PG No. 4 C_{s} $\quad m$ (b-axis setting) [monoclinic] (polar, internal polar dipole)

* Harmonics for rank 0

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

** 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

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

** symmetry

x

** expression

Q_x

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

** symmetry

z

** expression

Q_z

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

** symmetry

x

** expression

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

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

** symmetry

z

** expression

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

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

** symmetry

y

** expression

Q_y

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

** symmetry

y

** expression

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

* Harmonics for rank 2

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

** symmetry

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

** expression

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

$\vec{\mathbb{Q}}_2^{(1,-1)}[q](A',2)$
** symmetry

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

** expression

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

$\vec{\mathbb{Q}}_2^{(1,-1)}[q](A',3)$
** symmetry

$$\sqrt{3}xz$$

** expression

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

$\vec{\mathbb{Q}}_2^{(1,1)}[q](A',1)$
** symmetry

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

** expression

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

$\vec{\mathbb{Q}}_2^{(1,1)}[q](A',2)$
** symmetry

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

** expression

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

$\vec{\mathbb{Q}}_2^{(1,1)}[q](A',3)$
** symmetry

$$\sqrt{3}xz$$

** expression

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

$\vec{\mathbb{Q}}_2^{(1,-1)}[q](A'',1)$
** symmetry

$$\sqrt{3}yz$$

** expression

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

$\vec{\mathbb{Q}}_2^{(1,-1)}[q](A'',2)$
** symmetry

$$\sqrt{3}xy$$

** expression

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

$\vec{\mathbb{Q}}_2^{(1,1)}[q](A'',1)$
** symmetry

$$\sqrt{3}yz$$

** expression

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

$\vec{\mathbb{Q}}_2^{(1,1)}[q](A'', 2)$

** symmetry

$$\sqrt{3}xy$$

** expression

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

* Harmonics for rank 3

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

** symmetry

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

** expression

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

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

** symmetry

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

** expression

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

$\vec{\mathbb{Q}}_3^{(1,-1)}[q](A', 3)$

** symmetry

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

** expression

$$\frac{Q_x\left(y - z\right)\left(y + z\right)}{2} + Q_y xy - Q_z xz$$

$\vec{\mathbb{Q}}_3^{(1,-1)}[q](A', 4)$

** symmetry

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

** expression

$$Q_x xz - Q_y yz + \frac{Q_z\left(x - y\right)\left(x + y\right)}{2}$$

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

** symmetry

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

** expression

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

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

** symmetry

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

** expression

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

$\vec{\mathbb{Q}}_3^{(1,1)}[q](A', 3)$

** symmetry

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

** expression

$$\frac{\sqrt{15}Q_x\,(y-z)\,(y+z)\,(6x^2-y^2-z^2)}{12} - \frac{\sqrt{15}Q_y xy\,(2x^2-5y^2+9z^2)}{12} + \frac{\sqrt{15}Q_z xz\,(2x^2+9y^2-5z^2)}{12}$$

$\vec{\mathbb{Q}}_3^{(1,1)}[q](A',4)$

** symmetry

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

** expression

$$\frac{\sqrt{15}Q_x xz\,(5x^2-9y^2-2z^2)}{12} + \frac{\sqrt{15}Q_y yz\,(9x^2-5y^2+2z^2)}{12} - \frac{\sqrt{15}Q_z\,(x-y)\,(x+y)\,(x^2+y^2-6z^2)}{12}$$

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

** symmetry

$$\sqrt{15}xyz$$

** expression

$$Q_x yz + Q_y xz + Q_z xy$$

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

** symmetry

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

** expression

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

$\vec{\mathbb{Q}}_3^{(1,-1)}[q](A'',3)$

** symmetry

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

** expression

$$-Q_x xy - \frac{Q_y\,(x-z)\,(x+z)}{2} + Q_z yz$$

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

** symmetry

$$\sqrt{15}xyz$$

** expression

$$\frac{\sqrt{15}Q_x yz\,(6x^2-y^2-z^2)}{6} - \frac{\sqrt{15}Q_y xz\,(x^2-6y^2+z^2)}{6} - \frac{\sqrt{15}Q_z xy\,(x^2+y^2-6z^2)}{6}$$

