

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

\* Harmonics for rank 0

\* Harmonics for rank 1

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

\*\* symmetry

$z$

\*\* expression

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

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

\*\* 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

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

\*\* symmetry

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

\*\* expression

$$\frac{\sqrt{6}Q_xyz}{2} - \frac{\sqrt{6}Q_yxz}{2}$$

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

\*\* symmetry

$\sqrt{3}yz$

$-\sqrt{3}xz$

\*\* expression

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

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

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

\*\* 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

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

\*\* symmetry

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

\*\* expression

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

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

\*\* symmetry

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

\*\* expression

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

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

\*\* symmetry

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

\*\* expression

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

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

\*\* symmetry

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

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

\*\* expression

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

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

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

\*\* symmetry

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

$$\sqrt{15}xyz$$

\*\* expression

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

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

\* Harmonics for rank 4

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

\*\* symmetry

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

\*\* expression

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

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

\*\* symmetry

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

\*\* expression

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

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

\*\* symmetry

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

\*\* expression

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

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

\*\* symmetry

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

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

\*\* expression

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

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

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

\*\* 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

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

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

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

\*\* 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

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

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