

PG No. 8 D_{2h} mmm [orthorhombic] (polar, internal polar dipole)

* Harmonics for rank 0

$$\bar{Q}_0^{(1,1)}[q](A_g)$$

** 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

$$\bar{Q}_1^{(1,-1)}[q](B_{1u})$$

** symmetry

z

** expression

$$Q_z$$

$$\bar{Q}_1^{(1,1)}[q](B_{1u})$$

** symmetry

z

** expression

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

$$\bar{Q}_1^{(1,-1)}[q](B_{2u})$$

** symmetry

y

** expression

$$Q_y$$

$$\bar{Q}_1^{(1,1)}[q](B_{2u})$$

** symmetry

y

** expression

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

$$\bar{Q}_1^{(1,-1)}[q](B_{3u})$$

** symmetry

x

** expression

$$Q_x$$

$$\bar{Q}_1^{(1,1)}[q](B_{3u})$$

** symmetry

x

** expression

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

* Harmonics for rank 2

$$\bar{Q}_2^{(1,-1)}[q](A_g, 1)$$

** symmetry

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

** expression

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

$$\bar{Q}_2^{(1,-1)}[q](A_g, 2)$$

** symmetry

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

** expression

$$\frac{\sqrt{2}Q_{xx}}{2} - \frac{\sqrt{2}Q_{yy}}{2}$$

$$\bar{Q}_2^{(1,1)}[q](A_g, 1)$$

** symmetry

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

** expression

$$-\frac{\sqrt{21}Q_{xx}(x^2+y^2-4z^2)}{14} - \frac{\sqrt{21}Q_{yy}(x^2+y^2-4z^2)}{14} - \frac{\sqrt{21}Q_{zz}(3x^2+3y^2-2z^2)}{14}$$

$$\bar{Q}_2^{(1,1)}[q](A_g, 2)$$

** symmetry

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

** expression

$$\frac{\sqrt{7}Q_{xx}(3x^2-7y^2-2z^2)}{14} + \frac{\sqrt{7}Q_{yy}(7x^2-3y^2+2z^2)}{14} + \frac{5\sqrt{7}Q_{zz}(x-y)(x+y)}{14}$$

$$\bar{Q}_2^{(1,-1)}[q](B_{1g})$$

** symmetry

$$\sqrt{3}xy$$

** expression

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

$$\bar{Q}_2^{(1,1)}[q](B_{1g})$$

** symmetry

$$\sqrt{3}xy$$

** expression

$$\frac{\sqrt{7}Q_{xy}(4x^2-y^2-z^2)}{7} - \frac{\sqrt{7}Q_{yx}(x^2-4y^2+z^2)}{7} + \frac{5\sqrt{7}Q_{zxy}}{7}$$

$$\bar{Q}_2^{(1,-1)}[q](B_{2g})$$

** symmetry

$$\sqrt{3}xz$$

** expression

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

$$\bar{Q}_2^{(1,1)}[q](B_{2g})$$

** symmetry

$$\sqrt{3}xz$$

** expression

$$\frac{\sqrt{7}Q_{xz}(4x^2-y^2-z^2)}{7} + \frac{5\sqrt{7}Q_{yxyz}}{7} - \frac{\sqrt{7}Q_{zx}(x^2+y^2-4z^2)}{7}$$

