PG No. 23 C_{6h} $6/m$ [hexagonal] (polar, internal polar dipole)

* Harmonics for rank 0

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

** 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

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

** symmetry

z

** expression

Q_z

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

** symmetry

z

** expression

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

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

** 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

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

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

* Harmonics for rank 2

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

** symmetry

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

** expression

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

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

** symmetry

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

** expression

$$-\frac{\sqrt{21}Q_x x \left(x^2 + y^2 - 4z^2\right)}{14} - \frac{\sqrt{21}Q_y y \left(x^2 + y^2 - 4z^2\right)}{14} - \frac{\sqrt{21}Q_z z \left(3x^2 + 3y^2 - 2z^2\right)}{14}$$

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

** symmetry

$$\sqrt{3}yz$$

$$-\sqrt{3}xz$$

** expression

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

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

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

** symmetry

$$\sqrt{3}yz$$

$$-\sqrt{3}xz$$

** expression

$$\frac{5\sqrt{7}Q_x xyz}{7} - \frac{\sqrt{7}Q_y z \left(x^2 - 4y^2 + z^2\right)}{7} - \frac{\sqrt{7}Q_z y \left(x^2 + y^2 - 4z^2\right)}{7}$$

$$-\frac{\sqrt{7}Q_x z \left(4x^2 - y^2 - z^2\right)}{7} - \frac{5\sqrt{7}Q_y xyz}{7} + \frac{\sqrt{7}Q_z x \left(x^2 + y^2 - 4z^2\right)}{7}$$

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

** symmetry

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

$$-\sqrt{3}xy$$

** expression

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

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

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

** symmetry

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

$$-\sqrt{3}xy$$

** expression

$$\frac{\sqrt{7}Q_x x \left(3x^2 - 7y^2 - 2z^2\right)}{14} + \frac{\sqrt{7}Q_y y \left(7x^2 - 3y^2 + 2z^2\right)}{14} + \frac{5\sqrt{7}Q_z z \left(x - y\right)\left(x + y\right)}{14}$$

$$-\frac{\sqrt{7}Q_x y \left(4x^2 - y^2 - z^2\right)}{7} + \frac{\sqrt{7}Q_y x \left(x^2 - 4y^2 + z^2\right)}{7} - \frac{5\sqrt{7}Q_z xyz}{7}$$

* Harmonics for rank 3

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

** symmetry

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

2

** expression

$$-\frac{\sqrt{15}Q_x xz}{5} - \frac{\sqrt{15}Q_y yz}{5} - \frac{\sqrt{15}Q_z\left(x^2+y^2-2z^2\right)}{10}$$

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

** symmetry

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

** expression

$$-\frac{5Q_x xz\left(3x^2+3y^2-4z^2\right)}{12} - \frac{5Q_y yz\left(3x^2+3y^2-4z^2\right)}{12} + \frac{Q_z\left(3x^4+6x^2y^2-24x^2z^2+3y^4-24y^2z^2+8z^4\right)}{12}$$

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

** symmetry

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

** expression

$$\frac{\sqrt{6}Q_x xy}{2} + \frac{\sqrt{6}Q_y\left(x-y\right)\left(x+y\right)}{4}$$

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

** symmetry

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

** expression

$$\frac{\sqrt{6}Q_x\left(x-y\right)\left(x+y\right)}{4} - \frac{\sqrt{6}Q_y xy}{2}$$

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

** symmetry

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

** expression

$$\frac{\sqrt{10}Q_x xy\left(15x^2-13y^2-6z^2\right)}{24} - \frac{\sqrt{10}Q_y\left(3x^4-21x^2y^2+3x^2z^2+4y^4-3y^2z^2\right)}{24} + \frac{7\sqrt{10}Q_z yz\left(3x^2-y^2\right)}{24}$$

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

** symmetry

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

** expression

$$\frac{\sqrt{10}Q_x\left(4x^4-21x^2y^2-3x^2z^2+3y^4+3y^2z^2\right)}{24} + \frac{\sqrt{10}Q_y xy\left(13x^2-15y^2+6z^2\right)}{24} + \frac{7\sqrt{10}Q_z xz\left(x^2-3y^2\right)}{24}$$

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

** symmetry

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

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

** expression

$$-\frac{\sqrt{10}Q_x\left(3x^2+y^2-4z^2\right)}{20} - \frac{\sqrt{10}Q_y xy}{10} + \frac{2\sqrt{10}Q_z xz}{5}$$

$$-\frac{\sqrt{10}Q_x xy}{10} - \frac{\sqrt{10}Q_y\left(x^2+3y^2-4z^2\right)}{20} + \frac{2\sqrt{10}Q_z yz}{5}$$

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

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

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

** expression

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

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

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

** symmetry

$$\sqrt{15}xyz$$

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

** expression

$$Q_xyz+Q_yxz+Q_zxy$$

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

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

** symmetry

$$\sqrt{15}xyz$$

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

** expression

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

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

* Harmonics for rank 4

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

** symmetry

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

** expression

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

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

** symmetry

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

** expression

$$\frac{3\sqrt{55}Q_xx\left(x^4+2x^2y^2-12x^2z^2+y^4-12y^2z^2+8z^4\right)}{88}+\frac{3\sqrt{55}Q_yy\left(x^4+2x^2y^2-12x^2z^2+y^4-12y^2z^2+8z^4\right)}{88}$$

$$+\frac{\sqrt{55}Q_zz\left(15x^4+30x^2y^2-40x^2z^2+15y^4-40y^2z^2+8z^4\right)}{88}$$

