

PG No. 8  $D_{2h}$   $mmm$  [ orthorhombic ] (axial, internal axial dipole)

\* Harmonics for rank 0

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

\*\* 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

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

\*\* symmetry

$$z$$

\*\* expression

$$G_z$$

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

\*\* symmetry

$$z$$

\*\* expression

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

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

\*\* symmetry

$$y$$

\*\* expression

$$G_y$$

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

\*\* symmetry

$$y$$

\*\* expression

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

$$\vec{G}_1^{(1,-1)}[g](B_{3g})$$

\*\* symmetry

$$x$$

\*\* expression

$$G_x$$

$$\vec{G}_1^{(1,1)}[g](B_{3g})$$

\*\* symmetry

$$x$$

\*\* expression

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

\* Harmonics for rank 2

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

\*\* symmetry

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

\*\* expression

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

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

\*\* symmetry

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

\*\* expression

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

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

\*\* symmetry

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

\*\* expression

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

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

\*\* symmetry

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

\*\* expression

$$\frac{\sqrt{7}G_{xx}(3x^2-7y^2-2z^2)}{14} + \frac{\sqrt{7}G_{yy}(7x^2-3y^2+2z^2)}{14} + \frac{5\sqrt{7}G_{zz}(x-y)(x+y)}{14}$$

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

\*\* symmetry

$$\sqrt{3}xy$$

\*\* expression

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

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

\*\* symmetry

$$\sqrt{3}xy$$

\*\* expression

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

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

\*\* symmetry

$$\sqrt{3}xz$$

\*\* expression

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

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

\*\* symmetry

$$\sqrt{3}xz$$

\*\* expression

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

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

\*\* symmetry

$$\sqrt{3}yz$$

\*\* expression

$$\frac{\sqrt{2}G_{yz}}{2} + \frac{\sqrt{2}G_{zy}}{2}$$

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

\*\* symmetry

$$\sqrt{3}yz$$

\*\* expression

$$\frac{5\sqrt{7}G_xxyz}{7} - \frac{\sqrt{7}G_yz(x^2 - 4y^2 + z^2)}{7} - \frac{\sqrt{7}G_zy(x^2 + y^2 - 4z^2)}{7}$$

\* Harmonics for rank 3

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

\*\* symmetry

$$\sqrt{15}xyz$$

\*\* expression

$$G_xyz + G_yxz + G_zxy$$

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

\*\* symmetry

$$\sqrt{15}xyz$$

\*\* expression

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

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

\*\* symmetry

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

\*\* expression

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

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

\*\* symmetry

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

\*\* expression

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

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

\*\* symmetry

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

\*\* expression

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

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

\*\* symmetry

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

\*\* expression

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

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

\*\* symmetry

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

\*\* expression

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

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

\*\* symmetry

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

\*\* expression

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

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

\*\* symmetry

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

\*\* expression

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

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

\*\* symmetry

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

\*\* expression

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

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

\*\* symmetry

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

\*\* expression

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

$$\vec{\mathbb{G}}_3^{(1,-1)}[g](B_{3g},2)$$

\*\* symmetry

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

\*\* expression

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

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

\*\* symmetry

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

\*\* expression

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

$$\vec{\mathbb{G}}_3^{(1,1)}[g](B_{3g},2)$$

\*\* symmetry

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

\*\* expression

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

\* Harmonics for rank 4

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

\*\* symmetry

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

\*\* expression

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

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

\*\* symmetry

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

\*\* expression

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

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

\*\* symmetry

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

\*\* expression

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

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

\*\* symmetry

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

\*\* expression

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

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

\*\* symmetry

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

\*\* expression

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

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

\*\* symmetry

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

\*\* expression

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

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

\*\* symmetry

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

\*\* expression

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

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

\*\* symmetry

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

\*\* expression

$$-\frac{\sqrt{35}G_xy(3x^2+y^2-6z^2)}{28}-\frac{\sqrt{35}G_yx(x^2+3y^2-6z^2)}{28}+\frac{3\sqrt{35}G_zxyz}{7}$$

$$\vec{G}_4^{(1,1)}[g](B_{1u}, 1)$$

\*\* symmetry

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

\*\* expression

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

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

\*\* symmetry

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

\*\* expression

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

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

\*\* symmetry

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

\*\* expression

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

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

\*\* symmetry

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

\*\* expression

$$-\frac{\sqrt{35}G_xz(3x^2-6y^2+z^2)}{28}+\frac{3\sqrt{35}G_yxyz}{7}-\frac{\sqrt{35}G_zx(x^2-6y^2+3z^2)}{28}$$

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

\*\* symmetry

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

\*\* expression

$$-\frac{\sqrt{77}G_xz(6x^4-3x^2y^2-11x^2z^2+y^2z^2+z^4)}{22}-\frac{9\sqrt{77}G_yxyz(x-z)(x+z)}{22}+\frac{\sqrt{77}G_zx(x^4+x^2y^2-11x^2z^2-3y^2z^2+6z^4)}{22}$$

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

\*\* symmetry

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

\*\* expression

$$-\frac{\sqrt{11}G_xz(6x^4-51x^2y^2+5x^2z^2+6y^4+5y^2z^2-z^4)}{22}-\frac{21\sqrt{11}G_yxyz(x^2-2y^2+z^2)}{22}+\frac{\sqrt{11}G_zx(x^4-5x^2y^2-5x^2z^2-6y^4+51y^2z^2-6z^4)}{22}$$

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

\*\* symmetry

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

\*\* expression

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

$\vec{\mathbb{G}}_4^{(1,-1)}[g](B_{3u}, 2)$

\*\* symmetry

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

\*\* expression

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

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

\*\* symmetry

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

\*\* expression

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

$\vec{\mathbb{G}}_4^{(1,1)}[g](B_{3u}, 2)$

\*\* symmetry

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

\*\* expression

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