

PG No. 23  $C_{6h}$   $6/m$  [ hexagonal ] (polar, internal axial dipole)

\* Harmonics for rank 0

\* Harmonics for rank 1

$$\vec{Q}_1^{(1,0)}[g](A_u)$$

\*\* symmetry

$$z$$

\*\* expression

$$\frac{\sqrt{2}G_x y}{2} - \frac{\sqrt{2}G_y x}{2}$$

$$\vec{Q}_{1,1}^{(1,0)}[g](E_{1u}), \vec{Q}_{1,2}^{(1,0)}[g](E_{1u})$$

\*\* symmetry

$$x$$

$$y$$

\*\* expression

$$\frac{\sqrt{2}G_y z}{2} - \frac{\sqrt{2}G_z y}{2}$$

$$-\frac{\sqrt{2}G_x z}{2} + \frac{\sqrt{2}G_z x}{2}$$

\* Harmonics for rank 2

$$\vec{Q}_2^{(1,0)}[g](A_g)$$

\*\* symmetry

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

\*\* expression

$$\frac{\sqrt{6}G_x y z}{2} - \frac{\sqrt{6}G_y x z}{2}$$

$$\vec{Q}_{2,1}^{(1,0)}[g](E_{1g}), \vec{Q}_{2,2}^{(1,0)}[g](E_{1g})$$

\*\* symmetry

$$\sqrt{3}yz$$

$$-\sqrt{3}xz$$

\*\* expression

$$\frac{\sqrt{2}G_x (y-z)(y+z)}{2} - \frac{\sqrt{2}G_y xy}{2} + \frac{\sqrt{2}G_z xz}{2}$$

$$-\frac{\sqrt{2}G_x xy}{2} + \frac{\sqrt{2}G_y (x-z)(x+z)}{2} + \frac{\sqrt{2}G_z yz}{2}$$

$$\vec{Q}_{2,1}^{(1,0)}[g](E_{2g}), \vec{Q}_{2,2}^{(1,0)}[g](E_{2g})$$

\*\* symmetry

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

$$-\sqrt{3}xy$$

\*\* expression

$$\frac{\sqrt{2}G_x yz}{2} + \frac{\sqrt{2}G_y xz}{2} - \sqrt{2}G_z xy$$

$$\frac{\sqrt{2}G_x xz}{2} - \frac{\sqrt{2}G_y yz}{2} - \frac{\sqrt{2}G_z (x-y)(x+y)}{2}$$

\* Harmonics for rank 3

$$\vec{Q}_3^{(1,0)}[g](A_u)$$

\*\* symmetry

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

\*\* expression

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

$$\tilde{\mathcal{Q}}_3^{(1,0)}[g](B_u, 1)$$

\*\* symmetry

$$\frac{\sqrt{10}y (3x^2 - y^2)}{4}$$

\*\* expression

$$-\frac{\sqrt{30}G_x z (x - y) (x + y)}{8} + \frac{\sqrt{30}G_y x y z}{4} + \frac{\sqrt{30}G_z x (x^2 - 3y^2)}{8}$$

$$\tilde{\mathcal{Q}}_3^{(1,0)}[g](B_u, 2)$$

\*\* symmetry

$$\frac{\sqrt{10}x (x^2 - 3y^2)}{4}$$

\*\* expression

$$\frac{\sqrt{30}G_x x y z}{4} + \frac{\sqrt{30}G_y z (x - y) (x + y)}{8} - \frac{\sqrt{30}G_z y (3x^2 - y^2)}{8}$$

$$\tilde{\mathcal{Q}}_{3,1}^{(1,0)}[g](E_{1u}), \tilde{\mathcal{Q}}_{3,2}^{(1,0)}[g](E_{1u})$$

\*\* symmetry

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

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

\*\* expression

$$\frac{5\sqrt{2}G_x x y z}{4} - \frac{\sqrt{2}G_y z (11x^2 + y^2 - 4z^2)}{8} + \frac{\sqrt{2}G_z y (x^2 + y^2 - 4z^2)}{8}$$

$$\frac{\sqrt{2}G_x z (x^2 + 11y^2 - 4z^2)}{8} - \frac{5\sqrt{2}G_y x y z}{4} - \frac{\sqrt{2}G_z x (x^2 + y^2 - 4z^2)}{8}$$

$$\tilde{\mathcal{Q}}_{3,1}^{(1,0)}[g](E_{2u}), \tilde{\mathcal{Q}}_{3,2}^{(1,0)}[g](E_{2u})$$

