

PG No. 20  $D_{3d}$   $\bar{3}m$  (-3m1 setting) [ trigonal ] (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

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

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

\*\* symmetry

$$\sqrt{3}yz$$

$$-\sqrt{3}xz$$

\*\* expression

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

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

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

\*\* symmetry

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

$$-\sqrt{3}xy$$

\*\* expression

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

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

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

\*\* symmetry

$$\sqrt{3}yz$$

$$-\sqrt{3}xz$$

\*\* expression

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

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

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

\*\* symmetry

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

$$-\sqrt{3}xy$$

\*\* expression

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

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

\* Harmonics for rank 3

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

\*\* symmetry

$$\frac{\sqrt{10}x (x^2 - 3y^2)}{4}$$

\*\* expression

$$\frac{\sqrt{6}G_x(x-y)(x+y)}{4} - \frac{\sqrt{6}G_yxy}{2}$$

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

\*\* symmetry

$$\frac{\sqrt{10}x(x^2-3y^2)}{4}$$

\*\* expression

$$\frac{\sqrt{10}G_x(4x^4-21x^2y^2-3x^2z^2+3y^4+3y^2z^2)}{24} + \frac{\sqrt{10}G_yxy(13x^2-15y^2+6z^2)}{24} + \frac{7\sqrt{10}G_zxz(x^2-3y^2)}{24}$$

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

\*\* symmetry

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

\*\* expression

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

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

\*\* symmetry

$$\frac{\sqrt{10}y(3x^2-y^2)}{4}$$

\*\* expression

$$\frac{\sqrt{6}G_xxy}{2} + \frac{\sqrt{6}G_y(x-y)(x+y)}{4}$$

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

\*\* symmetry

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

\*\* expression

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

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

\*\* symmetry

$$\frac{\sqrt{10}y(3x^2-y^2)}{4}$$

\*\* expression

$$\frac{\sqrt{10}G_xxy(15x^2-13y^2-6z^2)}{24} - \frac{\sqrt{10}G_y(3x^4-21x^2y^2+3x^2z^2+4y^4-3y^2z^2)}{24} + \frac{7\sqrt{10}G_zyz(3x^2-y^2)}{24}$$

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

\*\* symmetry

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

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

\*\* expression

$$-\frac{\sqrt{10}G_x(3x^2+y^2-4z^2)}{20} - \frac{\sqrt{10}G_yxy}{10} + \frac{2\sqrt{10}G_zxz}{5}$$

$$-\frac{\sqrt{10}G_xxy}{10} - \frac{\sqrt{10}G_y(x^2+3y^2-4z^2)}{20} + \frac{2\sqrt{10}G_zyz}{5}$$

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

\*\* symmetry

$$\sqrt{15}xyz$$

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

\*\* expression

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

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

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

\*\* symmetry

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

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

\*\* expression

$$-\frac{\sqrt{6}G_x(4x^4+3x^2y^2-27x^2z^2-y^4+3y^2z^2+4z^4)}{24} - \frac{5\sqrt{6}G_yxy(x^2+y^2-6z^2)}{24} - \frac{5\sqrt{6}G_zxz(3x^2+3y^2-4z^2)}{24}$$

$$-\frac{5\sqrt{6}G_xxy(x^2+y^2-6z^2)}{24} + \frac{\sqrt{6}G_y(x^4-3x^2y^2-3x^2z^2-4y^4+27y^2z^2-4z^4)}{24} - \frac{5\sqrt{6}G_zyz(3x^2+3y^2-4z^2)}{24}$$

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

\*\* symmetry

$$\sqrt{15}xyz$$

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

\*\* expression

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

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

\* Harmonics for rank 4

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

\*\* symmetry

$$\frac{3x^4}{8} + \frac{3x^2y^2}{4} - 3x^2z^2 + \frac{3y^4}{8} - 3y^2z^2 + z^4$$

\*\* expression

$$\frac{3\sqrt{7}G_xx(x^2+y^2-4z^2)}{28} + \frac{3\sqrt{7}G_yy(x^2+y^2-4z^2)}{28} - \frac{\sqrt{7}G_zz(3x^2+3y^2-2z^2)}{7}$$

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

\*\* symmetry

$$\frac{\sqrt{70}yz(3x^2-y^2)}{4}$$

\*\* expression

$$\frac{3\sqrt{10}G_xxyz}{4} + \frac{3\sqrt{10}G_yz(x-y)(x+y)}{8} + \frac{\sqrt{10}G_zy(3x^2-y^2)}{8}$$

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

\*\* symmetry

$$\frac{3x^4}{8} + \frac{3x^2y^2}{4} - 3x^2z^2 + \frac{3y^4}{8} - 3y^2z^2 + z^4$$

