

PG No. 27 D_{6h} 6/mmm [hexagonal] (polar, internal polar dipole)

* Harmonics for rank 0

$$\vec{\mathbb{Q}}_0^{(1,1)}[q](A_{1g})$$

** symmetry

1

** expression

$$\frac{\sqrt{3}Q_x x}{3} + \frac{\sqrt{3}Q_y y}{3} + \frac{\sqrt{3}Q_z z}{3}$$

* Harmonics for rank 1

$$\vec{\mathbb{Q}}_1^{(1,-1)}[q](A_{2u})$$

** symmetry

z

** expression

Q_z

$$\vec{\mathbb{Q}}_1^{(1,1)}[q](A_{2u})$$

** symmetry

z

** expression

$$\frac{3\sqrt{10}Q_x x z}{10} + \frac{3\sqrt{10}Q_y y z}{10} - \frac{\sqrt{10}Q_z (x^2 + y^2 - 2z^2)}{10}$$

$$\vec{\mathbb{Q}}_{1,1}^{(1,-1)}[q](E_{1u}), \vec{\mathbb{Q}}_{1,2}^{(1,-1)}[q](E_{1u})$$

** symmetry

x

y

** expression

Q_x

Q_y

$$\vec{\mathbb{Q}}_{1,1}^{(1,1)}[q](E_{1u}), \vec{\mathbb{Q}}_{1,2}^{(1,1)}[q](E_{1u})$$

** symmetry

x

y

** expression

$$\frac{\sqrt{10}Q_x (2x^2 - y^2 - z^2)}{10} + \frac{3\sqrt{10}Q_y x y}{10} + \frac{3\sqrt{10}Q_z x z}{10}$$

$$\frac{3\sqrt{10}Q_x x y}{10} - \frac{\sqrt{10}Q_y (x^2 - 2y^2 + z^2)}{10} + \frac{3\sqrt{10}Q_z y z}{10}$$

* Harmonics for rank 2

$$\vec{\mathbb{Q}}_2^{(1,-1)}[q](A_{1g})$$

** symmetry

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

** expression

$$-\frac{\sqrt{6}Q_x x}{6} - \frac{\sqrt{6}Q_y y}{6} + \frac{\sqrt{6}Q_z z}{3}$$

$$\vec{\mathbb{Q}}_2^{(1,1)}[q](A_{1g})$$

** symmetry

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

** expression

$$-\frac{\sqrt{21}Q_xx(x^2+y^2-4z^2)}{14}-\frac{\sqrt{21}Q_yy(x^2+y^2-4z^2)}{14}-\frac{\sqrt{21}Q_zz(3x^2+3y^2-2z^2)}{14}$$

$\vec{\mathbb{Q}}_{2,1}^{(1,-1)}[q](E_{1g}), \vec{\mathbb{Q}}_{2,2}^{(1,-1)}[q](E_{1g})$

** symmetry

$$\sqrt{3}yz$$

$$-\sqrt{3}xz$$

** expression

$$\frac{\sqrt{2}Q_yz}{2}+\frac{\sqrt{2}Q_zy}{2}$$

$$-\frac{\sqrt{2}Q_xz}{2}-\frac{\sqrt{2}Q_zx}{2}$$

$\vec{\mathbb{Q}}_{2,1}^{(1,1)}[q](E_{1g}), \vec{\mathbb{Q}}_{2,2}^{(1,1)}[q](E_{1g})$

** symmetry

$$\sqrt{3}yz$$

$$-\sqrt{3}xz$$

** expression

$$\frac{5\sqrt{7}Q_xxyz}{7}-\frac{\sqrt{7}Q_yz(x^2-4y^2+z^2)}{7}-\frac{\sqrt{7}Q_zy(x^2+y^2-4z^2)}{7}$$

$$-\frac{\sqrt{7}Q_xz(4x^2-y^2-z^2)}{7}-\frac{5\sqrt{7}Q_yxyz}{7}+\frac{\sqrt{7}Q_zx(x^2+y^2-4z^2)}{7}$$

