

PG No. 13  $C_{4v}$   $4mm$  [ tetragonal ] (axial, internal polar dipole)

\* Harmonics for rank 0

\* Harmonics for rank 1

$$\vec{G}_1^{(1,0)}[q](A_2)$$

\*\* symmetry

$$z$$

\*\* expression

$$\frac{\sqrt{2}Q_{xy}}{2} - \frac{\sqrt{2}Q_{yx}}{2}$$

$$\vec{G}_{1,1}^{(1,0)}[q](E), \vec{G}_{1,2}^{(1,0)}[q](E)$$

\*\* symmetry

$$-y$$

$$x$$

\*\* expression

$$\frac{\sqrt{2}Q_{xz}}{2} - \frac{\sqrt{2}Q_{zx}}{2}$$

$$\frac{\sqrt{2}Q_{yz}}{2} - \frac{\sqrt{2}Q_{zy}}{2}$$

\* Harmonics for rank 2

$$\vec{G}_2^{(1,0)}[q](A_2)$$

\*\* symmetry

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

\*\* expression

$$\frac{\sqrt{6}Q_{xyz}}{2} - \frac{\sqrt{6}Q_{yxz}}{2}$$

$$\vec{G}_2^{(1,0)}[q](B_1)$$

\*\* symmetry

$$\sqrt{3}xy$$

\*\* expression

$$-\frac{\sqrt{2}Q_{xxz}}{2} + \frac{\sqrt{2}Q_{yyz}}{2} + \frac{\sqrt{2}Q_z(x-y)(x+y)}{2}$$

$$\vec{G}_2^{(1,0)}[q](B_2)$$

\*\* symmetry

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

\*\* expression

$$\frac{\sqrt{2}Q_{xyz}}{2} + \frac{\sqrt{2}Q_{yxz}}{2} - \sqrt{2}Q_zxy$$

$$\vec{G}_{2,1}^{(1,0)}[q](E), \vec{G}_{2,2}^{(1,0)}[q](E)$$

\*\* symmetry

$$\sqrt{3}yz$$

$$-\sqrt{3}xz$$

\*\* expression

$$\frac{\sqrt{2}Q_x(y-z)(y+z)}{2} - \frac{\sqrt{2}Q_yxy}{2} + \frac{\sqrt{2}Q_zxz}{2}$$

$$-\frac{\sqrt{2}Q_xxy}{2} + \frac{\sqrt{2}Q_y(x-z)(x+z)}{2} + \frac{\sqrt{2}Q_zyz}{2}$$

\* Harmonics for rank 3

$$\vec{\mathbb{G}}_3^{(1,0)}[q](A_2)$$

\*\* symmetry

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

\*\* expression

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

$$\vec{\mathbb{G}}_3^{(1,0)}[q](B_1)$$

\*\* symmetry

$$\sqrt{15}xyz$$

\*\* expression

$$\frac{\sqrt{5}Q_{xx}(y-z)(y+z)}{2} - \frac{\sqrt{5}Q_{yy}(x-z)(x+z)}{2} + \frac{\sqrt{5}Q_{zz}(x-y)(x+y)}{2}$$

$$\vec{\mathbb{G}}_3^{(1,0)}[q](B_2)$$

\*\* symmetry

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

\*\* expression

$$\frac{\sqrt{5}Q_{xy}(x^2 - y^2 + 2z^2)}{4} - \frac{\sqrt{5}Q_{yx}(x^2 - y^2 - 2z^2)}{4} - \sqrt{5}Q_{zxyz}$$

$$\vec{\mathbb{G}}_{3,1}^{(1,0)}[q](E, 1), \vec{\mathbb{G}}_{3,2}^{(1,0)}[q](E, 1)$$

\*\* symmetry

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

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

\*\* expression

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

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

$$\vec{\mathbb{G}}_{3,1}^{(1,0)}[q](E, 2), \vec{\mathbb{G}}_{3,2}^{(1,0)}[q](E, 2)$$

