

PG No. 5 C_{2h} $2/m$ (b-axis setting) [monoclinic] (axial, internal polar dipole)

* Harmonics for rank 0

* Harmonics for rank 1

$$\vec{G}_1^{(1,0)}[q](A_g)$$

** symmetry

$$y$$

** expression

$$-\frac{\sqrt{2}Q_x z}{2} + \frac{\sqrt{2}Q_z x}{2}$$

$$\vec{G}_1^{(1,0)}[q](B_g, 1)$$

** symmetry

$$x$$

** expression

$$\frac{\sqrt{2}Q_y z}{2} - \frac{\sqrt{2}Q_z y}{2}$$

$$\vec{G}_1^{(1,0)}[q](B_g, 2)$$

** symmetry

$$z$$

** expression

$$\frac{\sqrt{2}Q_x y}{2} - \frac{\sqrt{2}Q_y x}{2}$$

* Harmonics for rank 2

$$\vec{G}_2^{(1,0)}[q](A_u, 1)$$

** symmetry

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

** expression

$$\frac{\sqrt{6}Q_x y z}{2} - \frac{\sqrt{6}Q_y x z}{2}$$

$$\vec{G}_2^{(1,0)}[q](A_u, 2)$$

** symmetry

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

** expression

$$\frac{\sqrt{2}Q_x y z}{2} + \frac{\sqrt{2}Q_y x z}{2} - \sqrt{2}Q_z x y$$

$$\vec{G}_2^{(1,0)}[q](A_u, 3)$$

** symmetry

$$\sqrt{3}x z$$

** expression

$$\frac{\sqrt{2}Q_x x y}{2} - \frac{\sqrt{2}Q_y (x-z)(x+z)}{2} - \frac{\sqrt{2}Q_z y z}{2}$$

$$\vec{G}_2^{(1,0)}[q](B_u, 1)$$

** symmetry

$$\sqrt{3}y z$$

** expression

$$\frac{\sqrt{2}Q_x (y-z)(y+z)}{2} - \frac{\sqrt{2}Q_y x y}{2} + \frac{\sqrt{2}Q_z x z}{2}$$

$$\vec{G}_2^{(1,0)}[q](B_u, 2)$$

** symmetry

$$\sqrt{3}x y$$

** expression

$$-\frac{\sqrt{2}Q_{xx}z}{2} + \frac{\sqrt{2}Q_{yy}z}{2} + \frac{\sqrt{2}Q_z(x-y)(x+y)}{2}$$

* Harmonics for rank 3

$$\vec{\mathbb{G}}_3^{(1,0)}[q](A_g, 1)$$

** symmetry

$$\sqrt{15}xyz$$

** expression

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

$$\vec{\mathbb{G}}_3^{(1,0)}[q](A_g, 2)$$

** symmetry

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

** expression

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

$$\vec{\mathbb{G}}_3^{(1,0)}[q](A_g, 3)$$

** symmetry

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

** expression

$$\frac{\sqrt{5}Q_{xz}(x^2 + 2y^2 - z^2)}{4} - \sqrt{5}Q_yxyz - \frac{\sqrt{5}Q_zx(x^2 - 2y^2 - z^2)}{4}$$

$$\vec{\mathbb{G}}_3^{(1,0)}[q](B_g, 1)$$

** symmetry

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

** expression

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

$$\vec{\mathbb{G}}_3^{(1,0)}[q](B_g, 2)$$

** symmetry

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

** expression

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

$$\vec{\mathbb{G}}_3^{(1,0)}[q](B_g, 3)$$

** symmetry

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

** expression

$$-\sqrt{5}Q_{xyz} + \frac{\sqrt{5}Q_yz(2x^2 + y^2 - z^2)}{4} + \frac{\sqrt{5}Q_zy(2x^2 - y^2 + z^2)}{4}$$

$$\vec{\mathbb{G}}_3^{(1,0)}[q](B_g, 4)$$

** symmetry

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

** expression

$$\frac{\sqrt{5}Q_{xy}(x^2 - y^2 + 2z^2)}{4} - \frac{\sqrt{5}Q_yx(x^2 - y^2 - 2z^2)}{4} - \sqrt{5}Q_zxyz$$