$$\bar{Q}_2^{(1,-1)}[q](B_{3g})$$

** symmetry

$$\sqrt{3}yz$$

** expression

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

$$\bar{Q}_2^{(1,1)}[q](B_{3g})$$

** symmetry

$$\sqrt{3}yz$$

** expression

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

* Harmonics for rank 3

$$\bar{Q}_3^{(1,-1)}[q](A_u)$$

** symmetry

$$\sqrt{15}xyz$$

** expression

$$Q_xyz + Q_yxz + Q_zxy$$

$$\bar{Q}_3^{(1,1)}[q](A_u)$$

** symmetry

$$\sqrt{15}xyz$$

** expression

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

$$\bar{Q}_3^{(1,-1)}[q](B_{1u}, 1)$$

** symmetry

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

** expression

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

$$\bar{Q}_3^{(1,-1)}[q](B_{1u}, 2)$$

** symmetry

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

** expression

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

$$\bar{Q}_3^{(1,1)}[q](B_{1u}, 1)$$

** symmetry

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

** expression

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

$$\bar{Q}_3^{(1,1)}[q](B_{1u}, 2)$$

** symmetry

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

** expression

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

$$\bar{Q}_3^{(1,-1)}[q](B_{2u}, 1)$$

** symmetry

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

** expression

$$-\frac{\sqrt{15}Q_xxy}{5} - \frac{\sqrt{15}Q_y(x^2 - 2y^2 + z^2)}{10} - \frac{\sqrt{15}Q_zyz}{5}$$

$$\bar{Q}_3^{(1,-1)}[q](B_{2u}, 2)$$

** symmetry

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

** expression

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

$$\bar{Q}_3^{(1,1)}[q](B_{2u}, 1)$$

** symmetry

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

** expression

$$-\frac{5Q_xxy(3x^2 - 4y^2 + 3z^2)}{12} + \frac{Q_y(3x^4 - 24x^2y^2 + 6x^2z^2 + 8y^4 - 24y^2z^2 + 3z^4)}{12} - \frac{5Q_zyz(3x^2 - 4y^2 + 3z^2)}{12}$$

$$\bar{Q}_3^{(1,1)}[q](B_{2u}, 2)$$

** symmetry

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

** expression

$$-\frac{\sqrt{15}Q_xxy(5x^2 - 2y^2 - 9z^2)}{12} + \frac{\sqrt{15}Q_y(x-z)(x+z)(x^2 - 6y^2 + z^2)}{12} - \frac{\sqrt{15}Q_zyz(9x^2 + 2y^2 - 5z^2)}{12}$$

$$\bar{Q}_3^{(1,-1)}[q](B_{3u}, 1)$$

** symmetry

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

** expression

$$\frac{\sqrt{15}Q_x(2x^2 - y^2 - z^2)}{10} - \frac{\sqrt{15}Q_yxy}{5} - \frac{\sqrt{15}Q_zxz}{5}$$

$$\bar{Q}_3^{(1,-1)}[q](B_{3u}, 2)$$

** symmetry

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

** expression

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

$$\bar{Q}_3^{(1,1)}[q](B_{3u}, 1)$$

** symmetry

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

** expression

$$\frac{Q_x(8x^4 - 24x^2y^2 - 24x^2z^2 + 3y^4 + 6y^2z^2 + 3z^4)}{12} + \frac{5Q_yxy(4x^2 - 3y^2 - 3z^2)}{12} + \frac{5Q_zxz(4x^2 - 3y^2 - 3z^2)}{12}$$

$$\bar{Q}_3^{(1,1)}[q](B_{3u}, 2)$$

** symmetry

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

** expression

$$\frac{\sqrt{15}Q_x(y-z)(y+z)(6x^2 - y^2 - z^2)}{12} - \frac{\sqrt{15}Q_yxy(2x^2 - 5y^2 + 9z^2)}{12} + \frac{\sqrt{15}Q_zxz(2x^2 + 9y^2 - 5z^2)}{12}$$

* Harmonics for rank 4

$$\bar{Q}_4^{(1,-1)}[q](A_g, 1)$$

** symmetry

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

** expression

$$\frac{\sqrt{3}Q_{xx} (2x^2 - 3y^2 - 3z^2)}{6} - \frac{\sqrt{3}Q_{yy} (3x^2 - 2y^2 + 3z^2)}{6} - \frac{\sqrt{3}Q_{zz} (3x^2 + 3y^2 - 2z^2)}{6}$$