\*\* expression

$$\frac{3\sqrt{55}G_x x (x^4 + 2x^2y^2 - 12x^2z^2 + y^4 - 12y^2z^2 + 8z^4)}{88} + \frac{3\sqrt{55}G_y y (x^4 + 2x^2y^2 - 12x^2z^2 + y^4 - 12y^2z^2 + 8z^4)}{88} + \frac{\sqrt{55}G_z z (15x^4 + 30x^2y^2 - 40x^2z^2 + 15y^4 - 40y^2z^2 + 8z^4)}{88}$$

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

\*\* symmetry

$$\frac{\sqrt{70}yz (3x^2 - y^2)}{4}$$

\*\* expression

$$\frac{3\sqrt{154}G_x xy z (7x^2 - 5y^2 - 2z^2)}{44} - \frac{3\sqrt{154}G_y z (x^4 - 9x^2y^2 + x^2z^2 + 2y^4 - y^2z^2)}{44} - \frac{\sqrt{154}G_z y (3x^2 - y^2) (x^2 + y^2 - 8z^2)}{44}$$

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

\*\* symmetry

$$\frac{\sqrt{70}xz (x^2 - 3y^2)}{4}$$

\*\* expression

$$\frac{3\sqrt{10}G_x z (x - y) (x + y)}{8} - \frac{3\sqrt{10}G_y xyz}{4} + \frac{\sqrt{10}G_z x (x^2 - 3y^2)}{8}$$

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

\*\* symmetry

$$\frac{\sqrt{70}xz (x^2 - 3y^2)}{4}$$

\*\* expression

$$\frac{3\sqrt{154}G_x z (2x^4 - 9x^2y^2 - x^2z^2 + y^4 + y^2z^2)}{44} + \frac{3\sqrt{154}G_y xyz (5x^2 - 7y^2 + 2z^2)}{44} - \frac{\sqrt{154}G_z x (x^2 - 3y^2) (x^2 + y^2 - 8z^2)}{44}$$

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

\*\* symmetry

$$- \frac{\sqrt{10}yz (3x^2 + 3y^2 - 4z^2)}{4}$$

$$\frac{\sqrt{10}xz (3x^2 + 3y^2 - 4z^2)}{4}$$

\*\* expression

$$- \frac{3\sqrt{70}G_x xyz}{28} - \frac{\sqrt{70}G_y z (3x^2 + 9y^2 - 4z^2)}{56} - \frac{3\sqrt{70}G_z y (x^2 + y^2 - 4z^2)}{56}$$

$$\frac{\sqrt{70}G_x z (9x^2 + 3y^2 - 4z^2)}{56} + \frac{3\sqrt{70}G_y xyz}{28} + \frac{3\sqrt{70}G_z x (x^2 + y^2 - 4z^2)}{56}$$

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

\*\* symmetry

$$\frac{\sqrt{35} (x^2 - 2xy - y^2) (x^2 + 2xy - y^2)}{8}$$

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

\*\* expression

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

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

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

\*\* symmetry

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

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

\*\* expression

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

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

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

\*\* symmetry

$$-\frac{\sqrt{10}yz(3x^2 + 3y^2 - 4z^2)}{4}$$

$$\frac{\sqrt{10}xz(3x^2 + 3y^2 - 4z^2)}{4}$$

\*\* expression

$$-\frac{21\sqrt{22}G_x xyz(x^2 + y^2 - 2z^2)}{44} + \frac{\sqrt{22}G_y z(3x^4 - 15x^2y^2 - x^2z^2 - 18y^4 + 41y^2z^2 - 4z^4)}{44} + \frac{3\sqrt{22}G_z y(x^4 + 2x^2y^2 - 12x^2z^2 + y^4 - 12y^2z^2 + 8z^4)}{44}$$

$$\frac{\sqrt{22}G_x z(18x^4 + 15x^2y^2 - 41x^2z^2 - 3y^4 + y^2z^2 + 4z^4)}{44} + \frac{21\sqrt{22}G_y xyz(x^2 + y^2 - 2z^2)}{44} - \frac{3\sqrt{22}G_z x(x^4 + 2x^2y^2 - 12x^2z^2 + y^4 - 12y^2z^2 + 8z^4)}{44}$$

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

\*\* symmetry

$$\frac{\sqrt{35}(x^2 - 2xy - y^2)(x^2 + 2xy - y^2)}{8}$$

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

\*\* expression

$$\frac{\sqrt{77}G_x x(5x^4 - 46x^2y^2 - 4x^2z^2 + 21y^4 + 12y^2z^2)}{88} + \frac{\sqrt{77}G_y y(21x^4 - 46x^2y^2 + 12x^2z^2 + 5y^4 - 4y^2z^2)}{88} + \frac{9\sqrt{77}G_z z(x^2 - 2xy - y^2)(x^2 + 2xy - y^2)}{88}$$

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

$$\tilde{\mathbb{G}}_{4,1}^{(1,1)}[g](E_u, 3), \tilde{\mathbb{G}}_{4,2}^{(1,1)}[g](E_u, 3)$$

\*\* symmetry

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

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

\*\* expression

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

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