PG No. 5 $C_{2\mathrm{h}}$ $2/m$ (b-axis setting) [monoclinic] (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

$$y$$

** expression

$$Q_{y}$$

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

** symmetry

$$y$$

** expression

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

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

** symmetry

$$x$$

** expression

$$Q_{x}$$

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

** symmetry

$$z$$

** expression

$$Q_{z}$$

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

** symmetry

$$x$$

** expression

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

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

** symmetry

$$z$$

** expression

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

* Harmonics for rank 2

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

** symmetry

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

** expression

$$-\frac{\sqrt{6}Q_{x}x}{6}-\frac{\sqrt{6}Q_{y}y}{6}+\frac{\sqrt{6}Q_{z}z}{3}$$

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

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

** expression

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

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

$$\sqrt{3}xz$$

** expression

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

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

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

** expression

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

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

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

** expression

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

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

$$\sqrt{3}xz$$

** expression

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

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

$$\sqrt{3}yz$$

** expression

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

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

$$\sqrt{3}xy$$

** expression

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

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

$$\sqrt{3}yz$$

** expression

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

$\vec{\mathbb{Q}}_2^{(1,1)}[q](B_g,2)$
** 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
$\vec{\mathbb{Q}}_3^{(1,-1)}[q](A_u,1)$
** symmetry

$$\sqrt{15}xyz$$

** expression

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

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

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

** expression

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

$\vec{\mathbb{Q}}_3^{(1,-1)}[q](A_u,3)$
** symmetry

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

** expression

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

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

$$\sqrt{15}xyz$$

** expression

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

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

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

** expression

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

$\vec{\mathbb{Q}}_3^{(1,1)}[q](A_u,3)$
** symmetry

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

** expression

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

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

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

** expression

$$\frac{\sqrt{15}Q_x\left(2x^2-y^2-z^2\right)}{10}-\frac{\sqrt{15}Q_yxy}{5}-\frac{\sqrt{15}Q_zxz}{5}$$

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

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

** expression

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

$\vec{\mathbb{Q}}_3^{(1,-1)}[q](B_u,3)$
** symmetry

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

** expression

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

$\vec{\mathbb{Q}}_3^{(1,-1)}[q](B_u,4)$
** symmetry

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

** expression

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

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

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

** expression

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

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

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

** expression

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

$\vec{\mathbb{Q}}_3^{(1,1)}[q](B_u,3)$
** symmetry

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

** expression

$$\frac{\sqrt{15}Q_x\left(y-z\right)\left(y+z\right)\left(6x^2-y^2-z^2\right)}{12}-\frac{\sqrt{15}Q_yxy\left(2x^2-5y^2+9z^2\right)}{12}+\frac{\sqrt{15}Q_zxz\left(2x^2+9y^2-5z^2\right)}{12}$$

$\vec{\mathbb{Q}}_3^{(1,1)}[q](B_u,4)$
** symmetry

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

** expression

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

* Harmonics for rank 4

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

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

** expression

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

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

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

** expression

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

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

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

** expression

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

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

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

** expression

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

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

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

** expression

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

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

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

** expression

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

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

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

** expression

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

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

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

** expression

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

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

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

** expression

$$-\frac{\sqrt{77}Q_{x}z\left(6x^{4}-3x^{2}y^{2}-11x^{2}z^{2}+y^{2}z^{2}+z^{4}\right)}{22}-\frac{9\sqrt{77}Q_{y}xyz\left(x-z\right)\left(x+z\right)}{22}+\frac{\sqrt{77}Q_{z}x\left(x^{4}+x^{2}y^{2}-11x^{2}z^{2}-3y^{2}z^{2}+6z^{4}\right)}{22}$$

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

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

** expression

$$-\frac{\sqrt{11}Q_{x}z\left(6x^{4}-51x^{2}y^{2}+5x^{2}z^{2}+6y^{4}+5y^{2}z^{2}-z^{4}\right)}{22}-\frac{21\sqrt{11}Q_{y}xyz\left(x^{2}-2y^{2}+z^{2}\right)}{22}+\frac{\sqrt{11}Q_{z}x\left(x^{4}-5x^{2}y^{2}-5x^{2}z^{2}-6y^{4}+51y^{2}z^{2}-6z^{4}\right)}{22}$$

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

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

** expression

$$\frac{\sqrt{5}Q_{y}z\left(3y^{2}-z^{2}\right)}{4}+\frac{\sqrt{5}Q_{z}y\left(y^{2}-3z^{2}\right)}{4}$$

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

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

** expression

$$\frac{\sqrt{5}Q_{x}y\left(3x^{2}-y^{2}\right)}{4}+\frac{\sqrt{5}Q_{y}x\left(x^{2}-3y^{2}\right)}{4}$$

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

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

** expression

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

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

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

** expression

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

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

** symmetry

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

** expression

$$\frac{9\sqrt{77}Q_{x}xyz\left(y-z\right)\left(y+z\right)}{22}-\frac{\sqrt{77}Q_{y}z\left(3x^{2}y^{2}-x^{2}z^{2}-6y^{4}+11y^{2}z^{2}-z^{4}\right)}{22}-\frac{\sqrt{77}Q_{z}y\left(x^{2}y^{2}-3x^{2}z^{2}+y^{4}-11y^{2}z^{2}+6z^{4}\right)}{22}$$

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

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

** expression

$$\frac{\sqrt{77}Q_{x}y\left(6x^{4}-11x^{2}y^{2}-3x^{2}z^{2}+y^{4}+y^{2}z^{2}\right)}{22}-\frac{\sqrt{77}Q_{y}x\left(x^{4}-11x^{2}y^{2}+x^{2}z^{2}+6y^{4}-3y^{2}z^{2}\right)}{22}+\frac{9\sqrt{77}Q_{z}xyz\left(x-y\right)\left(x+y\right)}{22}$$

$\vec{\mathbb{Q}}_{4}^{(1,1)}[q](B_{g},3)$
** symmetry

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

** expression

$$\frac{21\sqrt{11}Q_{x}xyz\left(2x^{2}-y^{2}-z^{2}\right)}{22}-\frac{\sqrt{11}Q_{y}z\left(6x^{4}-51x^{2}y^{2}+5x^{2}z^{2}+6y^{4}+5y^{2}z^{2}-z^{4}\right)}{22}-\frac{\sqrt{11}Q_{z}y\left(6x^{4}+5x^{2}y^{2}-51x^{2}z^{2}-y^{4}+5y^{2}z^{2}+6z^{4}\right)}{22}$$

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

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

** expression

$$-\frac{\sqrt{11}Q_{x}y\left(6x^{4}+5x^{2}y^{2}-51x^{2}z^{2}-y^{4}+5y^{2}z^{2}+6z^{4}\right)}{22}+\frac{\sqrt{11}Q_{y}x\left(x^{4}-5x^{2}y^{2}-5x^{2}z^{2}-6y^{4}+51y^{2}z^{2}-6z^{4}\right)}{22}-\frac{21\sqrt{11}Q_{z}xyz\left(x^{2}+y^{2}-2z^{2}\right)}{22}$$