

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

* Harmonics for rank 0

* Harmonics for rank 1

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

** symmetry

$$z$$

** expression

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

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

** symmetry

$$x$$

$$-y$$

** expression

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

$$\frac{\sqrt{2}Q_{xz}}{2} - \frac{\sqrt{2}Q_{zx}}{2}$$

* Harmonics for rank 2

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

** symmetry

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

** expression

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

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

** symmetry

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

** expression

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

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

** symmetry

$$\sqrt{3}xy$$

** expression

$$-\frac{\sqrt{2}Q_{xxz}}{2} + \frac{\sqrt{2}Q_{yyz}}{2} + \frac{\sqrt{2}Q_z(x-y)(x+y)}{2}$$

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

** symmetry

$$\sqrt{3}yz$$

$$-\sqrt{3}xz$$

** expression

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

$$-\frac{\sqrt{2}Q_{xxy}}{2} + \frac{\sqrt{2}Q_y(x-z)(x+z)}{2} + \frac{\sqrt{2}Q_{zyz}}{2}$$

* Harmonics for rank 3

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

** symmetry

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

** expression

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

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

** symmetry

$$\sqrt{15}xyz$$

** expression

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

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

** symmetry

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

** expression

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

$$\vec{\mathbb{G}}_{3,1}^{(1,0)}[q](E_g,1), \vec{\mathbb{G}}_{3,2}^{(1,0)}[q](E_g,1)$$

** symmetry

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

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

** expression

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

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

$$\vec{\mathbb{G}}_{3,1}^{(1,0)}[q](E_g,2), \vec{\mathbb{G}}_{3,2}^{(1,0)}[q](E_g,2)$$

** symmetry

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

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

** expression

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

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

* Harmonics for rank 4

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

** symmetry

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

** expression

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

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

** symmetry

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

** expression

$$-\frac{\sqrt{3}Q_xyz(9x^2 + 2y^2 - 5z^2)}{6} + \frac{\sqrt{3}Q_yxz(2x^2 + 9y^2 - 5z^2)}{6} + \frac{7\sqrt{3}Q_zxy(x-y)(x+y)}{6}$$

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

** symmetry

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

** expression

$$-\frac{\sqrt{7}Q_xxz(x^2 - 3y^2)}{4} + \frac{\sqrt{7}Q_yyz(3x^2 - y^2)}{4} + \frac{\sqrt{7}Q_z(x^2 - 2xy - y^2)(x^2 + 2xy - y^2)}{4}$$

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

** symmetry

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

** expression

$$-\frac{Q_xyz(3x^2 - 4y^2 + 3z^2)}{2} + \frac{Q_yxz(4x^2 - 3y^2 - 3z^2)}{2} - \frac{Q_zxy(x^2 + y^2 - 6z^2)}{2}$$

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

** symmetry

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

** expression

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

$$\vec{\mathbb{G}}_{4,1}^{(1,0)}[q](E_u, 1), \vec{\mathbb{G}}_{4,2}^{(1,0)}[q](E_u, 1)$$

** symmetry

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

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

** expression

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

$$-\frac{\sqrt{7}Q_xxy(x^2 - 3z^2)}{4} + \frac{\sqrt{7}Q_y(x^2 - 2xz - z^2)(x^2 + 2xz - z^2)}{4} + \frac{\sqrt{7}Q_zyz(3x^2 - z^2)}{4}$$

$$\vec{\mathbb{G}}_{4,1}^{(1,0)}[q](E_u, 2), \vec{\mathbb{G}}_{4,2}^{(1,0)}[q](E_u, 2)$$

** symmetry

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

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

** expression

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

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