3y^2 - 4z^2)}{12} - \frac{5Q_yyz(3x^2 + 3y^2 - 4z^2)}{12} + \frac{Q_z(3x^4 + 6x^2y^2 - 24x^2z^2 + 3y^4 - 24y^2z^2 + 8z^4)}{12}$$

$\vec{\mathbb{Q}}_3^{(1,-1)}[q](B_{1u})$

\*\* symmetry

$$\sqrt{15}xyz$$

\*\* expression

$$Q_xyz + Q_yxz + Q_zxy$$

$\vec{\mathbb{Q}}_3^{(1,1)}[q](B_{1u})$

\*\* symmetry

$$\sqrt{15}xyz$$

\*\* expression

$$\frac{\sqrt{15}Q_xyz(6x^2 - y^2 - z^2)}{6} - \frac{\sqrt{15}Q_yxz(x^2 - 6y^2 + z^2)}{6} - \frac{\sqrt{15}Q_zxy(x^2 + y^2 - 6z^2)}{6}$$

$\vec{\mathbb{Q}}_3^{(1,-1)}[q](B_{2u})$

\*\* symmetry

$$\frac{\sqrt{15}z(x - y)(x + y)}{2}$$

\*\* expression

$$Q_xxz - Q_yyz + \frac{Q_z(x - y)(x + y)}{2}$$

$\vec{\mathbb{Q}}_3^{(1,1)}[q](B_{2u})$

\*\* symmetry

$$\frac{\sqrt{15}z(x - y)(x + y)}{2}$$

\*\* expression

$$\frac{\sqrt{15}Q_xxz(5x^2 - 9y^2 - 2z^2)}{12} + \frac{\sqrt{15}Q_yyz(9x^2 - 5y^2 + 2z^2)}{12} - \frac{\sqrt{15}Q_z(x - y)(x + y)(x^2 + y^2 - 6z^2)}{12}$$

$\vec{\mathbb{Q}}_{3,1}^{(1,-1)}[q](E_u, 1), \vec{\mathbb{Q}}_{3,2}^{(1,-1)}[q](E_u, 1)$

\*\* symmetry

$$\frac{x(2x^2 - 3y^2 - 3z^2)}{2}$$

$$-\frac{y(3x^2 - 2y^2 + 3z^2)}{2}$$

\*\* expression

$$\frac{\sqrt{15}Q_x(2x^2 - y^2 - z^2)}{10} - \frac{\sqrt{15}Q_yxy}{5} - \frac{\sqrt{15}Q_zxz}{5}$$

$$-\frac{\sqrt{15}Q_xxy}{5} - \frac{\sqrt{15}Q_y(x^2 - 2y^2 + z^2)}{10} - \frac{\sqrt{15}Q_zyz}{5}$$

$\tilde{\mathbb{Q}}_{3,1}^{(1,-1)}[q](E_u, 2), \tilde{\mathbb{Q}}_{3,2}^{(1,-1)}[q](E_u, 2)$   
\*\* symmetry

$$\frac{\sqrt{15}x(y-z)(y+z)}{2}$$

$$\frac{\sqrt{15}y(x-z)(x+z)}{2}$$

\*\* expression

$$\frac{Q_x(y-z)(y+z)}{2} + Q_yxy - Q_zxz$$

$$Q_xxy + \frac{Q_y(x-z)(x+z)}{2} - Q_zyz$$

$\tilde{\mathbb{Q}}_{3,1}^{(1,1)}[q](E_u, 1), \tilde{\mathbb{Q}}_{3,2}^{(1,1)}[q](E_u, 1)$

\*\* symmetry

$$\frac{x(2x^2 - 3y^2 - 3z^2)}{2}$$

$$-\frac{y(3x^2 - 2y^2 + 3z^2)}{2}$$

\*\* expression

$$\begin{aligned} & \frac{Q_x(8x^4 - 24x^2y^2 - 24x^2z^2 + 3y^4 + 6y^2z^2 + 3z^4)}{12} + \frac{5Q_yxy(4x^2 - 3y^2 - 3z^2)}{12} + \frac{5Q_zxz(4x^2 - 3y^2 - 3z^2)}{12} \\ & - \frac{5Q_xxy(3x^2 - 4y^2 + 3z^2)}{12} + \frac{Q_y(3x^4 - 24x^2y^2 + 6x^2z^2 + 8y^4 - 24y^2z^2 + 3z^4)}{12} - \frac{5Q_zyz(3x^2 - 4y^2 + 3z^2)}{12} \end{aligned}$$

