

PG No. 32  $O_h$   $m\bar{3}m$  [ cubic ] (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

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

\*\* symmetry

$x$

$y$

$z$

\*\* expression

$$G_x$$

$$G_y$$

$$G_z$$

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

\*\* symmetry

$x$

$y$

$z$

\*\* expression

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

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

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

\* Harmonics for rank 2

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

\*\* symmetry

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

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

\*\* expression

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

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

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

\*\* symmetry

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

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

\*\* expression

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

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

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

\*\* symmetry

$$\sqrt{3}yz$$

$$\sqrt{3}xz$$

$$\sqrt{3}xy$$

\*\* expression

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

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

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

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

\*\* symmetry

$$\sqrt{3}yz$$

$$\sqrt{3}xz$$

$$\sqrt{3}xy$$

\*\* expression

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

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

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

\* Harmonics for rank 3

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

\*\* symmetry

$$\sqrt{15}xyz$$

\*\* expression

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

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

\*\* symmetry

$$\sqrt{15}xyz$$

\*\* expression

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

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

\*\* symmetry

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

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

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

\*\* expression

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

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

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

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

\*\* symmetry

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

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

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

\*\* expression

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

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

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

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

\*\* symmetry

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

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

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

\*\* expression

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

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

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

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

\*\* symmetry

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

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

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

\*\* expression

$$\begin{aligned} & \frac{\sqrt{15}G_x(y-z)(y+z)(6x^2-y^2-z^2)}{12} - \frac{\sqrt{15}G_yxy(2x^2-5y^2+9z^2)}{12} + \frac{\sqrt{15}G_zxz(2x^2+9y^2-5z^2)}{12} \\ & - \frac{\sqrt{15}G_xy(5x^2-2y^2-9z^2)}{12} + \frac{\sqrt{15}G_y(x-z)(x+z)(x^2-6y^2+z^2)}{12} - \frac{\sqrt{15}G_zyz(9x^2+2y^2-5z^2)}{12} \\ & \frac{\sqrt{15}G_xxz(5x^2-9y^2-2z^2)}{12} + \frac{\sqrt{15}G_yyz(9x^2-5y^2+2z^2)}{12} - \frac{\sqrt{15}G_z(x-y)(x+y)(x^2+y^2-6z^2)}{12} \end{aligned}$$

\* Harmonics for rank 4

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

\*\* symmetry

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

\*\* expression

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

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

\*\* symmetry

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

\*\* expression

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

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

\*\* symmetry

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

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

\*\* expression

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

$$\frac{\sqrt{35}G_xx(x^2-3z^2)}{14} - \frac{\sqrt{35}G_yy(y^2-3z^2)}{14} - \frac{3\sqrt{35}G_zz(x-y)(x+y)}{14}$$

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

\*\* symmetry

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

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

\*\* expression

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

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

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

$$\vec{\mathbb{G}}_{4,1}^{(1,-1)}[g](T_{1u}), \vec{\mathbb{G}}_{4,2}^{(1,-1)}[g](T_{1u}), \vec{\mathbb{G}}_{4,3}^{(1,-1)}[g](T_{1u})$$

\*\* symmetry

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

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

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

\*\* expression

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

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

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

$$\vec{\mathbb{G}}_{4,1}^{(1,1)}[g](T_{1u}), \vec{\mathbb{G}}_{4,2}^{(1,1)}[g](T_{1u}), \vec{\mathbb{G}}_{4,3}^{(1,1)}[g](T_{1u})$$

\*\* symmetry

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

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

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

\*\* expression

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

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

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

$$\vec{\mathbb{G}}_{4,1}^{(1,-1)}[g](T_{2u}), \vec{\mathbb{G}}_{4,2}^{(1,-1)}[g](T_{2u}), \vec{\mathbb{G}}_{4,3}^{(1,-1)}[g](T_{2u})$$

\*\* symmetry

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

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

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

\*\* expression

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

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

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

$$\vec{\mathbb{G}}_{4,1}^{(1,1)}[g](T_{2u}), \vec{\mathbb{G}}_{4,2}^{(1,1)}[g](T_{2u}), \vec{\mathbb{G}}_{4,3}^{(1,1)}[g](T_{2u})$$

\*\* symmetry

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

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

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

\*\* expression

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

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

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