\*\* symmetry

$$\sqrt{15}x y z$$

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

\*\* expression

$$\frac{\sqrt{5}G_x x (y - z) (y + z)}{2} - \frac{\sqrt{5}G_y y (x - z) (x + z)}{2} + \frac{\sqrt{5}G_z z (x - y) (x + y)}{2}$$

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

\* Harmonics for rank 4

$$\tilde{\mathcal{Q}}_4^{(1,0)}[g](A_g)$$

\*\* symmetry

$$\frac{3x^4}{8} + \frac{3x^2 y^2}{4} - 3x^2 z^2 + \frac{3y^4}{8} - 3y^2 z^2 + z^4$$

\*\* expression

$$-\frac{\sqrt{5}G_x y z (3x^2 + 3y^2 - 4z^2)}{4} + \frac{\sqrt{5}G_y x z (3x^2 + 3y^2 - 4z^2)}{4}$$

$$\tilde{\mathcal{Q}}_4^{(1,0)}[g](B_g, 1)$$

\*\* symmetry

$$\frac{\sqrt{70}x z (x^2 - 3y^2)}{4}$$

\*\* expression

$$\frac{\sqrt{14}G_xxy(x^2-3y^2+6z^2)}{8} - \frac{\sqrt{14}G_y(x^4-3x^2y^2-3x^2z^2+3y^2z^2)}{8} - \frac{3\sqrt{14}G_zyz(3x^2-y^2)}{8}$$

$$\tilde{\mathbb{Q}}_4^{(1,0)}[g](B_g, 2)$$

\*\* symmetry

$$\frac{\sqrt{70}yz(3x^2-y^2)}{4}$$

\*\* expression

$$\frac{\sqrt{14}G_x(3x^2y^2-3x^2z^2-y^4+3y^2z^2)}{8} - \frac{\sqrt{14}G_yxy(3x^2-y^2-6z^2)}{8} + \frac{3\sqrt{14}G_zxz(x^2-3y^2)}{8}$$

$$\tilde{\mathbb{Q}}_{4,1}^{(1,0)}[g](E_{1g}), \tilde{\mathbb{Q}}_{4,2}^{(1,0)}[g](E_{1g})$$

\*\* symmetry

$$-\frac{\sqrt{10}yz(3x^2+3y^2-4z^2)}{4}$$

$$\frac{\sqrt{10}xz(3x^2+3y^2-4z^2)}{4}$$

\*\* expression

$$-\frac{\sqrt{2}G_x(3x^2y^2-3x^2z^2+3y^4-21y^2z^2+4z^4)}{8} + \frac{3\sqrt{2}G_yxy(x^2+y^2-6z^2)}{8} - \frac{\sqrt{2}G_zxz(3x^2+3y^2-4z^2)}{8}$$

$$\frac{3\sqrt{2}G_xxy(x^2+y^2-6z^2)}{8} - \frac{\sqrt{2}G_y(3x^4+3x^2y^2-21x^2z^2-3y^2z^2+4z^4)}{8} - \frac{\sqrt{2}G_zyz(3x^2+3y^2-4z^2)}{8}$$

$$\tilde{\mathbb{Q}}_{4,1}^{(1,0)}[g](E_{2g}, 1), \tilde{\mathbb{Q}}_{4,2}^{(1,0)}[g](E_{2g}, 1)$$

\*\* symmetry

$$\frac{\sqrt{35}(x^2-2xy-y^2)(x^2+2xy-y^2)}{8}$$

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

\*\* expression

$$\frac{\sqrt{7}G_xyz(3x^2-y^2)}{4} + \frac{\sqrt{7}G_yxz(x^2-3y^2)}{4} - \sqrt{7}G_zxy(x-y)(x+y)$$

$$-\frac{\sqrt{7}G_xxz(x^2-3y^2)}{4} + \frac{\sqrt{7}G_yyz(3x^2-y^2)}{4} + \frac{\sqrt{7}G_z(x^2-2xy-y^2)(x^2+2xy-y^2)}{4}$$

$$\tilde{\mathbb{Q}}_{4,1}^{(1,0)}[g](E_{2g}, 2), \tilde{\mathbb{Q}}_{4,2}^{(1,0)}[g](E_{2g}, 2)$$

\*\* symmetry

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

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

\*\* expression

$$\frac{G_xyz(3x^2-4y^2+3z^2)}{2} - \frac{G_yxz(4x^2-3y^2-3z^2)}{2} + \frac{G_zxy(x^2+y^2-6z^2)}{2}$$

$$-\frac{G_xxz(x^2+15y^2-6z^2)}{4} + \frac{G_yyz(15x^2+y^2-6z^2)}{4} + \frac{G_z(x-y)(x+y)(x^2+y^2-6z^2)}{4}$$