$\tilde{\mathbb{Q}}_{3,1}^{(1,1)}[q](E_u, 2), \tilde{\mathbb{Q}}_{3,2}^{(1,1)}[q](E_u, 2)$

\*\* symmetry

$$\frac{\sqrt{15}x(y-z)(y+z)}{2}$$

$$\frac{\sqrt{15}y(x-z)(x+z)}{2}$$

\*\* expression

$$\begin{aligned} & \frac{\sqrt{15}Q_x(y-z)(y+z)(6x^2 - y^2 - z^2)}{12} - \frac{\sqrt{15}Q_yxy(2x^2 - 5y^2 + 9z^2)}{12} + \frac{\sqrt{15}Q_zxz(2x^2 + 9y^2 - 5z^2)}{12} \\ & - \frac{\sqrt{15}Q_xxy(5x^2 - 2y^2 - 9z^2)}{12} - \frac{\sqrt{15}Q_y(x-z)(x+z)(x^2 - 6y^2 + z^2)}{12} + \frac{\sqrt{15}Q_zyz(9x^2 + 2y^2 - 5z^2)}{12} \end{aligned}$$

\* Harmonics for rank 4

$\tilde{\mathbb{Q}}_4^{(1,-1)}[q](A_{1g}, 1)$

\*\* symmetry

$$\frac{\sqrt{21}(x^4 - 3x^2y^2 - 3x^2z^2 + y^4 - 3y^2z^2 + z^4)}{6}$$

\*\* expression

$$\frac{\sqrt{3}Q_xx(2x^2 - 3y^2 - 3z^2)}{6} - \frac{\sqrt{3}Q_yy(3x^2 - 2y^2 + 3z^2)}{6} - \frac{\sqrt{3}Q_zz(3x^2 + 3y^2 - 2z^2)}{6}$$

$\tilde{\mathbb{Q}}_4^{(1,-1)}[q](A_{1g}, 2)$

\*\* symmetry

$$-\frac{\sqrt{15}(x^4 - 12x^2y^2 + 6x^2z^2 + y^4 + 6y^2z^2 - 2z^4)}{12}$$

\*\* expression

$$-\frac{\sqrt{105}Q_xx(x^2 - 6y^2 + 3z^2)}{42} + \frac{\sqrt{105}Q_yy(6x^2 - y^2 - 3z^2)}{42} - \frac{\sqrt{105}Q_zz(3x^2 + 3y^2 - 2z^2)}{42}$$

$\tilde{\mathbb{Q}}_4^{(1,1)}[q](A_{1g}, 1)$

\*\* symmetry

$$\frac{\sqrt{21} (x^4 - 3x^2y^2 - 3x^2z^2 + y^4 - 3y^2z^2 + z^4)}{6}$$

\*\* expression

$$\begin{aligned} & \frac{\sqrt{1155}Q_x x (x^4 - 5x^2y^2 - 5x^2z^2 + 3y^4 - 3y^2z^2 + 3z^4)}{66} + \frac{\sqrt{1155}Q_y y (3x^4 - 5x^2y^2 - 3x^2z^2 + y^4 - 5y^2z^2 + 3z^4)}{66} \\ & + \frac{\sqrt{1155}Q_z z (3x^4 - 3x^2y^2 - 5x^2z^2 + 3y^4 - 5y^2z^2 + z^4)}{66} \end{aligned}$$

$\vec{\mathbb{Q}}_4^{(1,1)}[q](A_{1g}, 2)$

\*\* symmetry

$$-\frac{\sqrt{15} (x^4 - 12x^2y^2 + 6x^2z^2 + y^4 + 6y^2z^2 - 2z^4)}{12}$$

\*\* expression

$$\begin{aligned} & -\frac{\sqrt{33}Q_x x (5x^4 - 88x^2y^2 + 38x^2z^2 + 33y^4 + 66y^2z^2 - 30z^4)}{132} - \frac{\sqrt{33}Q_y y (33x^4 - 88x^2y^2 + 66x^2z^2 + 5y^4 + 38y^2z^2 - 30z^4)}{132} \\ & + \frac{\sqrt{33}Q_z z (3x^4 + 132x^2y^2 - 50x^2z^2 + 3y^4 - 50y^2z^2 + 10z^4)}{132} \end{aligned}$$

