

PG No. 4 C_s m (b-axis setting) [monoclinic] (axial, internal axial dipole)

* Harmonics for rank 0

$$\bar{G}_0^{(1,1)}[g](A'')$$

** symmetry

$$1$$

** expression

$$\frac{\sqrt{3}G_x x}{3} + \frac{\sqrt{3}G_y y}{3} + \frac{\sqrt{3}G_z z}{3}$$

* Harmonics for rank 1

$$\bar{G}_1^{(1,-1)}[g](A')$$

** symmetry

$$y$$

** expression

$$G_y$$

$$\bar{G}_1^{(1,1)}[g](A')$$

** symmetry

$$y$$

** expression

$$\frac{3\sqrt{10}G_x xy}{10} - \frac{\sqrt{10}G_y (x^2 - 2y^2 + z^2)}{10} + \frac{3\sqrt{10}G_z yz}{10}$$

$$\bar{G}_1^{(1,-1)}[g](A'', 1)$$

** symmetry

$$x$$

** expression

$$G_x$$

$$\bar{G}_1^{(1,-1)}[g](A'', 2)$$

** symmetry

$$z$$

** expression

$$G_z$$

$$\bar{G}_1^{(1,1)}[g](A'', 1)$$

** symmetry

$$x$$

** expression

$$\frac{\sqrt{10}G_x (2x^2 - y^2 - z^2)}{10} + \frac{3\sqrt{10}G_y xy}{10} + \frac{3\sqrt{10}G_z xz}{10}$$

$$\bar{G}_1^{(1,1)}[g](A'', 2)$$

** symmetry

$$z$$

** expression

$$\frac{3\sqrt{10}G_x xz}{10} + \frac{3\sqrt{10}G_y yz}{10} - \frac{\sqrt{10}G_z (x^2 + y^2 - 2z^2)}{10}$$

* Harmonics for rank 2

$$\bar{G}_2^{(1,-1)}[g](A', 1)$$

** symmetry

$$\sqrt{3}yz$$

** expression

$$\frac{\sqrt{2}G_y z}{2} + \frac{\sqrt{2}G_z y}{2}$$

$$\vec{\mathbb{G}}_2^{(1,-1)}[g](A', 2)$$

** symmetry

$$\sqrt{3}xy$$

** expression

$$\frac{\sqrt{2}G_{xy}}{2} + \frac{\sqrt{2}G_{yx}}{2}$$

$$\vec{\mathbb{G}}_2^{(1,1)}[g](A', 1)$$

** symmetry

$$\sqrt{3}yz$$

** expression

$$\frac{5\sqrt{7}G_{xyz}}{7} - \frac{\sqrt{7}G_{yz}(x^2 - 4y^2 + z^2)}{7} - \frac{\sqrt{7}G_{zy}(x^2 + y^2 - 4z^2)}{7}$$

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

** symmetry

$$\sqrt{3}xy$$

** expression

$$\frac{\sqrt{7}G_{xy}(4x^2 - y^2 - z^2)}{7} - \frac{\sqrt{7}G_{yx}(x^2 - 4y^2 + z^2)}{7} + \frac{5\sqrt{7}G_{zxy}}{7}$$

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

** symmetry

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

** expression

$$-\frac{\sqrt{6}G_{xx}}{6} - \frac{\sqrt{6}G_{yy}}{6} + \frac{\sqrt{6}G_{zz}}{3}$$

$$\vec{\mathbb{G}}_2^{(1,-1)}[g](A'', 2)$$

** symmetry

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

** expression

$$\frac{\sqrt{2}G_{xx}}{2} - \frac{\sqrt{2}G_{yy}}{2}$$

$$\vec{\mathbb{G}}_2^{(1,-1)}[g](A'', 3)$$

** symmetry

$$\sqrt{3}xz$$

** expression

$$\frac{\sqrt{2}G_{xz}}{2} + \frac{\sqrt{2}G_{zx}}{2}$$

$$\vec{\mathbb{G}}_2^{(1,1)}[g](A'', 1)$$

** symmetry

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

** expression

$$-\frac{\sqrt{21}G_{xx}(x^2 + y^2 - 4z^2)}{14} - \frac{\sqrt{21}G_{yy}(x^2 + y^2 - 4z^2)}{14} - \frac{\sqrt{21}G_{zz}(3x^2 + 3y^2 - 2z^2)}{14}$$

