

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

* Harmonics for rank 0

* Harmonics for rank 1

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

** symmetry

$$z$$

** expression

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

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

** symmetry

$$y$$

** expression

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

$$\vec{G}_1^{(1,0)}[q](B_{3g})$$

** symmetry

$$x$$

** expression

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

* 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

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

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

** symmetry

$$\sqrt{3}xy$$

** expression

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

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

** symmetry

$$\sqrt{3}xz$$

** expression

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

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

** symmetry

$$\sqrt{3}yz$$

** expression

$$\frac{\sqrt{2}Q_x(y-z)(y+z)}{2} - \frac{\sqrt{2}Q_yxy}{2} + \frac{\sqrt{2}Q_zxz}{2}$$

* Harmonics for rank 3

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

** symmetry

$$\sqrt{15}xyz$$

** expression

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

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

** symmetry

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

** expression

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

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

** symmetry

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

** expression

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

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

** symmetry

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

** expression

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

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

** symmetry

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

** expression

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

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

** symmetry

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

** expression

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

$$\vec{\mathbb{G}}_3^{(1,0)}[q](B_{3g}, 2)$$

** symmetry

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

** expression

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

* 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

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

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

** symmetry

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

** expression

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

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

** symmetry

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

** expression

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

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

** symmetry

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

** expression

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

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

** symmetry

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

** expression

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

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

** symmetry

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

** expression

$$\frac{\sqrt{7}Q_x\left(y^2-2yz-z^2\right)\left(y^2+2yz-z^2\right)}{4}-\frac{\sqrt{7}Q_yxy\left(y^2-3z^2\right)}{4}+\frac{\sqrt{7}Q_zxz\left(3y^2-z^2\right)}{4}$$

$$\vec{\mathbb{G}}_4^{(1,0)}[q](B_{3u},2)$$

** symmetry

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

** expression

$$\frac{Q_x\left(y-z\right)\left(y+z\right)\left(6x^2-y^2-z^2\right)}{4}-\frac{Q_yxy\left(6x^2-y^2-15z^2\right)}{4}+\frac{Q_zxz\left(6x^2-15y^2-z^2\right)}{4}$$