

PG No. 3  $C_2$  2 (b-axis setting) [ monoclinic ] (axial, internal axial dipole)

\* Harmonics for rank 0

$$\vec{\mathbb{G}}_0^{(1,1)}[g](A)$$

\*\* 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

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

\*\* symmetry

$y$

\*\* expression

$$G_y$$

$$\vec{\mathbb{G}}_1^{(1,1)}[g](A)$$

\*\* symmetry

$y$

\*\* expression

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

$$\vec{\mathbb{G}}_1^{(1,-1)}[g](B, 1)$$

\*\* symmetry

$x$

\*\* expression

$$G_x$$

$$\vec{\mathbb{G}}_1^{(1,-1)}[g](B, 2)$$

\*\* symmetry

$z$

\*\* expression

$$G_z$$

$$\vec{\mathbb{G}}_1^{(1,1)}[g](B, 1)$$

\*\* symmetry

$x$

\*\* expression

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

$$\vec{\mathbb{G}}_1^{(1,1)}[g](B, 2)$$

\*\* 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

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

\*\* symmetry

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

\*\* expression

$$-\frac{\sqrt{6}G_x x}{6} - \frac{\sqrt{6}G_y y}{6} + \frac{\sqrt{6}G_z z}{3}$$

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

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

\*\* expression

$$\frac{\sqrt{2}G_x x}{2} - \frac{\sqrt{2}G_y y}{2}$$

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

$$\sqrt{3}xz$$

\*\* expression

$$\frac{\sqrt{2}G_x z}{2} + \frac{\sqrt{2}G_z x}{2}$$

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

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

\*\* expression

$$-\frac{\sqrt{21}G_x x (x^2 + y^2 - 4z^2)}{14} - \frac{\sqrt{21}G_y y (x^2 + y^2 - 4z^2)}{14} - \frac{\sqrt{21}G_z z (3x^2 + 3y^2 - 2z^2)}{14}$$

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

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

$\vec{\mathbb{G}}_2^{(1,-1)}[g](B, 1)$   
\*\* symmetry

$$\sqrt{3}yz$$

\*\* expression

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

$\vec{\mathbb{G}}_2^{(1,-1)}[g](B, 2)$   
\*\* symmetry

$$\sqrt{3}xy$$

\*\* expression

$$\frac{\sqrt{2}G_x y}{2} + \frac{\sqrt{2}G_y x}{2}$$

$\vec{\mathbb{G}}_2^{(1,1)}[g](B, 1)$   
\*\* symmetry

$$\sqrt{3}yz$$

\*\* expression

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

$$\tilde{\mathbb{G}}_2^{(1,1)}[g](B, 2)$$

\*\* symmetry

$$\sqrt{3}xy$$

\*\* expression

$$\frac{\sqrt{7}G_xy(4x^2-y^2-z^2)}{7}-\frac{\sqrt{7}G_yx(x^2-4y^2+z^2)}{7}+\frac{5\sqrt{7}G_zxyz}{7}$$

\* Harmonics for rank 3

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

\*\* symmetry

$$\sqrt{15}xyz$$

\*\* expression

$$G_xyz+G_yxz+G_zxy$$

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

\*\* symmetry

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

\*\* expression

$$-\frac{\sqrt{15}G_xxy}{5}-\frac{\sqrt{15}G_y(x^2-2y^2+z^2)}{10}-\frac{\sqrt{15}G_zyz}{5}$$

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

\*\* symmetry

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

\*\* expression

$$-G_xxy-\frac{G_y(x-z)(x+z)}{2}+G_zyz$$

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

\*\* symmetry

$$\sqrt{15}xyz$$

\*\* expression

$$\frac{\sqrt{15}G_xyz(6x^2-y^2-z^2)}{6}-\frac{\sqrt{15}G_yxz(x^2-6y^2+z^2)}{6}-\frac{\sqrt{15}G_zxy(x^2+y^2-6z^2)}{6}$$

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

\*\* symmetry

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

\*\* expression

$$-\frac{5G_xxy(3x^2-4y^2+3z^2)}{12}+\frac{G_y(3x^4-24x^2y^2+6x^2z^2+8y^4-24y^2z^2+3z^4)}{12}-\frac{5G_zyz(3x^2-4y^2+3z^2)}{12}$$

