

PG No. 15  $D_{4h}$   $4/mmm$  [ tetragonal ] (axial, internal axial dipole)

\* Harmonics for rank 0

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

\*\* 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

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

\*\* symmetry

$z$

\*\* expression

$G_z$

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

\*\* symmetry

$z$

\*\* expression

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

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

\*\* symmetry

$x$

$-y$

\*\* expression

$G_x$

$-G_y$

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

\*\* symmetry

$x$

$-y$

\*\* expression

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

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

\* Harmonics for rank 2

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

\*\* symmetry

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

\*\* expression

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

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

\*\* symmetry

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

\*\* expression

$$-\frac{\sqrt{21}G_xx(x^2+y^2-4z^2)}{14}-\frac{\sqrt{21}G_yy(x^2+y^2-4z^2)}{14}-\frac{\sqrt{21}G_zz(3x^2+3y^2-2z^2)}{14}$$

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

\*\* symmetry

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

\*\* expression

$$\frac{\sqrt{2}G_xx}{2}-\frac{\sqrt{2}G_yy}{2}$$

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

\*\* symmetry

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

\*\* expression

$$\frac{\sqrt{7}G_xx(3x^2-7y^2-2z^2)}{14}+\frac{\sqrt{7}G_yy(7x^2-3y^2+2z^2)}{14}+\frac{5\sqrt{7}G_zz(x-y)(x+y)}{14}$$

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

\*\* symmetry

$$\sqrt{3}xy$$

\*\* expression

$$\frac{\sqrt{2}G_xy}{2}+\frac{\sqrt{2}G_yx}{2}$$

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

\*\* symmetry

$$\sqrt{3}xy$$

\*\* expression

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

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

\*\* symmetry

$$\sqrt{3}yz$$

$$-\sqrt{3}xz$$

\*\* expression

$$\frac{\sqrt{2}G_yz}{2}+\frac{\sqrt{2}G_zy}{2}$$

$$-\frac{\sqrt{2}G_xz}{2}-\frac{\sqrt{2}G_zx}{2}$$

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

\*\* symmetry

$$\sqrt{3}yz$$

$$-\sqrt{3}xz$$

\*\* expression

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

$$-\frac{\sqrt{7}G_xz(4x^2-y^2-z^2)}{7}-\frac{5\sqrt{7}G_yxyz}{7}+\frac{\sqrt{7}G_zx(x^2+y^2-4z^2)}{7}$$

\* Harmonics for rank 3

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

\*\* symmetry

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

\*\* expression

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

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

\*\* symmetry

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

\*\* expression

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

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

\*\* symmetry

$$\sqrt{15}xyz$$

\*\* expression

$$G_xyz + G_yxz + G_zxy$$

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

\*\* symmetry

$$\sqrt{15}xyz$$

\*\* expression

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

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

\*\* symmetry

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

\*\* expression

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

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

\*\* symmetry

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

\*\* expression

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

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

\*\* symmetry

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

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

\*\* expression

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

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

$\vec{\mathbb{G}}_{3,1}^{(1,-1)}[g](E_g, 2), \vec{\mathbb{G}}_{3,2}^{(1,-1)}[g](E_g, 2)$   
\*\* symmetry

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

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

\*\* expression

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

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

$\vec{\mathbb{G}}_{3,1}^{(1,1)}[g](E_g, 1), \vec{\mathbb{G}}_{3,2}^{(1,1)}[g](E_g, 1)$   
\*\* symmetry

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

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

\*\* expression

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

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

$\vec{\mathbb{G}}_{3,1}^{(1,1)}[g](E_g, 2), \vec{\mathbb{G}}_{3,2}^{(1,1)}[g](E_g, 2)$   
\*\* symmetry

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

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

\*\* expression

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

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

\* Harmonics for rank 4

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

\*\* symmetry

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

\*\* expression

$$\frac{\sqrt{3}G_xx(2x^2 - 3y^2 - 3z^2)}{6} - \frac{\sqrt{3}G_yy(3x^2 - 2y^2 + 3z^2)}{6} - \frac{\sqrt{3}G_zz(3x^2 + 3y^2 - 2z^2)}{6}$$

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

\*\* symmetry

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

\*\* expression

$$-\frac{\sqrt{105}G_xx(x^2 - 6y^2 + 3z^2)}{42} + \frac{\sqrt{105}G_yy(6x^2 - y^2 - 3z^2)}{42} - \frac{\sqrt{105}G_zz(3x^2 + 3y^2 - 2z^2)}{42}$$

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

\*\* symmetry

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

\*\* expression

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

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

\*\* symmetry

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

\*\* expression

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

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

\*\* symmetry

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

\*\* expression

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

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

\*\* symmetry

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

\*\* expression

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

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

\*\* symmetry

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

\*\* expression

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

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

\*\* symmetry

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

\*\* expression

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

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

\*\* symmetry

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

\*\* expression

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

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

\*\* symmetry

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

\*\* expression

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

$$\vec{\mathbb{G}}_{4,1}^{(1,-1)}[g](E_u, 1), \vec{\mathbb{G}}_{4,2}^{(1,-1)}[g](E_u, 1)$$

\*\* symmetry

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

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

\*\* expression

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

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

$$\vec{\mathbb{G}}_{4,1}^{(1,-1)}[g](E_u, 2), \vec{\mathbb{G}}_{4,2}^{(1,-1)}[g](E_u, 2)$$

\*\* symmetry

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

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

\*\* expression

$$\frac{3\sqrt{35}G_xyxyz}{7} + \frac{\sqrt{35}G_yz(6x^2 - 3y^2 - z^2)}{28} + \frac{\sqrt{35}G_zy(6x^2 - y^2 - 3z^2)}{28}$$

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

$$\vec{\mathbb{G}}_{4,1}^{(1,1)}[g](E_u, 1), \vec{\mathbb{G}}_{4,2}^{(1,1)}[g](E_u, 1)$$

\*\* symmetry

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

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

\*\* expression

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

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

$$\vec{\mathbb{G}}_{4,1}^{(1,1)}[g](E_u, 2), \vec{\mathbb{G}}_{4,2}^{(1,1)}[g](E_u, 2)$$

\*\* symmetry

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

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

\*\* expression

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

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