

PG No. 36  $D_{3d}(1)$   $\bar{3}m$  (-31m setting) [ trigonal ] (axial, internal polar dipole)

\* Harmonics for rank 0

\* Harmonics for rank 1

$$\vec{G}_1^{(1,0)}[q](A_{2g})$$

\*\* symmetry

$$z$$

\*\* expression

$$\frac{\sqrt{2}Q_{xy}}{2} - \frac{\sqrt{2}Q_{yx}}{2}$$

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

\*\* symmetry

$$x$$

$$y$$

\*\* expression

$$\frac{\sqrt{2}Q_{yz}}{2} - \frac{\sqrt{2}Q_{zy}}{2}$$

$$-\frac{\sqrt{2}Q_{xz}}{2} + \frac{\sqrt{2}Q_{zx}}{2}$$

\* Harmonics for rank 2

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

\*\* symmetry

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

\*\* expression

$$\frac{\sqrt{6}Q_{xyz}}{2} - \frac{\sqrt{6}Q_{yxz}}{2}$$

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

\*\* symmetry

$$\sqrt{3}yz$$

$$-\sqrt{3}xz$$

\*\* expression

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

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

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

\*\* symmetry

$$\sqrt{3}xy$$

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

\*\* expression

$$-\frac{\sqrt{2}Q_{xxz}}{2} + \frac{\sqrt{2}Q_{yyz}}{2} + \frac{\sqrt{2}Q_z(x-y)(x+y)}{2}$$

$$\frac{\sqrt{2}Q_{xyz}}{2} + \frac{\sqrt{2}Q_{yxz}}{2} - \sqrt{2}Q_{zxy}$$

\* Harmonics for rank 3

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

\*\* symmetry

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

\*\* expression

$$-\frac{\sqrt{30}Q_x z (x-y) (x+y)}{8} + \frac{\sqrt{30}Q_y x y z}{4} + \frac{\sqrt{30}Q_z x (x^2 - 3y^2)}{8}$$

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

\*\* symmetry

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

\*\* expression

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

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

\*\* symmetry

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

\*\* expression

$$\frac{\sqrt{30}Q_x x y z}{4} + \frac{\sqrt{30}Q_y z (x-y) (x+y)}{8} - \frac{\sqrt{30}Q_z y (3x^2 - y^2)}{8}$$

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

\*\* symmetry

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

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

\*\* expression

$$\frac{5\sqrt{2}Q_x x y z}{4} - \frac{\sqrt{2}Q_y z (11x^2 + y^2 - 4z^2)}{8} + \frac{\sqrt{2}Q_z y (x^2 + y^2 - 4z^2)}{8}$$

$$\frac{\sqrt{2}Q_x z (x^2 + 11y^2 - 4z^2)}{8} - \frac{5\sqrt{2}Q_y x y z}{4} - \frac{\sqrt{2}Q_z x (x^2 + y^2 - 4z^2)}{8}$$

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

\*\* symmetry

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

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

\*\* expression

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

$$\frac{\sqrt{5}Q_x x (y-z) (y+z)}{2} - \frac{\sqrt{5}Q_y y (x-z) (x+z)}{2} + \frac{\sqrt{5}Q_z z (x-y) (x+y)}{2}$$

\* Harmonics for rank 4

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

\*\* 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

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

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

\*\* symmetry

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

\*\* expression

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

$$\tilde{\mathbb{G}}_4^{(1,0)}[q](A_{2u})$$

\*\* symmetry

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

\*\* expression

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

$$\tilde{\mathbb{G}}_{4,1}^{(1,0)}[q](E_u, 1), \tilde{\mathbb{G}}_{4,2}^{(1,0)}[q](E_u, 1)$$

\*\* symmetry

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

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

\*\* expression

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

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

$$\tilde{\mathbb{G}}_{4,1}^{(1,0)}[q](E_u, 2), \tilde{\mathbb{G}}_{4,2}^{(1,0)}[q](E_u, 2)$$

\*\* symmetry

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

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

\*\* expression

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

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

$$\tilde{\mathbb{G}}_{4,1}^{(1,0)}[q](E_u, 3), \tilde{\mathbb{G}}_{4,2}^{(1,0)}[q](E_u, 3)$$

\*\* symmetry

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

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

\*\* expression

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

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