$\vec{\mathbb{Q}}_4^{(1,-1)}[q](A_{2g})$

\*\* symmetry

$$\frac{\sqrt{35}xy(x-y)(x+y)}{2}$$

\*\* expression

$$\frac{\sqrt{5}Q_x y (3x^2 - y^2)}{4} + \frac{\sqrt{5}Q_y x (x^2 - 3y^2)}{4}$$

$\vec{\mathbb{Q}}_4^{(1,1)}[q](A_{2g})$

\*\* symmetry

$$\frac{\sqrt{35}xy(x-y)(x+y)}{2}$$

\*\* expression

$$\frac{\sqrt{77}Q_x y (6x^4 - 11x^2y^2 - 3x^2z^2 + y^4 + y^2z^2)}{22} - \frac{\sqrt{77}Q_y x (x^4 - 11x^2y^2 + x^2z^2 + 6y^4 - 3y^2z^2)}{22} + \frac{9\sqrt{77}Q_z xyz(x-y)(x+y)}{22}$$

$\vec{\mathbb{Q}}_4^{(1,-1)}[q](B_{1g})$

\*\* symmetry

$$\frac{\sqrt{5}(x-y)(x+y)(x^2 + y^2 - 6z^2)}{4}$$

\*\* expression

$$\frac{\sqrt{35}Q_x x (x^2 - 3z^2)}{14} - \frac{\sqrt{35}Q_y y (y^2 - 3z^2)}{14} - \frac{3\sqrt{35}Q_z z (x-y)(x+y)}{14}$$

$\vec{\mathbb{Q}}_4^{(1,1)}[q](B_{1g})$

\*\* symmetry

$$\frac{\sqrt{5}(x-y)(x+y)(x^2 + y^2 - 6z^2)}{4}$$

\*\* expression

$$\begin{aligned} & \frac{\sqrt{11}Q_x x (5x^4 - 4x^2y^2 - 46x^2z^2 - 9y^4 + 66y^2z^2 + 12z^4)}{44} \\ & + \frac{\sqrt{11}Q_y y (9x^4 + 4x^2y^2 - 66x^2z^2 - 5y^4 + 46y^2z^2 - 12z^4)}{44} + \frac{21\sqrt{11}Q_z z (x-y)(x+y)(x^2 + y^2 - 2z^2)}{44} \end{aligned}$$

$\vec{\mathbb{Q}}_4^{(1,-1)}[q](B_{2g})$

\*\* symmetry

$$-\frac{\sqrt{5}xy(x^2 + y^2 - 6z^2)}{2}$$

\*\* expression

$$-\frac{\sqrt{35}Q_x y (3x^2 + y^2 - 6z^2)}{28} - \frac{\sqrt{35}Q_y x (x^2 + 3y^2 - 6z^2)}{28} + \frac{3\sqrt{35}Q_z xyz}{7}$$

$$\vec{\mathbb{Q}}_4^{(1,1)}[q](B_{2g})$$

\*\* symmetry

$$-\frac{\sqrt{5}xy(x^2 + y^2 - 6z^2)}{2}$$

\*\* expression

$$-\frac{\sqrt{11}Q_xy(6x^4 + 5x^2y^2 - 51x^2z^2 - y^4 + 5y^2z^2 + 6z^4)}{22} + \frac{\sqrt{11}Q_yx(x^4 - 5x^2y^2 - 5x^2z^2 - 6y^4 + 51y^2z^2 - 6z^4)}{22} - \frac{21\sqrt{11}Q_zxyz(x^2 + y^2 - 2z^2)}{22}$$

$$\vec{\mathbb{Q}}_{4,1}^{(1,-1)}[q](E_g, 1), \vec{\mathbb{Q}}_{4,2}^{(1,-1)}[q](E_g, 1)$$