$\vec{\mathbb{Q}}_{2,1}^{(1,-1)}[q](E_{2g}), \vec{\mathbb{Q}}_{2,2}^{(1,-1)}[q](E_{2g})$

** symmetry

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

$$-\sqrt{3}xy$$

** expression

$$\frac{\sqrt{2}Q_xx}{2}-\frac{\sqrt{2}Q_yy}{2}$$

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

$\vec{\mathbb{Q}}_{2,1}^{(1,1)}[q](E_{2g}), \vec{\mathbb{Q}}_{2,2}^{(1,1)}[q](E_{2g})$

** symmetry

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

$$-\sqrt{3}xy$$

** expression

$$\frac{\sqrt{7}Q_xx(3x^2-7y^2-2z^2)}{14}+\frac{\sqrt{7}Q_yy(7x^2-3y^2+2z^2)}{14}+\frac{5\sqrt{7}Q_zz(x-y)(x+y)}{14}$$

$$-\frac{\sqrt{7}Q_xy(4x^2-y^2-z^2)}{7}+\frac{\sqrt{7}Q_yx(x^2-4y^2+z^2)}{7}-\frac{5\sqrt{7}Q_zxyz}{7}$$

* Harmonics for rank 3

$\vec{\mathbb{Q}}_3^{(1,-1)}[q](A_{2u})$

** symmetry

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

** expression

$$-\frac{\sqrt{15}Q_xxz}{5} - \frac{\sqrt{15}Q_yyz}{5} - \frac{\sqrt{15}Q_z(x^2 + y^2 - 2z^2)}{10}$$

$\vec{\mathbb{Q}}_3^{(1,1)}[q](A_{2u})$

** symmetry

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

** expression

$$-\frac{5Q_xxz(3x^2 + 3y^2 - 4z^2)}{12} - \frac{5Q_yyz(3x^2 + 3y^2 - 4z^2)}{12} + \frac{Q_z(3x^4 + 6x^2y^2 - 24x^2z^2 + 3y^4 - 24y^2z^2 + 8z^4)}{12}$$

$\vec{\mathbb{Q}}_3^{(1,-1)}[q](B_{1u})$

** symmetry

$$\frac{\sqrt{10}y(3x^2 - y^2)}{4}$$

** expression

$$\frac{\sqrt{6}Q_xxy}{2} + \frac{\sqrt{6}Q_y(x-y)(x+y)}{4}$$

$\vec{\mathbb{Q}}_3^{(1,1)}[q](B_{1u})$

** symmetry

$$\frac{\sqrt{10}y(3x^2 - y^2)}{4}$$

** expression

$$\frac{\sqrt{10}Q_xxy(15x^2 - 13y^2 - 6z^2)}{24} - \frac{\sqrt{10}Q_y(3x^4 - 21x^2y^2 + 3x^2z^2 + 4y^4 - 3y^2z^2)}{24} + \frac{7\sqrt{10}Q_yyz(3x^2 - y^2)}{24}$$

$\vec{\mathbb{Q}}_3^{(1,-1)}[q](B_{2u})$

** symmetry

$$\frac{\sqrt{10}x(x^2 - 3y^2)}{4}$$

** expression

$$\frac{\sqrt{6}Q_x(x-y)(x+y)}{4} - \frac{\sqrt{6}Q_yxy}{2}$$

$\vec{\mathbb{Q}}_3^{(1,1)}[q](B_{2u})$

** symmetry

$$\frac{\sqrt{10}x(x^2 - 3y^2)}{4}$$

** expression

$$\frac{\sqrt{10}Q_x(4x^4 - 21x^2y^2 - 3x^2z^2 + 3y^4 + 3y^2z^2)}{24} + \frac{\sqrt{10}Q_yxy(13x^2 - 15y^2 + 6z^2)}{24} + \frac{7\sqrt{10}Q_zxz(x^2 - 3y^2)}{24}$$

$\vec{\mathbb{Q}}_{3,1}^{(1,-1)}[q](E_{1u}), \vec{\mathbb{Q}}_{3,2}^{(1,-1)}[q](E_{1u})$

