

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

* Harmonics for rank 0

* Harmonics for rank 1

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

** symmetry

z

** expression

$$\frac{\sqrt{2}Q_xy}{2} - \frac{\sqrt{2}Q_yx}{2}$$

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

** 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

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

** symmetry

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

** expression

$$\frac{\sqrt{6}Q_xyz}{2} - \frac{\sqrt{6}Q_yxz}{2}$$

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

** symmetry

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

** expression

$$\frac{\sqrt{2}Q_xyz}{2} + \frac{\sqrt{2}Q_yxz}{2} - \sqrt{2}Q_zxy$$

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

** symmetry

$$\sqrt{3}xy$$

** expression

$$-\frac{\sqrt{2}Q_xxz}{2} + \frac{\sqrt{2}Q_yyz}{2} + \frac{\sqrt{2}Q_z(x-y)(x+y)}{2}$$

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

** 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

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

** 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

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

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

* 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

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

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

** 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

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

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

** 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

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

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