

PG No. 33  $D_{2d}(1)$   $\bar{4}2m$  (-4m2 setting) [ tetragonal ] (polar, internal axial dipole)

\* Harmonics for rank 0

\* Harmonics for rank 1

$$\bar{Q}_1^{(1,0)}[g](B_2)$$

\*\* symmetry

$$z$$

\*\* expression

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

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

\*\* symmetry

$$x$$

$$y$$

\*\* expression

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

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

\* Harmonics for rank 2

$$\bar{Q}_2^{(1,0)}[g](A_1)$$

\*\* symmetry

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

\*\* expression

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

$$\bar{Q}_2^{(1,0)}[g](B_1)$$

\*\* symmetry

$$\sqrt{3}xy$$

\*\* expression

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

$$\bar{Q}_2^{(1,0)}[g](B_2)$$

\*\* symmetry

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

\*\* expression

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

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

\*\* symmetry

$$-\sqrt{3}xz$$

$$\sqrt{3}yz$$

\*\* expression

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

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

\* Harmonics for rank 3

$$\bar{Q}_3^{(1,0)}[g](A_1)$$

\*\* symmetry

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

\*\* expression

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

$$\bar{Q}_3^{(1,0)}[g](A_2)$$

\*\* symmetry

$$\sqrt{15}xyz$$

\*\* expression

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

$$\bar{Q}_3^{(1,0)}[g](B_2)$$

\*\* symmetry

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

\*\* expression

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

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

\*\* symmetry

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

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

\*\* expression

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

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

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

\*\* symmetry

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

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

\*\* expression

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

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

\* Harmonics for rank 4

$$\bar{Q}_4^{(1,0)}[g](A_1,1)$$

\*\* symmetry

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

\*\* expression

$$-\frac{\sqrt{105}G_{xyz}(y-z)(y+z)}{6} + \frac{\sqrt{105}G_{yxz}(x-z)(x+z)}{6} - \frac{\sqrt{105}G_{zxy}(x-y)(x+y)}{6}$$

$$\bar{Q}_4^{(1,0)}[g](A_1,2)$$

\*\* symmetry

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

\*\* expression

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

$\vec{Q}_4^{(1,0)}[g](A_2)$

\*\* symmetry

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

\*\* expression

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

$\vec{Q}_4^{(1,0)}[g](B_1)$

\*\* symmetry

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

\*\* expression

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

$\vec{Q}_4^{(1,0)}[g](B_2)$

\*\* symmetry

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

\*\* expression

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

$\vec{Q}_{4,1}^{(1,0)}[g](E, 1), \vec{Q}_{4,2}^{(1,0)}[g](E, 1)$

\*\* symmetry

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

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

\*\* expression

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

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

$\vec{Q}_{4,1}^{(1,0)}[g](E, 2), \vec{Q}_{4,2}^{(1,0)}[g](E, 2)$

\*\* symmetry

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

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

\*\* expression

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

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