** symmetry

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

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

** expression

$$-\frac{\sqrt{10}Q_x(3x^2 + y^2 - 4z^2)}{20} - \frac{\sqrt{10}Q_yxy}{10} + \frac{2\sqrt{10}Q_zxz}{5}$$

$$-\frac{\sqrt{10}Q_xxy}{10} - \frac{\sqrt{10}Q_y(x^2 + 3y^2 - 4z^2)}{20} + \frac{2\sqrt{10}Q_yyz}{5}$$

$\vec{\mathbb{Q}}_{3,1}^{(1,1)}[q](E_{1u}), \vec{\mathbb{Q}}_{3,2}^{(1,1)}[q](E_{1u})$

** symmetry

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

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

** expression

$$-\frac{\sqrt{6}Q_x(4x^4 + 3x^2y^2 - 27x^2z^2 - y^4 + 3y^2z^2 + 4z^4)}{24} - \frac{5\sqrt{6}Q_yxy(x^2 + y^2 - 6z^2)}{24} - \frac{5\sqrt{6}Q_zxz(3x^2 + 3y^2 - 4z^2)}{24}$$

$$-\frac{5\sqrt{6}Q_xy(x^2 + y^2 - 6z^2)}{24} + \frac{\sqrt{6}Q_y(x^4 - 3x^2y^2 - 3x^2z^2 - 4y^4 + 27y^2z^2 - 4z^4)}{24} - \frac{5\sqrt{6}Q_zyz(3x^2 + 3y^2 - 4z^2)}{24}$$

$\vec{\mathbb{Q}}_{3,1}^{(1,-1)}[q](E_{2u}), \vec{\mathbb{Q}}_{3,2}^{(1,-1)}[q](E_{2u})$

** symmetry

$$\sqrt{15}xyz$$

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

** expression

$$Q_xyz + Q_yxz + Q_zyy$$

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

$\vec{\mathbb{Q}}_{3,1}^{(1,1)}[q](E_{2u}), \vec{\mathbb{Q}}_{3,2}^{(1,1)}[q](E_{2u})$

** symmetry

$$\sqrt{15}xyz$$

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

** expression

$$\frac{\sqrt{15}Q_xy(x^2 - y^2 - z^2)}{6} - \frac{\sqrt{15}Q_yxz(x^2 - 6y^2 + z^2)}{6} - \frac{\sqrt{15}Q_zxy(x^2 + y^2 - 6z^2)}{6}$$

$$\frac{\sqrt{15}Q_xxz(5x^2 - 9y^2 - 2z^2)}{12} + \frac{\sqrt{15}Q_yyz(9x^2 - 5y^2 + 2z^2)}{12} - \frac{\sqrt{15}Q_z(x - y)(x + y)(x^2 + y^2 - 6z^2)}{12}$$

* Harmonics for rank 4

$\vec{\mathbb{Q}}_4^{(1,-1)}[q](A_{1g})$

** symmetry

$$\frac{3x^4}{8} + \frac{3x^2y^2}{4} - 3x^2z^2 + \frac{3y^4}{8} - 3y^2z^2 + z^4$$

** expression

$$\frac{3\sqrt{7}Q_xx(x^2 + y^2 - 4z^2)}{28} + \frac{3\sqrt{7}Q_yy(x^2 + y^2 - 4z^2)}{28} - \frac{\sqrt{7}Q_zz(3x^2 + 3y^2 - 2z^2)}{7}$$

$\vec{\mathbb{Q}}_4^{(1,1)}[q](A_{1g})$

** symmetry

$$\frac{3x^4}{8} + \frac{3x^2y^2}{4} - 3x^2z^2 + \frac{3y^4}{8} - 3y^2z^2 + z^4$$

** expression

$$\begin{aligned} & \frac{3\sqrt{55}Q_xx(x^4 + 2x^2y^2 - 12x^2z^2 + y^4 - 12y^2z^2 + 8z^4)}{88} + \frac{3\sqrt{55}Q_yy(x^4 + 2x^2y^2 - 12x^2z^2 + y^4 - 12y^2z^2 + 8z^4)}{88} \\ & + \frac{\sqrt{55}Q_zz(15x^4 + 30x^2y^2 - 40x^2z^2 + 15y^4 - 40y^2z^2 + 8z^4)}{88} \end{aligned}$$

