

PG No. 32  $O_h$   $m\bar{3}m$  [ cubic ] (polar, internal axial dipole)

\* Harmonics for rank 0

\* Harmonics for rank 1

$$\bar{Q}_{1,1}^{(1,0)}[g](T_{1u}), \bar{Q}_{1,2}^{(1,0)}[g](T_{1u}), \bar{Q}_{1,3}^{(1,0)}[g](T_{1u})$$

\*\* symmetry

$$x$$

$$y$$

$$z$$

\*\* expression

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

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

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

\* Harmonics for rank 2

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

\*\* symmetry

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

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

\*\* expression

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

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

$$\bar{Q}_{2,1}^{(1,0)}[g](T_{2g}), \bar{Q}_{2,2}^{(1,0)}[g](T_{2g}), \bar{Q}_{2,3}^{(1,0)}[g](T_{2g})$$

\*\* symmetry

$$\sqrt{3}yz$$

$$\sqrt{3}xz$$

$$\sqrt{3}xy$$

\*\* expression

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

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

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

\* Harmonics for rank 3

$$\bar{Q}_3^{(1,0)}[g](A_{2u})$$

\*\* symmetry

$$\sqrt{15}xyz$$

\*\* expression

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

$$\bar{Q}_{3,1}^{(1,0)}[g](T_{1u}), \bar{Q}_{3,2}^{(1,0)}[g](T_{1u}), \bar{Q}_{3,3}^{(1,0)}[g](T_{1u})$$

\*\* symmetry

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

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

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

\*\* expression

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

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

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

$$\bar{\mathbb{Q}}_{3,1}^{(1,0)}[g](T_{2u}), \bar{\mathbb{Q}}_{3,2}^{(1,0)}[g](T_{2u}), \bar{\mathbb{Q}}_{3,3}^{(1,0)}[g](T_{2u})$$

\*\* symmetry

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

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

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

\*\* expression

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

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

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

\* Harmonics for rank 4

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

\*\* symmetry

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

\*\* expression

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

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

\*\* symmetry

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

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

\*\* expression

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

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

$$\bar{\mathbb{Q}}_{4,1}^{(1,0)}[g](T_{1g}), \bar{\mathbb{Q}}_{4,2}^{(1,0)}[g](T_{1g}), \bar{\mathbb{Q}}_{4,3}^{(1,0)}[g](T_{1g})$$

\*\* symmetry

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

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

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

\*\* expression

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

$$-\frac{\sqrt{7}G_xxy(x^2-3z^2)}{4} + \frac{\sqrt{7}G_y(x^2-2xz-z^2)(x^2+2xz-z^2)}{4} + \frac{\sqrt{7}G_zyz(3x^2-z^2)}{4}$$

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

$$\bar{\mathbb{Q}}_{4,1}^{(1,0)}[g](T_{2g}), \bar{\mathbb{Q}}_{4,2}^{(1,0)}[g](T_{2g}), \bar{\mathbb{Q}}_{4,3}^{(1,0)}[g](T_{2g})$$

\*\* symmetry

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

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

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

\*\* expression

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

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

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