

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

\* Harmonics for rank 0

\* Harmonics for rank 1

$$\vec{G}_1^{(1,0)}[q](A_g)$$

\*\* symmetry

$$z$$

\*\* expression

$$\frac{\sqrt{2}Q_x y}{2} - \frac{\sqrt{2}Q_y x}{2}$$

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

\*\* symmetry

$$x$$

$$y$$

\*\* expression

$$\frac{\sqrt{2}Q_y z}{2} - \frac{\sqrt{2}Q_z y}{2}$$

$$-\frac{\sqrt{2}Q_x z}{2} + \frac{\sqrt{2}Q_z x}{2}$$

\* Harmonics for rank 2

$$\vec{G}_2^{(1,0)}[q](A_u)$$

\*\* symmetry

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

\*\* expression

$$\frac{\sqrt{6}Q_x y z}{2} - \frac{\sqrt{6}Q_y x z}{2}$$

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

\*\* symmetry

$$\sqrt{3}yz$$

$$-\sqrt{3}xz$$

\*\* expression

$$\frac{\sqrt{2}Q_x (y-z)(y+z)}{2} - \frac{\sqrt{2}Q_y xy}{2} + \frac{\sqrt{2}Q_z xz}{2}$$

$$-\frac{\sqrt{2}Q_x xy}{2} + \frac{\sqrt{2}Q_y (x-z)(x+z)}{2} + \frac{\sqrt{2}Q_z yz}{2}$$

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

\*\* symmetry

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

$$-\sqrt{3}xy$$

\*\* expression

$$\frac{\sqrt{2}Q_x yz}{2} + \frac{\sqrt{2}Q_y xz}{2} - \sqrt{2}Q_z xy$$

$$\frac{\sqrt{2}Q_x xz}{2} - \frac{\sqrt{2}Q_y yz}{2} - \frac{\sqrt{2}Q_z (x-y)(x+y)}{2}$$

\* Harmonics for rank 3

$$\vec{G}_3^{(1,0)}[q](A_g)$$

\*\* symmetry

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

\*\* expression

$$-\frac{\sqrt{3}Q_{xy}(x^2+y^2-4z^2)}{4}+\frac{\sqrt{3}Q_yx(x^2+y^2-4z^2)}{4}$$

$$\vec{\mathbb{G}}_3^{(1,0)}[q](B_g, 1)$$

\*\* symmetry

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

\*\* expression

$$-\frac{\sqrt{30}Q_xz(x-y)(x+y)}{8}+\frac{\sqrt{30}Q_yxyz}{4}+\frac{\sqrt{30}Q_zx(x^2-3y^2)}{8}$$

$$\vec{\mathbb{G}}_3^{(1,0)}[q](B_g, 2)$$

\*\* symmetry

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

\*\* expression

$$\frac{\sqrt{30}Q_xxyz}{4}+\frac{\sqrt{30}Q_yz(x-y)(x+y)}{8}-\frac{\sqrt{30}Q_zy(3x^2-y^2)}{8}$$

$$\vec{\mathbb{G}}_{3,1}^{(1,0)}[q](E_{1g}), \vec{\mathbb{G}}_{3,2}^{(1,0)}[q](E_{1g})$$

\*\* symmetry

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

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

\*\* expression

$$\frac{5\sqrt{2}Q_xxyz}{4}-\frac{\sqrt{2}Q_yz(11x^2+y^2-4z^2)}{8}+\frac{\sqrt{2}Q_zy(x^2+y^2-4z^2)}{8}$$

$$\frac{\sqrt{2}Q_xz(x^2+11y^2-4z^2)}{8}-\frac{5\sqrt{2}Q_yxyz}{4}-\frac{\sqrt{2}Q_zx(x^2+y^2-4z^2)}{8}$$

$$\vec{\mathbb{G}}_{3,1}^{(1,0)}[q](E_{2g}), \vec{\mathbb{G}}_{3,2}^{(1,0)}[q](E_{2g})$$

\*\* symmetry

$$\sqrt{15}xyz$$

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

\*\* expression

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

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

\* Harmonics for rank 4

$$\vec{\mathbb{G}}_4^{(1,0)}[q](A_u)$$

\*\* symmetry

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

\*\* expression

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

$$\vec{\mathbb{G}}_4^{(1,0)}[q](B_u, 1)$$

\*\* symmetry

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

\*\* expression

$$\frac{\sqrt{14}Q_xxy(x^2-3y^2+6z^2)}{8} - \frac{\sqrt{14}Q_y(x^4-3x^2y^2-3x^2z^2+3y^2z^2)}{8} - \frac{3\sqrt{14}Q_zyz(3x^2-y^2)}{8}$$

$$\vec{\mathbb{G}}_4^{(1,0)}[q](B_u, 2)$$

\*\* symmetry

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

\*\* expression

$$\frac{\sqrt{14}Q_x(3x^2y^2-3x^2z^2-y^4+3y^2z^2)}{8} - \frac{\sqrt{14}Q_yxy(3x^2-y^2-6z^2)}{8} + \frac{3\sqrt{14}Q_zxz(x^2-3y^2)}{8}$$

$$\vec{\mathbb{G}}_{4,1}^{(1,0)}[q](E_{1u}), \vec{\mathbb{G}}_{4,2}^{(1,0)}[q](E_{1u})$$

\*\* symmetry

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

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

\*\* expression

$$-\frac{\sqrt{2}Q_x(3x^2y^2-3x^2z^2+3y^4-21y^2z^2+4z^4)}{8} + \frac{3\sqrt{2}Q_yxy(x^2+y^2-6z^2)}{8} - \frac{\sqrt{2}Q_zxz(3x^2+3y^2-4z^2)}{8}$$

$$\frac{3\sqrt{2}Q_xxy(x^2+y^2-6z^2)}{8} - \frac{\sqrt{2}Q_y(3x^4+3x^2y^2-21x^2z^2-3y^2z^2+4z^4)}{8} - \frac{\sqrt{2}Q_zyz(3x^2+3y^2-4z^2)}{8}$$

$$\vec{\mathbb{G}}_{4,1}^{(1,0)}[q](E_{2u}, 1), \vec{\mathbb{G}}_{4,2}^{(1,0)}[q](E_{2u}, 1)$$

\*\* 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

$$\frac{\sqrt{7}Q_xyz(3x^2-y^2)}{4} + \frac{\sqrt{7}Q_yxz(x^2-3y^2)}{4} - \sqrt{7}Q_zxy(x-y)(x+y)$$

$$-\frac{\sqrt{7}Q_xxz(x^2-3y^2)}{4} + \frac{\sqrt{7}Q_yyz(3x^2-y^2)}{4} + \frac{\sqrt{7}Q_z(x^2-2xy-y^2)(x^2+2xy-y^2)}{4}$$

$$\vec{\mathbb{G}}_{4,1}^{(1,0)}[q](E_{2u}, 2), \vec{\mathbb{G}}_{4,2}^{(1,0)}[q](E_{2u}, 2)$$

\*\* 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

$$\frac{Q_xyz(3x^2-4y^2+3z^2)}{2} - \frac{Q_yxz(4x^2-3y^2-3z^2)}{2} + \frac{Q_zxy(x^2+y^2-6z^2)}{2}$$

$$-\frac{Q_xxz(x^2+15y^2-6z^2)}{4} + \frac{Q_yyz(15x^2+y^2-6z^2)}{4} + \frac{Q_z(x-y)(x+y)(x^2+y^2-6z^2)}{4}$$