$\vec{\mathbb{Q}}_4^{(1,-1)}[q](B_{1g})$

** symmetry

$$\frac{\sqrt{70}xz(x^2 - 3y^2)}{4}$$

** expression

$$\frac{3\sqrt{10}Q_xz(x-y)(x+y)}{8} - \frac{3\sqrt{10}Q_yxyz}{4} + \frac{\sqrt{10}Q_zx(x^2-3y^2)}{8}$$

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

** symmetry

$$\frac{\sqrt{70}xz(x^2-3y^2)}{4}$$

** expression

$$\frac{3\sqrt{154}Q_xz(2x^4-9x^2y^2-x^2z^2+y^4+y^2z^2)}{44} + \frac{3\sqrt{154}Q_yxyz(5x^2-7y^2+2z^2)}{44} - \frac{\sqrt{154}Q_zx(x^2-3y^2)(x^2+y^2-8z^2)}{44}$$

$\vec{\mathbb{Q}}_4^{(1,-1)}[q](B_{2g})$

** symmetry

$$\frac{\sqrt{70}yz(3x^2-y^2)}{4}$$

** expression

$$\frac{3\sqrt{10}Q_xyxyz}{4} + \frac{3\sqrt{10}Q_yz(x-y)(x+y)}{8} + \frac{\sqrt{10}Q_zy(3x^2-y^2)}{8}$$

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

** symmetry

$$\frac{\sqrt{70}yz(3x^2-y^2)}{4}$$

** expression

$$\frac{3\sqrt{154}Q_xyxyz(7x^2-5y^2-2z^2)}{44} - \frac{3\sqrt{154}Q_yz(x^4-9x^2y^2+x^2z^2+2y^4-y^2z^2)}{44} - \frac{\sqrt{154}Q_zy(3x^2-y^2)(x^2+y^2-8z^2)}{44}$$

$\vec{\mathbb{Q}}_{4,1}^{(1,-1)}[q](E_{1g}), \vec{\mathbb{Q}}_{4,2}^{(1,-1)}[q](E_{1g})$

** symmetry

$$- \frac{\sqrt{10}yz(3x^2+3y^2-4z^2)}{4}$$

$$\frac{\sqrt{10}xz(3x^2+3y^2-4z^2)}{4}$$

** expression

$$- \frac{3\sqrt{70}Q_xyxyz}{28} - \frac{\sqrt{70}Q_yz(3x^2+9y^2-4z^2)}{56} - \frac{3\sqrt{70}Q_zy(x^2+y^2-4z^2)}{56}$$

$$\frac{\sqrt{70}Q_xz(9x^2+3y^2-4z^2)}{56} + \frac{3\sqrt{70}Q_yxyz}{28} + \frac{3\sqrt{70}Q_zx(x^2+y^2-4z^2)}{56}$$

$\vec{\mathbb{Q}}_{4,1}^{(1,1)}[q](E_{1g}), \vec{\mathbb{Q}}_{4,2}^{(1,1)}[q](E_{1g})$

** symmetry

$$- \frac{\sqrt{10}yz(3x^2+3y^2-4z^2)}{4}$$

$$\frac{\sqrt{10}xz(3x^2+3y^2-4z^2)}{4}$$

** expression

$$- \frac{21\sqrt{22}Q_xyxyz(x^2+y^2-2z^2)}{44} + \frac{\sqrt{22}Q_yz(3x^4-15x^2y^2-x^2z^2-18y^4+41y^2z^2-4z^4)}{44} + \frac{3\sqrt{22}Q_zy(x^4+2x^2y^2-12x^2z^2+y^4-12y^2z^2+8z^4)}{44}$$

$$\frac{\sqrt{22}Q_xz(18x^4+15x^2y^2-41x^2z^2-3y^4+y^2z^2+4z^4)}{44} + \frac{21\sqrt{22}Q_yxyz(x^2+y^2-2z^2)}{44} - \frac{3\sqrt{22}Q_zx(x^4+2x^2y^2-12x^2z^2+y^4-12y^2z^2+8z^4)}{44}$$

