

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

\* Harmonics for rank 0

\* Harmonics for rank 1

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

\*\* symmetry

$$z$$

\*\* expression

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

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

\*\* symmetry

$$y$$

\*\* expression

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

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

\*\* symmetry

$$x$$

\*\* expression

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

\* Harmonics for rank 2

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

\*\* symmetry

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

\*\* expression

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

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

\*\* symmetry

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

\*\* expression

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

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

\*\* symmetry

$$\sqrt{3}xy$$

\*\* expression

$$-\frac{\sqrt{2}G_{xxz}}{2} + \frac{\sqrt{2}G_{yyz}}{2} + \frac{\sqrt{2}G_z(x-y)(x+y)}{2}$$

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

\*\* symmetry

$$\sqrt{3}xz$$

\*\* expression

$$\frac{\sqrt{2}G_{xxy}}{2} - \frac{\sqrt{2}G_y(x-z)(x+z)}{2} - \frac{\sqrt{2}G_zyz}{2}$$

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

\*\* 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

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

\*\* symmetry

$$\sqrt{15}xyz$$

\*\* expression

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

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

\*\* symmetry

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

\*\* expression

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

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

\*\* symmetry

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

\*\* expression

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

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

\*\* symmetry

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

\*\* expression

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

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

\*\* symmetry

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

\*\* expression

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

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

\*\* symmetry

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

\*\* expression

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

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

\*\* symmetry

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

\*\* expression

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

\* Harmonics for rank 4

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

\*\* symmetry

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

\*\* expression

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

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

\*\* symmetry

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

\*\* expression

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

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

\*\* symmetry

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

\*\* expression

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

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

\*\* symmetry

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

\*\* expression

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

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

\*\* symmetry

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

\*\* expression

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

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

\*\* symmetry

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

\*\* expression

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

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

\*\* symmetry

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

\*\* expression

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

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

\*\* symmetry

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

\*\* expression

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

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

\*\* symmetry

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

\*\* expression

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