

PG No. 19  $C_{3v}$   $3m$  (3m1 setting) [ trigonal ] (polar, internal polar dipole)

\* Harmonics for rank 0

$$\vec{\mathbb{Q}}_0^{(1,1)}[q](A_1)$$

\*\* symmetry

1

\*\* expression

$$\frac{\sqrt{3}Q_x x}{3} + \frac{\sqrt{3}Q_y y}{3} + \frac{\sqrt{3}Q_z z}{3}$$

\* Harmonics for rank 1

$$\vec{\mathbb{Q}}_1^{(1,-1)}[q](A_1)$$

\*\* symmetry

$z$

\*\* expression

$Q_z$

$$\vec{\mathbb{Q}}_1^{(1,1)}[q](A_1)$$

\*\* symmetry

$z$

\*\* expression

$$\frac{3\sqrt{10}Q_x xz}{10} + \frac{3\sqrt{10}Q_y yz}{10} - \frac{\sqrt{10}Q_z (x^2 + y^2 - 2z^2)}{10}$$

$$\vec{\mathbb{Q}}_{1,1}^{(1,-1)}[q](E), \vec{\mathbb{Q}}_{1,2}^{(1,-1)}[q](E)$$

\*\* symmetry

$x$

$y$

\*\* expression

$Q_x$

$Q_y$

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

\*\* symmetry

$x$

$y$

\*\* expression

$$\frac{\sqrt{10}Q_x (2x^2 - y^2 - z^2)}{10} + \frac{3\sqrt{10}Q_y xy}{10} + \frac{3\sqrt{10}Q_z xz}{10}$$

$$\frac{3\sqrt{10}Q_x xy}{10} - \frac{\sqrt{10}Q_y (x^2 - 2y^2 + z^2)}{10} + \frac{3\sqrt{10}Q_z yz}{10}$$

\* Harmonics for rank 2

$$\vec{\mathbb{Q}}_2^{(1,-1)}[q](A_1)$$

\*\* symmetry

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

\*\* expression

$$-\frac{\sqrt{6}Q_x x}{6} - \frac{\sqrt{6}Q_y y}{6} + \frac{\sqrt{6}Q_z z}{3}$$

$$\vec{\mathbb{Q}}_2^{(1,1)}[q](A_1)$$

\*\* symmetry

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

\*\* expression

$$-\frac{\sqrt{21}Q_xx(x^2+y^2-4z^2)}{14}-\frac{\sqrt{21}Q_yy(x^2+y^2-4z^2)}{14}-\frac{\sqrt{21}Q_zz(3x^2+3y^2-2z^2)}{14}$$

$$\vec{\mathbb{Q}}_{2,1}^{(1,-1)}[q](E,1), \vec{\mathbb{Q}}_{2,2}^{(1,-1)}[q](E,1)$$

\*\* symmetry

$$\sqrt{3}xz$$

$$\sqrt{3}yz$$

\*\* expression

$$\frac{\sqrt{2}Q_xz}{2}+\frac{\sqrt{2}Q_zx}{2}$$

$$\frac{\sqrt{2}Q_yz}{2}+\frac{\sqrt{2}Q_zy}{2}$$

$$\vec{\mathbb{Q}}_{2,1}^{(1,-1)}[q](E,2), \vec{\mathbb{Q}}_{2,2}^{(1,-1)}[q](E,2)$$

\*\* symmetry

$$\sqrt{3}xy$$

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

\*\* expression

$$\frac{\sqrt{2}Q_xy}{2}+\frac{\sqrt{2}Q_yx}{2}$$

$$\frac{\sqrt{2}Q_xx}{2}-\frac{\sqrt{2}Q_yy}{2}$$

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

\*\* symmetry

$$\sqrt{3}xz$$

$$\sqrt{3}yz$$

\*\* expression

$$\frac{\sqrt{7}Q_xz(4x^2-y^2-z^2)}{7}+\frac{5\sqrt{7}Q_yxyz}{7}-\frac{\sqrt{7}Q_zx(x^2+y^2-4z^2)}{7}$$

$$\frac{5\sqrt{7}Q_xxyz}{7}-\frac{\sqrt{7}Q_yz(x^2-4y^2+z^2)}{7}-\frac{\sqrt{7}Q_zy(x^2+y^2-4z^2)}{7}$$