\*\* symmetry

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

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

\*\* expression

$$\frac{\sqrt{5}Q_{xz}(x^2 + 2y^2 - z^2)}{4} - \sqrt{5}Q_{yxyz} - \frac{\sqrt{5}Q_{zx}(x^2 - 2y^2 - z^2)}{4}$$

$$-\sqrt{5}Q_{xxyz} + \frac{\sqrt{5}Q_{yz}(2x^2 + y^2 - z^2)}{4} + \frac{\sqrt{5}Q_{zy}(2x^2 - y^2 + z^2)}{4}$$

\* Harmonics for rank 4

$$\vec{\mathbb{G}}_4^{(1,0)}[q](A_1)$$

\*\* symmetry

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

\*\* expression

$$-\frac{\sqrt{7}Q_{xxz}(x^2 - 3y^2)}{4} + \frac{\sqrt{7}Q_{yyz}(3x^2 - y^2)}{4} + \frac{\sqrt{7}Q_z(x^2 - 2xy - y^2)(x^2 + 2xy - y^2)}{4}$$

$$\vec{\mathbb{G}}_4^{(1,0)}[q](A_2, 1)$$

\*\* symmetry

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

\*\* expression

$$-\frac{\sqrt{105}Q_xyz (y-z)(y+z)}{6} + \frac{\sqrt{105}Q_yxz (x-z)(x+z)}{6} - \frac{\sqrt{105}Q_zxy (x-y)(x+y)}{6}$$

$$\vec{\mathbb{G}}_4^{(1,0)}[q](A_2, 2)$$

\*\* symmetry

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

\*\* expression

$$-\frac{\sqrt{3}Q_xyz (9x^2 + 2y^2 - 5z^2)}{6} + \frac{\sqrt{3}Q_yxz (2x^2 + 9y^2 - 5z^2)}{6} + \frac{7\sqrt{3}Q_zxy (x-y)(x+y)}{6}$$

$$\vec{\mathbb{G}}_4^{(1,0)}[q](B_1)$$

\*\* symmetry

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

\*\* expression

$$\frac{Q_xxz (x^2 + 15y^2 - 6z^2)}{4} - \frac{Q_yyz (15x^2 + y^2 - 6z^2)}{4} - \frac{Q_z (x-y)(x+y)(x^2 + y^2 - 6z^2)}{4}$$

$$\vec{\mathbb{G}}_4^{(1,0)}[q](B_2)$$

\*\* symmetry

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

\*\* expression

$$-\frac{Q_xyz (3x^2 - 4y^2 + 3z^2)}{2} + \frac{Q_yxz (4x^2 - 3y^2 - 3z^2)}{2} - \frac{Q_zxy (x^2 + y^2 - 6z^2)}{2}$$

$$\vec{\mathbb{G}}_{4,1}^{(1,0)}[q](E, 1), \vec{\mathbb{G}}_{4,2}^{(1,0)}[q](E, 1)$$

\*\* symmetry

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

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

\*\* expression

$$\frac{\sqrt{7}Q_x (y^2 - 2yz - z^2)(y^2 + 2yz - z^2)}{4} - \frac{\sqrt{7}Q_yxy (y^2 - 3z^2)}{4} + \frac{\sqrt{7}Q_zxz (3y^2 - z^2)}{4}$$

$$-\frac{\sqrt{7}Q_xxy (x^2 - 3z^2)}{4} + \frac{\sqrt{7}Q_y (x^2 - 2xz - z^2)(x^2 + 2xz - z^2)}{4} + \frac{\sqrt{7}Q_zyz (3x^2 - z^2)}{4}$$

$$\vec{\mathbb{G}}_{4,1}^{(1,0)}[q](E, 2), \vec{\mathbb{G}}_{4,2}^{(1,0)}[q](E, 2)$$

\*\* symmetry

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

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

\*\* expression

$$\frac{Q_x (y-z)(y+z)(6x^2 - y^2 - z^2)}{4} - \frac{Q_yxy (6x^2 - y^2 - 15z^2)}{4} + \frac{Q_zxz (6x^2 - 15y^2 - z^2)}{4}$$

$$\frac{Q_xxy (x^2 - 6y^2 + 15z^2)}{4} - \frac{Q_y (x-z)(x+z)(x^2 - 6y^2 + z^2)}{4} - \frac{Q_zyz (15x^2 - 6y^2 + z^2)}{4}$$