$\vec{\mathbb{Q}}_{4,1}^{(1,-1)}[q](E_{2g}, 1), \vec{\mathbb{Q}}_{4,2}^{(1,-1)}[q](E_{2g}, 1)$

** symmetry

$$\frac{\sqrt{35}(x^2-2xy-y^2)(x^2+2xy-y^2)}{8}$$

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

** expression

$$\frac{\sqrt{5}Q_xx(x^2-3y^2)}{4} - \frac{\sqrt{5}Q_yy(3x^2-y^2)}{4}$$

$$\frac{\sqrt{5}Q_xy(3x^2-y^2)}{4} + \frac{\sqrt{5}Q_yx(x^2-3y^2)}{4}$$

$$\vec{\mathbb{Q}}_{4,1}^{(1,-1)}[q](E_{2g}, 2), \vec{\mathbb{Q}}_{4,2}^{(1,-1)}[q](E_{2g}, 2)$$

** symmetry

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

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

** expression

$$-\frac{\sqrt{35}Q_xx(x^2-3z^2)}{14} + \frac{\sqrt{35}Q_yy(y^2-3z^2)}{14} + \frac{3\sqrt{35}Q_zz(x-y)(x+y)}{14}$$

$$\frac{\sqrt{35}Q_xy(3x^2+y^2-6z^2)}{28} + \frac{\sqrt{35}Q_yx(x^2+3y^2-6z^2)}{28} - \frac{3\sqrt{35}Q_zxyz}{7}$$

$$\vec{\mathbb{Q}}_{4,1}^{(1,1)}[q](E_{2g}, 1), \vec{\mathbb{Q}}_{4,2}^{(1,1)}[q](E_{2g}, 1)$$

** symmetry

$$\frac{\sqrt{35}(x^2-2xy-y^2)(x^2+2xy-y^2)}{8}$$

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

** expression

$$\frac{\sqrt{77}Q_xx(5x^4-46x^2y^2-4x^2z^2+21y^4+12y^2z^2)}{88} + \frac{\sqrt{77}Q_yy(21x^4-46x^2y^2+12x^2z^2+5y^4-4y^2z^2)}{88} + \frac{9\sqrt{77}Q_zz(x^2-2xy-y^2)(x^2+2xy-y^2)}{88}$$

$$\frac{\sqrt{77}Q_xy(6x^4-11x^2y^2-3x^2z^2+y^4+y^2z^2)}{22} - \frac{\sqrt{77}Q_yx(x^4-11x^2y^2+x^2z^2+6y^4-3y^2z^2)}{22} + \frac{9\sqrt{77}Q_zxyz(x-y)(x+y)}{22}$$

$$\vec{\mathbb{Q}}_{4,1}^{(1,1)}[q](E_{2g}, 2), \vec{\mathbb{Q}}_{4,2}^{(1,1)}[q](E_{2g}, 2)$$

** symmetry

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

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

** expression

$$-\frac{\sqrt{11}Q_xx(5x^4-4x^2y^2-46x^2z^2-9y^4+66y^2z^2+12z^4)}{44}$$

$$-\frac{\sqrt{11}Q_yy(9x^4+4x^2y^2-66x^2z^2-5y^4+46y^2z^2-12z^4)}{44} - \frac{21\sqrt{11}Q_zz(x-y)(x+y)(x^2+y^2-2z^2)}{44}$$

$$\frac{\sqrt{11}Q_xy(6x^4+5x^2y^2-51x^2z^2-y^4+5y^2z^2+6z^4)}{22} - \frac{\sqrt{11}Q_yx(x^4-5x^2y^2-5x^2z^2-6y^4+51y^2z^2-6z^4)}{22} + \frac{21\sqrt{11}Q_zxyz(x^2+y^2-2z^2)}{22}$$