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

\*\* symmetry

$$\sqrt{3}xy$$

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

\*\* expression

$$\frac{\sqrt{7}Q_xy(4x^2-y^2-z^2)}{7}-\frac{\sqrt{7}Q_yx(x^2-4y^2+z^2)}{7}+\frac{5\sqrt{7}Q_zyxyz}{7}$$

$$\frac{\sqrt{7}Q_xx(3x^2-7y^2-2z^2)}{14}+\frac{\sqrt{7}Q_yy(7x^2-3y^2+2z^2)}{14}+\frac{5\sqrt{7}Q_zz(x-y)(x+y)}{14}$$

\* Harmonics for rank 3

$$\vec{\mathbb{Q}}_3^{(1,-1)}[q](A_1,1)$$

\*\* symmetry

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

\*\* expression

$$-\frac{\sqrt{15}Q_xxz}{5} - \frac{\sqrt{15}Q_yyz}{5} - \frac{\sqrt{15}Q_z(x^2 + y^2 - 2z^2)}{10}$$

$\vec{\mathbb{Q}}_3^{(1,-1)}[q](A_1, 2)$

\*\* symmetry

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

\*\* expression

$$\frac{\sqrt{6}Q_xxy}{2} + \frac{\sqrt{6}Q_y(x - y)(x + y)}{4}$$

$\vec{\mathbb{Q}}_3^{(1,1)}[q](A_1, 1)$

\*\* symmetry

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

\*\* expression

$$-\frac{5Q_xxz(3x^2 + 3y^2 - 4z^2)}{12} - \frac{5Q_yyz(3x^2 + 3y^2 - 4z^2)}{12} + \frac{Q_z(3x^4 + 6x^2y^2 - 24x^2z^2 + 3y^4 - 24y^2z^2 + 8z^4)}{12}$$

$\vec{\mathbb{Q}}_3^{(1,1)}[q](A_1, 2)$

\*\* symmetry

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

\*\* expression

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

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

\*\* symmetry

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

\*\* expression

$$\frac{\sqrt{6}Q_x(x - y)(x + y)}{4} - \frac{\sqrt{6}Q_yxy}{2}$$

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

\*\* symmetry

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

\*\* expression

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

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

\*\* symmetry

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

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

\*\* expression

$$-\frac{\sqrt{10}Q_x(3x^2 + y^2 - 4z^2)}{20} - \frac{\sqrt{10}Q_yxy}{10} + \frac{2\sqrt{10}Q_zxz}{5}$$

$$-\frac{\sqrt{10}Q_xxy}{10} - \frac{\sqrt{10}Q_y(x^2 + 3y^2 - 4z^2)}{20} + \frac{2\sqrt{10}Q_zyz}{5}$$

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

\*\* symmetry

$$\sqrt{15}xyz$$

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

\*\* expression

$$Q_xxyz + Q_yxz + Q_zxy$$

$$Q_xxz - Q_yyz + \frac{Q_z(x-y)(x+y)}{2}$$

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

\*\* symmetry

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

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

\*\* expression

$$-\frac{\sqrt{6}Q_x(4x^4+3x^2y^2-27x^2z^2-y^4+3y^2z^2+4z^4)}{24} - \frac{5\sqrt{6}Q_yxy(x^2+y^2-6z^2)}{24} - \frac{5\sqrt{6}Q_zxz(3x^2+3y^2-4z^2)}{24}$$

$$-\frac{5\sqrt{6}Q_xy(x^2+y^2-6z^2)}{24} + \frac{\sqrt{6}Q_y(x^4-3x^2y^2-3x^2z^2-4y^4+27y^2z^2-4z^4)}{24} - \frac{5\sqrt{6}Q_zyz(3x^2+3y^2-4z^2)}{24}$$