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

** symmetry

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

** expression

$$\frac{\sqrt{7}G_x x (3x^2 - 7y^2 - 2z^2)}{14} + \frac{\sqrt{7}G_y y (7x^2 - 3y^2 + 2z^2)}{14} + \frac{5\sqrt{7}G_z z (x - y) (x + y)}{14}$$

$$\vec{\mathbb{G}}_2^{(1,1)}[g](A'', 3)$$

** symmetry

$$\sqrt{3}xz$$

** expression

$$\frac{\sqrt{7}G_x z (4x^2 - y^2 - z^2)}{7} + \frac{5\sqrt{7}G_y xyz}{7} - \frac{\sqrt{7}G_z x (x^2 + y^2 - 4z^2)}{7}$$

* Harmonics for rank 3

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

** symmetry

$$\sqrt{15}xyz$$

** expression

$$G_x y z + G_y x z + G_z x y$$

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

** symmetry

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

** expression

$$-\frac{\sqrt{15}G_x xy}{5} - \frac{\sqrt{15}G_y (x^2 - 2y^2 + z^2)}{10} - \frac{\sqrt{15}G_z yz}{5}$$

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

** symmetry

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

** expression

$$-G_x xy - \frac{G_y(x-z)(x+z)}{2} + G_z yz$$

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

** symmetry

$$\sqrt{15}xyz$$

** expression

$$\frac{\sqrt{15}G_x yz (6x^2 - y^2 - z^2)}{6} - \frac{\sqrt{15}G_y xz (x^2 - 6y^2 + z^2)}{6} - \frac{\sqrt{15}G_z xy (x^2 + y^2 - 6z^2)}{6}$$

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

** symmetry

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

** expression

$$-\frac{5G_x xy (3x^2 - 4y^2 + 3z^2)}{12} + \frac{G_y (3x^4 - 24x^2 y^2 + 6x^2 z^2 + 8y^4 - 24y^2 z^2 + 3z^4)}{12} - \frac{5G_z yz (3x^2 - 4y^2 + 3z^2)}{12}$$

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

** symmetry

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

** expression

$$-\frac{\sqrt{15}G_x xy (5x^2 - 2y^2 - 9z^2)}{12} + \frac{\sqrt{15}G_y (x-z)(x+z)(x^2 - 6y^2 + z^2)}{12} - \frac{\sqrt{15}G_z yz (9x^2 + 2y^2 - 5z^2)}{12}$$

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

** symmetry

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

** expression

$$\frac{\sqrt{15}G_x(2x^2 - y^2 - z^2)}{10} - \frac{\sqrt{15}G_yxy}{5} - \frac{\sqrt{15}G_zxz}{5}$$

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

** symmetry

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

** expression

$$-\frac{\sqrt{15}G_xxz}{5} - \frac{\sqrt{15}G_yyz}{5} - \frac{\sqrt{15}G_z(x^2 + y^2 - 2z^2)}{10}$$

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

** symmetry

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

** expression

$$\frac{G_x(y-z)(y+z)}{2} + G_yxy - G_zxz$$

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

** symmetry

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

** expression

$$G_xxz - G_yyz + \frac{G_z(x-y)(x+y)}{2}$$

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

** symmetry

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

** expression

$$\frac{G_x(8x^4 - 24x^2y^2 - 24x^2z^2 + 3y^4 + 6y^2z^2 + 3z^4)}{12} + \frac{5G_yxy(4x^2 - 3y^2 - 3z^2)}{12} + \frac{5G_zxz(4x^2 - 3y^2 - 3z^2)}{12}$$

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

** symmetry

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

** expression

$$-\frac{5G_xxz(3x^2 + 3y^2 - 4z^2)}{12} - \frac{5G_yyz(3x^2 + 3y^2 - 4z^2)}{12} + \frac{G_z(3x^4 + 6x^2y^2 - 24x^2z^2 + 3y^4 - 24y^2z^2 + 8z^4)}{12}$$