* Harmonics for rank 4

$$\vec{\mathbb{G}}_4^{(1,0)}[q](A_u, 1)$$

** symmetry

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

** expression

$$-\frac{\sqrt{105}Q_x y z (y - z) (y + z)}{6} + \frac{\sqrt{105}Q_y x z (x - z) (x + z)}{6} - \frac{\sqrt{105}Q_z x y (x - y) (x + y)}{6}$$

$$\vec{\mathbb{G}}_4^{(1,0)}[q](A_u, 2)$$

** symmetry

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

** expression

$$-\frac{\sqrt{3}Q_x y z (9x^2 + 2y^2 - 5z^2)}{6} + \frac{\sqrt{3}Q_y x z (2x^2 + 9y^2 - 5z^2)}{6} + \frac{7\sqrt{3}Q_z x y (x - y) (x + y)}{6}$$

$$\vec{\mathbb{G}}_4^{(1,0)}[q](A_u, 3)$$

** symmetry

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

** expression

$$-\frac{Q_x y z (3x^2 - 4y^2 + 3z^2)}{2} + \frac{Q_y x z (4x^2 - 3y^2 - 3z^2)}{2} - \frac{Q_z x y (x^2 + y^2 - 6z^2)}{2}$$

$$\vec{\mathbb{G}}_4^{(1,0)}[q](A_u, 4)$$

** symmetry

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

** expression

$$-\frac{\sqrt{7}Q_x x y (x^2 - 3z^2)}{4} + \frac{\sqrt{7}Q_y (x^2 - 2x z - z^2) (x^2 + 2x z - z^2)}{4} + \frac{\sqrt{7}Q_z y z (3x^2 - z^2)}{4}$$

$$\vec{\mathbb{G}}_4^{(1,0)}[q](A_u, 5)$$

** symmetry

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

** expression

$$-\frac{Q_x x y (x^2 - 6y^2 + 15z^2)}{4} + \frac{Q_y (x - z) (x + z) (x^2 - 6y^2 + z^2)}{4} + \frac{Q_z y z (15x^2 - 6y^2 + z^2)}{4}$$

$$\vec{\mathbb{G}}_4^{(1,0)}[q](B_u, 1)$$

** symmetry

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

** expression

$$\frac{\sqrt{7}Q_x (y^2 - 2y z - z^2) (y^2 + 2y z - z^2)}{4} - \frac{\sqrt{7}Q_y x y (y^2 - 3z^2)}{4} + \frac{\sqrt{7}Q_z x z (3y^2 - z^2)}{4}$$

$$\vec{\mathbb{G}}_4^{(1,0)}[q](B_u, 2)$$

** symmetry

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

** expression

$$-\frac{\sqrt{7}Q_x x z (x^2 - 3y^2)}{4} + \frac{\sqrt{7}Q_y y z (3x^2 - y^2)}{4} + \frac{\sqrt{7}Q_z (x^2 - 2x y - y^2) (x^2 + 2x y - y^2)}{4}$$

$$\vec{\mathbb{G}}_4^{(1,0)}[q](B_u, 3)$$

** symmetry

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

** expression

$$\frac{Q_x (y - z) (y + z) (6x^2 - y^2 - z^2)}{4} - \frac{Q_y xy (6x^2 - y^2 - 15z^2)}{4} + \frac{Q_z xz (6x^2 - 15y^2 - z^2)}{4}$$

$$\vec{\mathbb{G}}_4^{(1,0)}[q](B_u, 4)$$

** symmetry

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

** expression

$$\frac{Q_x xz \left(x^2+15y^2-6z^2\right)}{4} - \frac{Q_y yz \left(15x^2+y^2-6z^2\right)}{4} - \frac{Q_z \left(x-y\right) \left(x+y\right) \left(x^2+y^2-6z^2\right)}{4}$$