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

\*\* symmetry

$$\sqrt{15}xyz$$

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

\*\* expression

$$\frac{\sqrt{15}Q_xxyz(6x^2-y^2-z^2)}{6} - \frac{\sqrt{15}Q_yxz(x^2-6y^2+z^2)}{6} - \frac{\sqrt{15}Q_zxy(x^2+y^2-6z^2)}{6}$$

$$\frac{\sqrt{15}Q_xxz(5x^2-9y^2-2z^2)}{12} + \frac{\sqrt{15}Q_yyz(9x^2-5y^2+2z^2)}{12} - \frac{\sqrt{15}Q_z(x-y)(x+y)(x^2+y^2-6z^2)}{12}$$

\* Harmonics for rank 4

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

\*\* symmetry

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

\*\* expression

$$\frac{3\sqrt{7}Q_xx(x^2+y^2-4z^2)}{28} + \frac{3\sqrt{7}Q_yy(x^2+y^2-4z^2)}{28} - \frac{\sqrt{7}Q_zz(3x^2+3y^2-2z^2)}{7}$$

$$\vec{\mathbb{Q}}_4^{(1,-1)}[q](A_1,2)$$

\*\* symmetry

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

\*\* expression

$$\frac{3\sqrt{10}Q_xxyz}{4} + \frac{3\sqrt{10}Q_yz(x-y)(x+y)}{8} + \frac{\sqrt{10}Q_zy(3x^2-y^2)}{8}$$

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

\*\* symmetry

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

\*\* expression

$$\begin{aligned} & \frac{3\sqrt{55}Q_xx(x^4 + 2x^2y^2 - 12x^2z^2 + y^4 - 12y^2z^2 + 8z^4)}{88} + \frac{3\sqrt{55}Q_yy(x^4 + 2x^2y^2 - 12x^2z^2 + y^4 - 12y^2z^2 + 8z^4)}{88} \\ & + \frac{\sqrt{55}Q_zz(15x^4 + 30x^2y^2 - 40x^2z^2 + 15y^4 - 40y^2z^2 + 8z^4)}{88} \end{aligned}$$

$\vec{\mathbb{Q}}_4^{(1,1)}[q](A_1, 2)$

\*\* symmetry

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

\*\* expression

$$\frac{3\sqrt{154}Q_xxyz(7x^2 - 5y^2 - 2z^2)}{44} - \frac{3\sqrt{154}Q_yyz(x^4 - 9x^2y^2 + x^2z^2 + 2y^4 - y^2z^2)}{44} - \frac{\sqrt{154}Q_zy(3x^2 - y^2)(x^2 + y^2 - 8z^2)}{44}$$

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

\*\* symmetry

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

\*\* expression

$$\frac{3\sqrt{10}Q_xz(x - y)(x + y)}{8} - \frac{3\sqrt{10}Q_yxyz}{4} + \frac{\sqrt{10}Q_zx(x^2 - 3y^2)}{8}$$

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

\*\* symmetry

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

\*\* expression

$$\frac{3\sqrt{154}Q_xz(2x^4 - 9x^2y^2 - x^2z^2 + y^4 + y^2z^2)}{44} + \frac{3\sqrt{154}Q_yxyz(5x^2 - 7y^2 + 2z^2)}{44} - \frac{\sqrt{154}Q_zx(x^2 - 3y^2)(x^2 + y^2 - 8z^2)}{44}$$

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

\*\* symmetry

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

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

\*\* expression

$$-\frac{\sqrt{70}Q_xz(9x^2 + 3y^2 - 4z^2)}{56} - \frac{3\sqrt{70}Q_yxyz}{28} - \frac{3\sqrt{70}Q_zx(x^2 + y^2 - 4z^2)}{56}$$

$$-\frac{3\sqrt{70}Q_xxyz}{28} - \frac{\sqrt{70}Q_yz(3x^2 + 9y^2 - 4z^2)}{56} - \frac{3\sqrt{70}Q_zy(x^2 + y^2 - 4z^2)}{56}$$