\*\* symmetry

$$\frac{\sqrt{35}yz(y - z)(y + z)}{2}$$

$$\frac{\sqrt{35}xz(x - z)(x + z)}{2}$$

\*\* expression

$$\frac{\sqrt{5}Q_yz(3y^2 - z^2)}{4} + \frac{\sqrt{5}Q_zy(y^2 - 3z^2)}{4}$$

$$\frac{\sqrt{5}Q_xz(3x^2 - z^2)}{4} + \frac{\sqrt{5}Q_zx(x^2 - 3z^2)}{4}$$

$$\vec{\mathbb{Q}}_{4,1}^{(1,-1)}[q](E_g, 2), \vec{\mathbb{Q}}_{4,2}^{(1,-1)}[q](E_g, 2)$$

\*\* symmetry

$$\frac{\sqrt{5}yz(6x^2 - y^2 - z^2)}{2}$$

$$-\frac{\sqrt{5}xz(x^2 - 6y^2 + z^2)}{2}$$

\*\* expression

$$\frac{3\sqrt{35}Q_xxyz}{7} + \frac{\sqrt{35}Q_yz(6x^2 - 3y^2 - z^2)}{28} + \frac{\sqrt{35}Q_zy(6x^2 - y^2 - 3z^2)}{28}$$

$$-\frac{\sqrt{35}Q_xz(3x^2 - 6y^2 + z^2)}{28} + \frac{3\sqrt{35}Q_yxyz}{7} - \frac{\sqrt{35}Q_zx(x^2 - 6y^2 + 3z^2)}{28}$$

$$\vec{\mathbb{Q}}_{4,1}^{(1,1)}[q](E_g, 1), \vec{\mathbb{Q}}_{4,2}^{(1,1)}[q](E_g, 1)$$

\*\* symmetry

$$\frac{\sqrt{35}yz(y - z)(y + z)}{2}$$

$$\frac{\sqrt{35}xz(x - z)(x + z)}{2}$$

\*\* expression

$$\frac{9\sqrt{77}Q_xxyz(y - z)(y + z)}{22} - \frac{\sqrt{77}Q_yz(3x^2y^2 - x^2z^2 - 6y^4 + 11y^2z^2 - z^4)}{22} - \frac{\sqrt{77}Q_zy(x^2y^2 - 3x^2z^2 + y^4 - 11y^2z^2 + 6z^4)}{22}$$

$$\frac{\sqrt{77}Q_xz(6x^4 - 3x^2y^2 - 11x^2z^2 + y^2z^2 + z^4)}{22} + \frac{9\sqrt{77}Q_yxyz(x - z)(x + z)}{22} - \frac{\sqrt{77}Q_zx(x^4 + x^2y^2 - 11x^2z^2 - 3y^2z^2 + 6z^4)}{22}$$

$$\vec{\mathbb{Q}}_{4,1}^{(1,1)}[q](E_g, 2), \vec{\mathbb{Q}}_{4,2}^{(1,1)}[q](E_g, 2)$$

\*\* symmetry

$$\frac{\sqrt{5}yz(6x^2 - y^2 - z^2)}{2}$$

$$-\frac{\sqrt{5}xz(x^2 - 6y^2 + z^2)}{2}$$

\*\* expression

$$\frac{21\sqrt{11}Q_xxyz(2x^2 - y^2 - z^2)}{22} - \frac{\sqrt{11}Q_yz(6x^4 - 51x^2y^2 + 5x^2z^2 + 6y^4 + 5y^2z^2 - z^4)}{22} - \frac{\sqrt{11}Q_zy(6x^4 + 5x^2y^2 - 51x^2z^2 - y^4 + 5y^2z^2 + 6z^4)}{22}$$

$$-\frac{\sqrt{11}Q_xz(6x^4 - 51x^2y^2 + 5x^2z^2 + 6y^4 + 5y^2z^2 - z^4)}{22} - \frac{21\sqrt{11}Q_yxyz(x^2 - 2y^2 + z^2)}{22} + \frac{\sqrt{11}Q_zx(x^4 - 5x^2y^2 - 5x^2z^2 - 6y^4 + 51y^2z^2 - 6z^4)}{22}$$