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

\*\* symmetry

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

\*\* expression

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

$$\tilde{\mathbb{G}}_3^{(1,-1)}[g](B, 1)$$

\*\* symmetry

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

\*\* expression

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

$\tilde{\mathbb{G}}_3^{(1,-1)}[g](B, 2)$

\*\* symmetry

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

\*\* expression

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

$\tilde{\mathbb{G}}_3^{(1,-1)}[g](B, 3)$

\*\* symmetry

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

\*\* expression

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

$\tilde{\mathbb{G}}_3^{(1,-1)}[g](B, 4)$

\*\* symmetry

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

\*\* expression

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

$\tilde{\mathbb{G}}_3^{(1,1)}[g](B, 1)$

\*\* symmetry

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

\*\* expression

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

$\tilde{\mathbb{G}}_3^{(1,1)}[g](B, 2)$

\*\* symmetry

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

\*\* expression

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

$\tilde{\mathbb{G}}_3^{(1,1)}[g](B, 3)$

\*\* symmetry

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

\*\* expression

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

$\tilde{\mathbb{G}}_3^{(1,1)}[g](B, 4)$

\*\* symmetry

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

\*\* expression

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

\* Harmonics for rank 4

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

\*\* symmetry

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

\*\* expression

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

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

\*\* symmetry

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

\*\* expression

$$-\frac{\sqrt{105}G_x x (x^2 - 6y^2 + 3z^2)}{42} + \frac{\sqrt{105}G_y y (6x^2 - y^2 - 3z^2)}{42} - \frac{\sqrt{105}G_z z (3x^2 + 3y^2 - 2z^2)}{42}$$

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

\*\* symmetry

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

\*\* expression

$$\frac{\sqrt{35}G_x x (x^2 - 3z^2)}{14} - \frac{\sqrt{35}G_y y (y^2 - 3z^2)}{14} - \frac{3\sqrt{35}G_z z (x - y) (x + y)}{14}$$

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

\*\* symmetry

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

\*\* expression

$$-\frac{\sqrt{5}G_x z (3x^2 - z^2)}{4} - \frac{\sqrt{5}G_z x (x^2 - 3z^2)}{4}$$

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

\*\* symmetry

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

\*\* expression

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

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

\*\* symmetry

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

\*\* expression

$$\begin{aligned} & \frac{\sqrt{1155}G_x x (x^4 - 5x^2y^2 - 5x^2z^2 + 3y^4 - 3y^2z^2 + 3z^4)}{66} + \frac{\sqrt{1155}G_y y (3x^4 - 5x^2y^2 - 3x^2z^2 + y^4 - 5y^2z^2 + 3z^4)}{66} \\ & + \frac{\sqrt{1155}G_z z (3x^4 - 3x^2y^2 - 5x^2z^2 + 3y^4 - 5y^2z^2 + z^4)}{66} \end{aligned}$$

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

\*\* symmetry

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

\*\* expression

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

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

\*\* symmetry

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

\*\* expression

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

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

\*\* symmetry

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

\*\* expression

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

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

\*\* symmetry

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

\*\* expression

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

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

\*\* symmetry

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

\*\* expression

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

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

\*\* symmetry

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

\*\* expression

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

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

\*\* symmetry

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

\*\* expression

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

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

\*\* symmetry

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

\*\* expression

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

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

\*\* symmetry

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

\*\* expression

$$\frac{9\sqrt{77}G_xxyz(y-z)(y+z)}{22} - \frac{\sqrt{77}G_yz(3x^2y^2-x^2z^2-6y^4+11y^2z^2-z^4)}{22} - \frac{\sqrt{77}G_zy(x^2y^2-3x^2z^2+y^4-11y^2z^2+6z^4)}{22}$$

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

\*\* symmetry

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

\*\* expression

$$\frac{\sqrt{77}G_xy(6x^4-11x^2y^2-3x^2z^2+y^4+y^2z^2)}{22} - \frac{\sqrt{77}G_yx(x^4-11x^2y^2+x^2z^2+6y^4-3y^2z^2)}{22} + \frac{9\sqrt{77}G_zxyz(x-y)(x+y)}{22}$$

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

\*\* symmetry

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

\*\* expression

$$\frac{21\sqrt{11}G_xxyz(2x^2-y^2-z^2)}{22} - \frac{\sqrt{11}G_yz(6x^4-51x^2y^2+5x^2z^2+6y^4+5y^2z^2-z^4)}{22} - \frac{\sqrt{11}G_zy(6x^4+5x^2y^2-51x^2z^2-y^4+5y^2z^2+6z^4)}{22}$$

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

\*\* symmetry

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

\*\* expression

$$-\frac{\sqrt{11}G_xy(6x^4+5x^2y^2-51x^2z^2-y^4+5y^2z^2+6z^4)}{22} + \frac{\sqrt{11}G_yx(x^4-5x^2y^2-5x^2z^2-6y^4+51y^2z^2-6z^4)}{22} - \frac{21\sqrt{11}G_zxyz(x^2+y^2-2z^2)}{22}$$