

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

* Harmonics for rank 0

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

** 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

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

** symmetry

$$z$$

** expression

$$G_z$$

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

** symmetry

$$z$$

** expression

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

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

** symmetry

$$x$$

$$-y$$

** expression

$$G_x$$

$$-G_y$$

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

** symmetry

$$x$$

$$-y$$

** expression

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

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

* Harmonics for rank 2

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

** symmetry

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

** expression

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

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

** symmetry

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

** expression

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

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

** symmetry

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

** expression

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

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

** symmetry

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

** expression

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

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

** symmetry

$$\sqrt{3}xy$$

** expression

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

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

** symmetry

$$\sqrt{3}xy$$

** expression

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

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

** symmetry

$$\sqrt{3}yz$$

$$-\sqrt{3}xz$$

** expression

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

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

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

** symmetry

$$\sqrt{3}yz$$

$$-\sqrt{3}xz$$

** expression

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

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

* Harmonics for rank 3

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

** symmetry

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

** expression

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

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

** symmetry

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

** expression

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

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

** symmetry

$$\sqrt{15}xyz$$

** expression

$$G_x yz + G_y xz + G_z xy$$

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

** symmetry

$$\sqrt{15}xyz$$

** expression

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

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

** symmetry

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

** expression

$$G_x xz - G_y yz + \frac{G_z(x-y)(x+y)}{2}$$

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

** symmetry

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

** expression

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

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

** symmetry

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

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

** expression

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

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

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

** 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

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

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

** symmetry

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

** expression

$$-\frac{\sqrt{33}G_{xx} (5x^4 - 88x^2y^2 + 38x^2z^2 + 33y^4 + 66y^2z^2 - 30z^4)}{132} - \frac{\sqrt{33}G_{yy} (33x^4 - 88x^2y^2 + 66x^2z^2 + 5y^4 + 38y^2z^2 - 30z^4)}{132} + \frac{\sqrt{33}G_{zz} (3x^4 + 132x^2y^2 - 50x^2z^2 + 3y^4 - 50y^2z^2 + 10z^4)}{132}$$

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

** symmetry

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

** expression

$$\frac{\sqrt{5}G_{xy} (3x^2 - y^2)}{4} + \frac{\sqrt{5}G_{yx} (x^2 - 3y^2)}{4}$$

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

** symmetry

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

** expression

$$\frac{\sqrt{77}G_{xy} (6x^4 - 11x^2y^2 - 3x^2z^2 + y^4 + y^2z^2)}{22} - \frac{\sqrt{77}G_{yx} (x^4 - 11x^2y^2 + x^2z^2 + 6y^4 - 3y^2z^2)}{22} + \frac{9\sqrt{77}G_{zz}xyz (x - y) (x + y)}{22}$$

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

** symmetry

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

** expression

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

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

** symmetry

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

** expression

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

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

** symmetry

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

** expression

$$-\frac{\sqrt{35}G_{xy} (3x^2 + y^2 - 6z^2)}{28} - \frac{\sqrt{35}G_{yx} (x^2 + 3y^2 - 6z^2)}{28} + \frac{3\sqrt{35}G_{zz}xyz}{7}$$

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

** symmetry

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

** expression

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

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

** symmetry

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

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

** expression

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

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

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

** symmetry

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

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

** expression

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

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

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

** symmetry

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

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

** expression

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

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

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

** symmetry

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

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

** expression

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

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