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

** symmetry

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

** expression

$$\frac{3\sqrt{10}Q_x z\left(x-y\right)\left(x+y\right)}{8} - \frac{3\sqrt{10}Q_y xyz}{4} + \frac{\sqrt{10}Q_z x\left(x^2-3y^2\right)}{8}$$

$\vec{\mathbb{Q}}_4^{(1,-1)}[q](B_g, 2)$
** symmetry

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

** expression

$$\frac{3\sqrt{10}Q_x xyz}{4} + \frac{3\sqrt{10}Q_y z\left(x-y\right)\left(x+y\right)}{8} + \frac{\sqrt{10}Q_z y\left(3x^2-y^2\right)}{8}$$

$\vec{\mathbb{Q}}_4^{(1,1)}[q](B_g, 1)$
** symmetry

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

** expression

$$\frac{3\sqrt{154}Q_x z\left(2x^4-9x^2y^2-x^2z^2+y^4+y^2z^2\right)}{44} + \frac{3\sqrt{154}Q_y xyz\left(5x^2-7y^2+2z^2\right)}{44} - \frac{\sqrt{154}Q_z x\left(x^2-3y^2\right)\left(x^2+y^2-8z^2\right)}{44}$$

$\vec{\mathbb{Q}}_4^{(1,1)}[q](B_g, 2)$
** symmetry

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

** expression

$$\frac{3\sqrt{154}Q_x xyz\left(7x^2-5y^2-2z^2\right)}{44} - \frac{3\sqrt{154}Q_y z\left(x^4-9x^2y^2+x^2z^2+2y^4-y^2z^2\right)}{44} - \frac{\sqrt{154}Q_z y\left(3x^2-y^2\right)\left(x^2+y^2-8z^2\right)}{44}$$

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

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

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

** expression

$$-\frac{3\sqrt{70}Q_x xyz}{28} - \frac{\sqrt{70}Q_y z\left(3x^2+9y^2-4z^2\right)}{56} - \frac{3\sqrt{70}Q_z y\left(x^2+y^2-4z^2\right)}{56}$$

$$\frac{\sqrt{70}Q_x z\left(9x^2+3y^2-4z^2\right)}{56} + \frac{3\sqrt{70}Q_y xyz}{28} + \frac{3\sqrt{70}Q_z x\left(x^2+y^2-4z^2\right)}{56}$$

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

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

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

** expression

$$-\frac{21\sqrt{22}Q_x xyz\left(x^2+y^2-2z^2\right)}{44} + \frac{\sqrt{22}Q_y z\left(3x^4-15x^2y^2-x^2z^2-18y^4+41y^2z^2-4z^4\right)}{44} + \frac{3\sqrt{22}Q_z y\left(x^4+2x^2y^2-12x^2z^2+y^4-12y^2z^2+8z^4\right)}{44}$$

$$\frac{\sqrt{22}Q_x z\left(18x^4+15x^2y^2-41x^2z^2-3y^4+y^2z^2+4z^4\right)}{44} + \frac{21\sqrt{22}Q_y xyz\left(x^2+y^2-2z^2\right)}{44} - \frac{3\sqrt{22}Q_z x\left(x^4+2x^2y^2-12x^2z^2+y^4-12y^2z^2+8z^4\right)}{44}$$

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

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

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

** expression

$$\frac{\sqrt{5}Q_x x\,(x^2-3y^2)}{4}-\frac{\sqrt{5}Q_y y\,(3x^2-y^2)}{4}$$

$$\frac{\sqrt{5}Q_x y\,(3x^2-y^2)}{4}+\frac{\sqrt{5}Q_y x\,(x^2-3y^2)}{4}$$

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

$$-\frac{\sqrt{35}Q_x x\,(x^2-3z^2)}{14}+\frac{\sqrt{35}Q_y y\,(y^2-3z^2)}{14}+\frac{3\sqrt{35}Q_z z\,(x-y)\,(x+y)}{14}$$

$$\frac{\sqrt{35}Q_x y\,(3x^2+y^2-6z^2)}{28}+\frac{\sqrt{35}Q_y x\,(x^2+3y^2-6z^2)}{28}-\frac{3\sqrt{35}Q_z xyz}{7}$$

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

$$\frac{\sqrt{77}Q_x x\,(5x^4-46x^2y^2-4x^2z^2+21y^4+12y^2z^2)}{88}+\frac{\sqrt{77}Q_y y\,(21x^4-46x^2y^2+12x^2z^2+5y^4-4y^2z^2)}{88}+\frac{9\sqrt{77}Q_z z\,(x^2-2xy-y^2)\,(x^2+2xy-y^2)}{88}$$

$$\frac{\sqrt{77}Q_x y\,(6x^4-11x^2y^2-3x^2z^2+y^4+y^2z^2)}{22}-\frac{\sqrt{77}Q_y x\,(x^4-11x^2y^2+x^2z^2+6y^4-3y^2z^2)}{22}+\frac{9\sqrt{77}Q_z xyz\,(x-y)\,(x+y)}{22}$$

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

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

$$\frac{\sqrt{11}Q_x y\,(6x^4+5x^2y^2-51x^2z^2-y^4+5y^2z^2+6z^4)}{22}-\frac{\sqrt{11}Q_y x\,(x^4-5x^2y^2-5x^2z^2-6y^4+51y^2z^2-6z^4)}{22}+\frac{21\sqrt{11}Q_z xyz\,(x^2+y^2-2z^2)}{22}$$