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

** symmetry

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

** expression

$$\frac{\sqrt{15}G_x(y-z)(y+z)(6x^2 - y^2 - z^2)}{12} - \frac{\sqrt{15}G_yxy(2x^2 - 5y^2 + 9z^2)}{12} + \frac{\sqrt{15}G_zxz(2x^2 + 9y^2 - 5z^2)}{12}$$

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

** symmetry

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

** expression

$$\frac{\sqrt{15}G_x x z (5x^2 - 9y^2 - 2z^2)}{12} + \frac{\sqrt{15}G_y y z (9x^2 - 5y^2 + 2z^2)}{12} - \frac{\sqrt{15}G_z (x - y)(x + y)(x^2 + y^2 - 6z^2)}{12}$$

* Harmonics for rank 4

$$\bar{\mathbb{G}}_4^{(1,-1)}[g](A', 1)$$

** symmetry

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

** expression

$$\frac{\sqrt{5}G_y z (3y^2 - z^2)}{4} + \frac{\sqrt{5}G_z y (y^2 - 3z^2)}{4}$$

$$\bar{\mathbb{G}}_4^{(1,-1)}[g](A', 2)$$

** symmetry

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

** expression

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

$$\bar{\mathbb{G}}_4^{(1,-1)}[g](A', 3)$$

** symmetry

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

** expression

$$\frac{3\sqrt{35}G_x x y z}{7} + \frac{\sqrt{35}G_y z (6x^2 - 3y^2 - z^2)}{28} + \frac{\sqrt{35}G_z y (6x^2 - y^2 - 3z^2)}{28}$$

$$\bar{\mathbb{G}}_4^{(1,-1)}[g](A', 4)$$

** symmetry

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

** expression

$$-\frac{\sqrt{35}G_x y (3x^2 + y^2 - 6z^2)}{28} - \frac{\sqrt{35}G_y x (x^2 + 3y^2 - 6z^2)}{28} + \frac{3\sqrt{35}G_z x y z}{7}$$

$$\bar{\mathbb{G}}_4^{(1,1)}[g](A', 1)$$

** symmetry

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

** expression

$$\frac{9\sqrt{77}G_x x y z (y - z)(y + z)}{22} - \frac{\sqrt{77}G_y z (3x^2 y^2 - x^2 z^2 - 6y^4 + 11y^2 z^2 - z^4)}{22} - \frac{\sqrt{77}G_z y (x^2 y^2 - 3x^2 z^2 + y^4 - 11y^2 z^2 + 6z^4)}{22}$$

$$\bar{\mathbb{G}}_4^{(1,1)}[g](A', 2)$$

** symmetry

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

** expression

$$\frac{\sqrt{77}G_x y (6x^4 - 11x^2 y^2 - 3x^2 z^2 + y^4 + y^2 z^2)}{22} - \frac{\sqrt{77}G_y x (x^4 - 11x^2 y^2 + x^2 z^2 + 6y^4 - 3y^2 z^2)}{22} + \frac{9\sqrt{77}G_z x y z (x - y)(x + y)}{22}$$

$$\bar{\mathbb{G}}_4^{(1,1)}[g](A', 3)$$

** symmetry

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

** expression

$$\frac{21\sqrt{11}G_x x y z (2x^2 - y^2 - z^2)}{22} - \frac{\sqrt{11}G_y z (6x^4 - 51x^2 y^2 + 5x^2 z^2 + 6y^4 + 5y^2 z^2 - z^4)}{22} - \frac{\sqrt{11}G_z y (6x^4 + 5x^2 y^2 - 51x^2 z^2 - y^4 + 5y^2 z^2 + 6z^4)}{22}$$

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

** symmetry

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

** expression

$$-\frac{\sqrt{11}G_{xy}(6x^4 + 5x^2y^2 - 51x^2z^2 - y^4 + 5y^2z^2 + 6z^4)}{22} + \frac{\sqrt{11}G_{yx}(x^4 - 5x^2y^2 - 5x^2z^2 - 6y^4 + 51y^2z^2 - 6z^4)}{22} - \frac{21\sqrt{11}G_{zxyz}(x^2 + y^2 - 2z^2)}{22}$$

