

PG No. 15 D_{4h} $4/mmm$ [tetragonal] (polar, internal axial dipole)

* Harmonics for rank 0

* Harmonics for rank 1

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

** symmetry

$$z$$

** expression

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

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

** symmetry

$$x$$

$$y$$

** expression

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

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

* Harmonics for rank 2

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

** symmetry

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

** expression

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

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

** symmetry

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

** expression

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

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

** symmetry

$$\sqrt{3}xy$$

** expression

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

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

** symmetry

$$\sqrt{3}yz$$

$$\sqrt{3}xz$$

** expression

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

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

* Harmonics for rank 3

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

** symmetry

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

** expression

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

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

** symmetry

$$\sqrt{15}xyz$$

** expression

$$\frac{\sqrt{5}G_xx(y-z)(y+z)}{2}-\frac{\sqrt{5}G_yy(x-z)(x+z)}{2}+\frac{\sqrt{5}G_zz(x-y)(x+y)}{2}$$

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

** symmetry

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

** expression

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

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

** symmetry

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

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

** expression

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

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

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

** symmetry

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

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

** expression

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

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

* Harmonics for rank 4

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

** symmetry

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

** expression

$$-\frac{\sqrt{105}G_xyz(y-z)(y+z)}{6}+\frac{\sqrt{105}G_yxz(x-z)(x+z)}{6}-\frac{\sqrt{105}G_zxy(x-y)(x+y)}{6}$$

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

** symmetry

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

** expression

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

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

** symmetry

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

** expression

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

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

** symmetry

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

** expression

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

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

** symmetry

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

** expression

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

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

** symmetry

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

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

** expression

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

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

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

** symmetry

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

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

** expression

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

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