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

\*\* symmetry

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

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

\*\* expression

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

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

$\vec{\mathbb{Q}}_{4,1}^{(1,-1)}[q](E, 3), \vec{\mathbb{Q}}_{4,2}^{(1,-1)}[q](E, 3)$

\*\* symmetry

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

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

\*\* expression

$$-\frac{\sqrt{35} Q_x y (3 x^2 + y^2 - 6 z^2)}{28} - \frac{\sqrt{35} Q_y x (x^2 + 3 y^2 - 6 z^2)}{28} + \frac{3 \sqrt{35} Q_z x y z}{7}$$

$$-\frac{\sqrt{35} Q_x x (x^2 - 3 z^2)}{14} + \frac{\sqrt{35} Q_y y (y^2 - 3 z^2)}{14} + \frac{3 \sqrt{35} Q_z z (x-y) (x+y)}{14}$$

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

\*\* symmetry

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

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

\*\* expression

$$-\frac{\sqrt{22} Q_x z (18 x^4 + 15 x^2 y^2 - 41 x^2 z^2 - 3 y^4 + y^2 z^2 + 4 z^4)}{44} - \frac{21 \sqrt{22} Q_y x y z (x^2 + y^2 - 2 z^2)}{44} + \frac{3 \sqrt{22} Q_z x (x^4 + 2 x^2 y^2 - 12 x^2 z^2 + y^4 - 12 y^2 z^2 + 8 z^4)}{44}$$

$$-\frac{21 \sqrt{22} Q_x x y z (x^2 + y^2 - 2 z^2)}{44} + \frac{\sqrt{22} Q_y z (3 x^4 - 15 x^2 y^2 - x^2 z^2 - 18 y^4 + 41 y^2 z^2 - 4 z^4)}{44} + \frac{3 \sqrt{22} Q_z y (x^4 + 2 x^2 y^2 - 12 x^2 z^2 + y^4 - 12 y^2 z^2 + 8 z^4)}{44}$$

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

\*\* symmetry

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

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

\*\* expression

$$-\frac{\sqrt{77} Q_x y (6 x^4 - 11 x^2 y^2 - 3 x^2 z^2 + y^4 + y^2 z^2)}{22} + \frac{\sqrt{77} Q_y x (x^4 - 11 x^2 y^2 + x^2 z^2 + 6 y^4 - 3 y^2 z^2)}{22} - \frac{9 \sqrt{77} Q_z x y z (x-y) (x+y)}{22}$$

$$\frac{\sqrt{77} Q_x x (5 x^4 - 46 x^2 y^2 - 4 x^2 z^2 + 21 y^4 + 12 y^2 z^2)}{88} + \frac{\sqrt{77} Q_y y (21 x^4 - 46 x^2 y^2 + 12 x^2 z^2 + 5 y^4 - 4 y^2 z^2)}{88} + \frac{9 \sqrt{77} Q_z z (x^2 - 2 x y - y^2) (x^2 + 2 x y - y^2)}{88}$$

$$\vec{\mathbb{Q}}_{4,1}^{(1,1)}[q](E,3), \vec{\mathbb{Q}}_{4,2}^{(1,1)}[q](E,3)$$

\*\* symmetry

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

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

\*\* expression

$$-\frac{\sqrt{11} Q_x y (6 x^4 + 5 x^2 y^2 - 51 x^2 z^2 - y^4 + 5 y^2 z^2 + 6 z^4)}{22} + \frac{\sqrt{11} Q_y x (x^4 - 5 x^2 y^2 - 5 x^2 z^2 - 6 y^4 + 51 y^2 z^2 - 6 z^4)}{22} - \frac{21 \sqrt{11} Q_z x y z (x^2 + y^2 - 2 z^2)}{22}$$

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

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