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

** symmetry

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

** expression

$$\frac{\sqrt{3}G_{xx}(2x^2 - 3y^2 - 3z^2)}{6} - \frac{\sqrt{3}G_{yy}(3x^2 - 2y^2 + 3z^2)}{6} - \frac{\sqrt{3}G_{zz}(3x^2 + 3y^2 - 2z^2)}{6}$$

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

** symmetry

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

** expression

$$-\frac{\sqrt{105}G_{xx}(x^2 - 6y^2 + 3z^2)}{42} + \frac{\sqrt{105}G_{yy}(6x^2 - y^2 - 3z^2)}{42} - \frac{\sqrt{105}G_{zz}(3x^2 + 3y^2 - 2z^2)}{42}$$

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

** symmetry

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

** expression

$$\frac{\sqrt{35}G_{xx}(x^2 - 3z^2)}{14} - \frac{\sqrt{35}G_{yy}(y^2 - 3z^2)}{14} - \frac{3\sqrt{35}G_{zz}(x-y)(x+y)}{14}$$

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

** symmetry

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

** expression

$$-\frac{\sqrt{5}G_{xz}(3x^2 - z^2)}{4} - \frac{\sqrt{5}G_{zx}(x^2 - 3z^2)}{4}$$

$$\vec{\mathbb{G}}_4^{(1,-1)}[g](A'', 5)$$

** symmetry

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

** expression

$$-\frac{\sqrt{35}G_{xz}(3x^2 - 6y^2 + z^2)}{28} + \frac{3\sqrt{35}G_{yxyz}}{7} - \frac{\sqrt{35}G_{zx}(x^2 - 6y^2 + 3z^2)}{28}$$

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

** symmetry

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

** expression

$$\frac{\sqrt{1155}G_{xx}(x^4 - 5x^2y^2 - 5x^2z^2 + 3y^4 - 3y^2z^2 + 3z^4)}{66} + \frac{\sqrt{1155}G_{yy}(3x^4 - 5x^2y^2 - 3x^2z^2 + y^4 - 5y^2z^2 + 3z^4)}{66} + \frac{\sqrt{1155}G_{zz}(3x^4 - 3x^2y^2 - 5x^2z^2 + 3y^4 - 5y^2z^2 + z^4)}{66}$$

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

** symmetry

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

** expression

$$-\frac{\sqrt{33}G_x x (5x^4 - 88x^2y^2 + 38x^2z^2 + 33y^4 + 66y^2z^2 - 30z^4)}{132} - \frac{\sqrt{33}G_y y (33x^4 - 88x^2y^2 + 66x^2z^2 + 5y^4 + 38y^2z^2 - 30z^4)}{132} + \frac{\sqrt{33}G_z z (3x^4 + 132x^2y^2 - 50x^2z^2 + 3y^4 - 50y^2z^2 + 10z^4)}{132}$$

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

** symmetry

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

** expression

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

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

** symmetry

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

** expression

$$-\frac{\sqrt{77}G_x z (6x^4 - 3x^2y^2 - 11x^2z^2 + y^2z^2 + z^4)}{22} - \frac{9\sqrt{77}G_y xyz(x-z)(x+z)}{22} + \frac{\sqrt{77}G_z x (x^4 + x^2y^2 - 11x^2z^2 - 3y^2z^2 + 6z^4)}{22}$$

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

** symmetry

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

** expression

$$-\frac{\sqrt{11}G_x z (6x^4 - 51x^2y^2 + 5x^2z^2 + 6y^4 + 5y^2z^2 - z^4)}{22} - \frac{21\sqrt{11}G_y xyz(x^2 - 2y^2 + z^2)}{22} + \frac{\sqrt{11}G_z x (x^4 - 5x^2y^2 - 5x^2z^2 - 6y^4 + 51y^2z^2 - 6z^4)}{22}$$