

PG No. 8  $D_{2h}$   $mmm$  [ orthorhombic ] (polar, internal axial dipole)

\* Harmonics for rank 0

\* Harmonics for rank 1

$$\tilde{Q}_1^{(1,0)}[g](B_{1u})$$

\*\* symmetry

$$z$$

\*\* expression

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

$$\tilde{Q}_1^{(1,0)}[g](B_{2u})$$

\*\* symmetry

$$y$$

\*\* expression

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

$$\tilde{Q}_1^{(1,0)}[g](B_{3u})$$

\*\* symmetry

$$x$$

\*\* expression

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

\* Harmonics for rank 2

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

\*\* symmetry

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

\*\* expression

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

$$\tilde{Q}_2^{(1,0)}[g](A_g, 2)$$

\*\* symmetry

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

\*\* expression

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

$$\tilde{Q}_2^{(1,0)}[g](B_{1g})$$

\*\* symmetry

$$\sqrt{3}xy$$

\*\* expression

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

$$\tilde{Q}_2^{(1,0)}[g](B_{2g})$$

\*\* symmetry

$$\sqrt{3}xz$$

\*\* expression

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

$$\tilde{Q}_2^{(1,0)}[g](B_{3g})$$

\*\* symmetry

$$\sqrt{3}yz$$

\*\* expression

$$\frac{\sqrt{2}G_x(y-z)(y+z)}{2} - \frac{\sqrt{2}G_yxy}{2} + \frac{\sqrt{2}G_zxz}{2}$$

\* Harmonics for rank 3

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

\*\* symmetry

$$\sqrt{15}xyz$$

\*\* expression

$$\frac{\sqrt{5}G_{xx}(y-z)(y+z)}{2} - \frac{\sqrt{5}G_{yy}(x-z)(x+z)}{2} + \frac{\sqrt{5}G_{zz}(x-y)(x+y)}{2}$$

$$\tilde{\mathbb{Q}}_3^{(1,0)}[g](B_{1u}, 1)$$

\*\* symmetry

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

\*\* expression

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

$$\tilde{\mathbb{Q}}_3^{(1,0)}[g](B_{1u}, 2)$$

\*\* symmetry

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

\*\* expression

$$\frac{\sqrt{5}G_{xy}(x^2 - y^2 + 2z^2)}{4} - \frac{\sqrt{5}G_{yx}(x^2 - y^2 + 2z^2)}{4} - \sqrt{5}G_{zz}xyz$$

$$\tilde{\mathbb{Q}}_3^{(1,0)}[g](B_{2u}, 1)$$

\*\* symmetry

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

\*\* expression

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

$$\tilde{\mathbb{Q}}_3^{(1,0)}[g](B_{2u}, 2)$$

\*\* symmetry

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

\*\* expression

$$\frac{\sqrt{5}G_{xz}(x^2 + 2y^2 - z^2)}{4} - \sqrt{5}G_{yxyz} - \frac{\sqrt{5}G_{zx}(x^2 - 2y^2 - z^2)}{4}$$

$$\tilde{\mathbb{Q}}_3^{(1,0)}[g](B_{3u}, 1)$$

\*\* symmetry

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

\*\* expression

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

$$\tilde{\mathbb{Q}}_3^{(1,0)}[g](B_{3u}, 2)$$

\*\* symmetry

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

\*\* expression

$$-\sqrt{5}G_{xyz} + \frac{\sqrt{5}G_{yz}(2x^2 + y^2 - z^2)}{4} + \frac{\sqrt{5}G_{zy}(2x^2 - y^2 + z^2)}{4}$$

\* Harmonics for rank 4

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

\*\* symmetry

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

\*\* expression

$$-\frac{\sqrt{105}G_x y z (y - z) (y + z)}{6} + \frac{\sqrt{105}G_y x z (x - z) (x + z)}{6} - \frac{\sqrt{105}G_z x y (x - y) (x + y)}{6}$$

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

\*\* symmetry

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

\*\* expression

$$-\frac{\sqrt{3}G_x y z (9x^2 + 2y^2 - 5z^2)}{6} + \frac{\sqrt{3}G_y x z (2x^2 + 9y^2 - 5z^2)}{6} + \frac{7\sqrt{3}G_z x y (x - y) (x + y)}{6}$$

$$\bar{\mathbb{Q}}_4^{(1,0)}[g](A_g, 3)$$

\*\* symmetry

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

\*\* expression

$$-\frac{G_x y z (3x^2 - 4y^2 + 3z^2)}{2} + \frac{G_y x z (4x^2 - 3y^2 - 3z^2)}{2} - \frac{G_z x y (x^2 + y^2 - 6z^2)}{2}$$

$$\bar{\mathbb{Q}}_4^{(1,0)}[g](B_{1g}, 1)$$

\*\* symmetry

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

\*\* expression

$$-\frac{\sqrt{7}G_x x z (x^2 - 3y^2)}{4} + \frac{\sqrt{7}G_y y z (3x^2 - y^2)}{4} + \frac{\sqrt{7}G_z (x^2 - 2xy - y^2) (x^2 + 2xy - y^2)}{4}$$

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

\*\* symmetry

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

\*\* expression

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

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

\*\* symmetry

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

\*\* expression

$$-\frac{\sqrt{7}G_x x y (x^2 - 3z^2)}{4} + \frac{\sqrt{7}G_y (x^2 - 2xz - z^2) (x^2 + 2xz - z^2)}{4} + \frac{\sqrt{7}G_z y z (3x^2 - z^2)}{4}$$

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

\*\* symmetry

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

\*\* expression

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

$$\bar{\mathbb{Q}}_4^{(1,0)}[g](B_{3g}, 1)$$

\*\* symmetry

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

\*\* expression

$$\frac{\sqrt{7}G_x\left(y^2-2yz-z^2\right)\left(y^2+2yz-z^2\right)}{4}-\frac{\sqrt{7}G_yxy\left(y^2-3z^2\right)}{4}+\frac{\sqrt{7}G_zxz\left(3y^2-z^2\right)}{4}$$

$$\tilde{\mathbb{Q}}_4^{(1,0)}[g](B_{3g},2)$$

\*\* symmetry

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

\*\* expression

$$\frac{G_x\left(y-z\right)\left(y+z\right)\left(6x^2-y^2-z^2\right)}{4}-\frac{G_yxy\left(6x^2-y^2-15z^2\right)}{4}+\frac{G_zxz\left(6x^2-15y^2-z^2\right)}{4}$$