

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

\* Harmonics for rank 0

\* Harmonics for rank 1

$$\vec{\mathbb{Q}}_1^{(1,0)}[g](A_{2u})$$

\*\* symmetry

$z$

\*\* expression

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

$$\vec{\mathbb{Q}}_{1,1}^{(1,0)}[g](E_u), \vec{\mathbb{Q}}_{1,2}^{(1,0)}[g](E_u)$$

\*\* symmetry

$x$

$y$

\*\* expression

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

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

\* Harmonics for rank 2

$$\vec{\mathbb{Q}}_2^{(1,0)}[g](A_{1g})$$

\*\* symmetry

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

\*\* expression

$$\frac{\sqrt{6}G_xyz}{2} - \frac{\sqrt{6}G_yxz}{2}$$

$$\vec{\mathbb{Q}}_2^{(1,0)}[g](B_{1g})$$

\*\* symmetry

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

\*\* expression

$$\frac{\sqrt{2}G_xyz}{2} + \frac{\sqrt{2}G_yxz}{2} - \sqrt{2}G_zxy$$

$$\vec{\mathbb{Q}}_2^{(1,0)}[g](B_{2g})$$

\*\* symmetry

$$\sqrt{3}xy$$

\*\* expression

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

$$\vec{\mathbb{Q}}_{2,1}^{(1,0)}[g](E_g), \vec{\mathbb{Q}}_{2,2}^{(1,0)}[g](E_g)$$

\*\* symmetry

$$\sqrt{3}yz$$

$$\sqrt{3}xz$$

\*\* expression

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

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

\* Harmonics for rank 3

$$\vec{\mathbb{Q}}_3^{(1,0)}[g](A_{2u})$$

\*\* symmetry

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

\*\* expression

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

$\vec{\mathbb{Q}}_3^{(1,0)}[g](B_{1u})$

\*\* symmetry

$$\sqrt{15}xyz$$

\*\* expression

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

$\vec{\mathbb{Q}}_3^{(1,0)}[g](B_{2u})$

\*\* symmetry

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

\*\* expression

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

$\vec{\mathbb{Q}}_{3,1}^{(1,0)}[g](E_u, 1), \vec{\mathbb{Q}}_{3,2}^{(1,0)}[g](E_u, 1)$

\*\* symmetry

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

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

\*\* expression

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

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

$\vec{\mathbb{Q}}_{3,1}^{(1,0)}[g](E_u, 2), \vec{\mathbb{Q}}_{3,2}^{(1,0)}[g](E_u, 2)$

\*\* symmetry

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

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

\*\* expression

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

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

\* Harmonics for rank 4

$\vec{\mathbb{Q}}_4^{(1,0)}[g](A_{1g}, 1)$

\*\* symmetry

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

\*\* expression

$$-\frac{\sqrt{105}G_xyz(y-z)(y+z)}{6} + \frac{\sqrt{105}G_yxz(x-z)(x+z)}{6} - \frac{\sqrt{105}G_zxy(x-y)(x+y)}{6}$$

$\vec{\mathbb{Q}}_4^{(1,0)}[g](A_{1g}, 2)$

\*\* symmetry

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

\*\* expression

$$-\frac{\sqrt{3}G_xyz(9x^2 + 2y^2 - 5z^2)}{6} + \frac{\sqrt{3}G_yxz(2x^2 + 9y^2 - 5z^2)}{6} + \frac{7\sqrt{3}G_zxy(x - y)(x + y)}{6}$$

$\vec{\mathbb{Q}}_4^{(1,0)}[g](A_{2g})$

\*\* symmetry

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

\*\* expression

$$-\frac{\sqrt{7}G_xxz(x^2 - 3y^2)}{4} + \frac{\sqrt{7}G_yyz(3x^2 - y^2)}{4} + \frac{\sqrt{7}G_z(x^2 - 2xy - y^2)(x^2 + 2xy - y^2)}{4}$$

$\vec{\mathbb{Q}}_4^{(1,0)}[g](B_{1g})$

\*\* symmetry

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

\*\* expression

$$-\frac{G_xyz(3x^2 - 4y^2 + 3z^2)}{2} + \frac{G_yxz(4x^2 - 3y^2 - 3z^2)}{2} - \frac{G_zxy(x^2 + y^2 - 6z^2)}{2}$$

$\vec{\mathbb{Q}}_4^{(1,0)}[g](B_{2g})$

\*\* symmetry

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

\*\* expression

$$\frac{G_xxz(x^2 + 15y^2 - 6z^2)}{4} - \frac{G_yyz(15x^2 + y^2 - 6z^2)}{4} - \frac{G_z(x - y)(x + y)(x^2 + y^2 - 6z^2)}{4}$$

$\vec{\mathbb{Q}}_{4,1}^{(1,0)}[g](E_g, 1), \vec{\mathbb{Q}}_{4,2}^{(1,0)}[g](E_g, 1)$

\*\* symmetry

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

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

\*\* expression

$$\frac{\sqrt{7}G_x(y^2 - 2yz - z^2)(y^2 + 2yz - z^2)}{4} - \frac{\sqrt{7}G_yxy(y^2 - 3z^2)}{4} + \frac{\sqrt{7}G_zxz(3y^2 - z^2)}{4}$$

$$\frac{\sqrt{7}G_xxy(x^2 - 3z^2)}{4} - \frac{\sqrt{7}G_y(x^2 - 2xz - z^2)(x^2 + 2xz - z^2)}{4} - \frac{\sqrt{7}G_zyz(3x^2 - z^2)}{4}$$

$\vec{\mathbb{Q}}_{4,1}^{(1,0)}[g](E_g, 2), \vec{\mathbb{Q}}_{4,2}^{(1,0)}[g](E_g, 2)$

\*\* symmetry

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

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

\*\* expression

$$\frac{G_x(y - z)(y + z)(6x^2 - y^2 - z^2)}{4} - \frac{G_yxy(6x^2 - y^2 - 15z^2)}{4} + \frac{G_zxz(6x^2 - 15y^2 - z^2)}{4}$$

$$-\frac{G_xxy(x^2 - 6y^2 + 15z^2)}{4} + \frac{G_y(x - z)(x + z)(x^2 - 6y^2 + z^2)}{4} + \frac{G_zyz(15x^2 - 6y^2 + z^2)}{4}$$