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

** symmetry

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

** expression

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

$\vec{\mathbb{Q}}_3^{(1,1)}[q](A'',3)$

** symmetry

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

** expression

$$-\frac{\sqrt{15}Q_x xy\,(5x^2-2y^2-9z^2)}{12} + \frac{\sqrt{15}Q_y\,(x-z)\,(x+z)\,(x^2-6y^2+z^2)}{12} - \frac{\sqrt{15}Q_z yz\,(9x^2+2y^2-5z^2)}{12}$$

* Harmonics for rank 4

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

** symmetry

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

** expression

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

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

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

** expression

$$-\frac{\sqrt{105}Q_x x\left(x^2 - 6y^2 + 3z^2\right)}{42} + \frac{\sqrt{105}Q_y y\left(6x^2 - y^2 - 3z^2\right)}{42} - \frac{\sqrt{105}Q_z z\left(3x^2 + 3y^2 - 2z^2\right)}{42}$$

$\vec{\mathbb{Q}}_4^{(1,-1)}[q](A',3)$
** symmetry

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

** expression

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

$\vec{\mathbb{Q}}_4^{(1,-1)}[q](A',4)$
** symmetry

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

** expression

$$-\frac{\sqrt{5}Q_x z\left(3x^2 - z^2\right)}{4} - \frac{\sqrt{5}Q_z x\left(x^2 - 3z^2\right)}{4}$$

$\vec{\mathbb{Q}}_4^{(1,-1)}[q](A',5)$
** symmetry

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

** expression

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

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

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

** expression

$$\frac{\sqrt{1155}Q_x x\left(x^4 - 5x^2y^2 - 5x^2z^2 + 3y^4 - 3y^2z^2 + 3z^4\right)}{66} + \frac{\sqrt{1155}Q_y y\left(3x^4 - 5x^2y^2 - 3x^2z^2 + y^4 - 5y^2z^2 + 3z^4\right)}{66}$$
$$+ \frac{\sqrt{1155}Q_z z\left(3x^4 - 3x^2y^2 - 5x^2z^2 + 3y^4 - 5y^2z^2 + z^4\right)}{66}$$

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

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

** expression

$$-\frac{\sqrt{33}Q_x x\left(5x^4 - 88x^2y^2 + 38x^2z^2 + 33y^4 + 66y^2z^2 - 30z^4\right)}{132} - \frac{\sqrt{33}Q_y y\left(33x^4 - 88x^2y^2 + 66x^2z^2 + 5y^4 + 38y^2z^2 - 30z^4\right)}{132}$$
$$+ \frac{\sqrt{33}Q_z z\left(3x^4 + 132x^2y^2 - 50x^2z^2 + 3y^4 - 50y^2z^2 + 10z^4\right)}{132}$$

$\vec{\mathbb{Q}}_4^{(1,1)}[q](A',3)$

** symmetry

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

** expression

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

$\vec{\mathbb{Q}}_4^{(1,1)}[q](A',4)$

** symmetry

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

** expression

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

$\vec{\mathbb{Q}}_4^{(1,1)}[q](A',5)$

** symmetry

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

** expression

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

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

** symmetry

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

** expression

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

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

** symmetry

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

** expression

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

$\vec{\mathbb{Q}}_4^{(1,-1)}[q](A'',3)$

** symmetry

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

** expression

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

$\vec{\mathbb{Q}}_4^{(1,-1)}[q](A'',4)$

** symmetry

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

** expression

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

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

** symmetry

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

** expression

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

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

** symmetry

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

** expression

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

$\vec{\mathbb{Q}}_4^{(1,1)}[q](A'',3)$

** symmetry

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

** expression

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

$\vec{\mathbb{Q}}_4^{(1,1)}[q](A'',4)$

** symmetry

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

** expression

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