

PG No. 27  $D_{6h}$  6/mmm [ hexagonal ] (polar, internal axial dipole)

\* Harmonics for rank 0

\* Harmonics for rank 1

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

\*\* symmetry

$z$

\*\* expression

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

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

\*\* 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

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

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

\*\* symmetry

$\sqrt{3}yz$

$-\sqrt{3}xz$

\*\* expression

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

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

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

\*\* symmetry

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

$-\sqrt{3}xy$

\*\* expression

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

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

\* 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

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

\*\* expression

$$-\frac{\sqrt{30}G_xz(x-y)(x+y)}{8} + \frac{\sqrt{30}G_yxyz}{4} + \frac{\sqrt{30}G_zx(x^2-3y^2)}{8}$$

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

\*\* symmetry

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

\*\* expression

$$\frac{\sqrt{30}G_xxyz}{4} + \frac{\sqrt{30}G_yz(x-y)(x+y)}{8} - \frac{\sqrt{30}G_zy(3x^2-y^2)}{8}$$

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

\*\* symmetry

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

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

\*\* expression

$$\frac{5\sqrt{2}G_xxyz}{4} - \frac{\sqrt{2}G_yz(11x^2+y^2-4z^2)}{8} + \frac{\sqrt{2}G_zy(x^2+y^2-4z^2)}{8}$$

$$\frac{\sqrt{2}G_xz(x^2+11y^2-4z^2)}{8} - \frac{5\sqrt{2}G_yxyz}{4} - \frac{\sqrt{2}G_zx(x^2+y^2-4z^2)}{8}$$

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

\*\* symmetry

$$\sqrt{15}xyz$$

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

\*\* expression

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

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

\* Harmonics for rank 4

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

\*\* symmetry

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

\*\* expression

$$-\frac{\sqrt{5}G_xyz(3x^2+3y^2-4z^2)}{4} + \frac{\sqrt{5}G_yxz(3x^2+3y^2-4z^2)}{4}$$

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

\*\* symmetry

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

\*\* expression

$$\frac{\sqrt{14}G_xxy(x^2 - 3y^2 + 6z^2)}{8} - \frac{\sqrt{14}G_y(x^4 - 3x^2y^2 - 3x^2z^2 + 3y^2z^2)}{8} - \frac{3\sqrt{14}G_zyz(3x^2 - y^2)}{8}$$

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

\*\* symmetry

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

\*\* expression

$$\frac{\sqrt{14}G_x(3x^2y^2 - 3x^2z^2 - y^4 + 3y^2z^2)}{8} - \frac{\sqrt{14}G_yxy(3x^2 - y^2 - 6z^2)}{8} + \frac{3\sqrt{14}G_zxz(x^2 - 3y^2)}{8}$$

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

\*\* symmetry

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

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

\*\* expression

$$-\frac{\sqrt{2}G_x(3x^2y^2 - 3x^2z^2 + 3y^4 - 21y^2z^2 + 4z^4)}{8} + \frac{3\sqrt{2}G_yxy(x^2 + y^2 - 6z^2)}{8} - \frac{\sqrt{2}G_zxz(3x^2 + 3y^2 - 4z^2)}{8}$$

$$\frac{3\sqrt{2}G_xxy(x^2 + y^2 - 6z^2)}{8} - \frac{\sqrt{2}G_y(3x^4 + 3x^2y^2 - 21x^2z^2 - 3y^2z^2 + 4z^4)}{8} - \frac{\sqrt{2}G_zyz(3x^2 + 3y^2 - 4z^2)}{8}$$

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

\*\* 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

$$\frac{\sqrt{7}G_xyz(3x^2 - y^2)}{4} + \frac{\sqrt{7}G_yxz(x^2 - 3y^2)}{4} - \sqrt{7}G_zyy(x - y)(x + y)$$

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

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

\*\* 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

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

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