$$\bar{Q}_4^{(1,-1)}[q](A_g, 2)$$

** symmetry

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

** expression

$$-\frac{\sqrt{105}Q_{xx} (x^2 - 6y^2 + 3z^2)}{42} + \frac{\sqrt{105}Q_{yy} (6x^2 - y^2 - 3z^2)}{42} - \frac{\sqrt{105}Q_{zz} (3x^2 + 3y^2 - 2z^2)}{42}$$

$$\bar{Q}_4^{(1,-1)}[q](A_g, 3)$$

** symmetry

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

** expression

$$\frac{\sqrt{35}Q_{xx} (x^2 - 3z^2)}{14} - \frac{\sqrt{35}Q_{yy} (y^2 - 3z^2)}{14} - \frac{3\sqrt{35}Q_{zz} (x - y) (x + y)}{14}$$

$$\bar{Q}_4^{(1,1)}[q](A_g, 1)$$

** symmetry

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

** expression

$$\frac{\sqrt{1155}Q_{xx} (x^4 - 5x^2y^2 - 5x^2z^2 + 3y^4 - 3y^2z^2 + 3z^4)}{66} + \frac{\sqrt{1155}Q_{yy} (3x^4 - 5x^2y^2 - 3x^2z^2 + y^4 - 5y^2z^2 + 3z^4)}{66} + \frac{\sqrt{1155}Q_{zz} (3x^4 - 3x^2y^2 - 5x^2z^2 + 3y^4 - 5y^2z^2 + z^4)}{66}$$

$$\bar{Q}_4^{(1,1)}[q](A_g, 2)$$

** symmetry

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

** expression

$$-\frac{\sqrt{33}Q_{xx} (5x^4 - 88x^2y^2 + 38x^2z^2 + 33y^4 + 66y^2z^2 - 30z^4)}{132} - \frac{\sqrt{33}Q_{yy} (33x^4 - 88x^2y^2 + 66x^2z^2 + 5y^4 + 38y^2z^2 - 30z^4)}{132} + \frac{\sqrt{33}Q_{zz} (3x^4 + 132x^2y^2 - 50x^2z^2 + 3y^4 - 50y^2z^2 + 10z^4)}{132}$$

$$\bar{Q}_4^{(1,1)}[q](A_g, 3)$$

** symmetry

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

** expression

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

$$\bar{Q}_4^{(1,-1)}[q](B_{1g}, 1)$$

** symmetry

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

** expression

$$\frac{\sqrt{5}Q_{xy} (3x^2 - y^2)}{4} + \frac{\sqrt{5}Q_{yx} (x^2 - 3y^2)}{4}$$

$$\bar{Q}_4^{(1,-1)}[q](B_{1g}, 2)$$

** symmetry

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

** expression

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

$$\bar{Q}_4^{(1,1)}[q](B_{1g}, 1)$$

** symmetry

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

** expression

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

$$\bar{Q}_4^{(1,1)}[q](B_{1g}, 2)$$

** symmetry

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

** expression

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

$$\bar{Q}_4^{(1,-1)}[q](B_{2g}, 1)$$

** symmetry

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

** expression

$$-\frac{\sqrt{5}Q_x z(3x^2 - z^2)}{4} - \frac{\sqrt{5}Q_z x(x^2 - 3z^2)}{4}$$

$$\bar{Q}_4^{(1,-1)}[q](B_{2g}, 2)$$

** symmetry

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

** expression

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

$$\bar{Q}_4^{(1,1)}[q](B_{2g}, 1)$$

** symmetry

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

** expression

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

$$\bar{Q}_4^{(1,1)}[q](B_{2g}, 2)$$

** symmetry

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

** expression

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

$$\bar{Q}_4^{(1,-1)}[q](B_{3g}, 1)$$

** symmetry

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

** expression

$$\frac{\sqrt{5}Q_y z (3y^2 - z^2)}{4} + \frac{\sqrt{5}Q_z y (y^2 - 3z^2)}{4}$$

$\bar{Q}_4^{(1,-1)}[q](B_{3g}, 2)$

** symmetry

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

** expression

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

$\bar{Q}_4^{(1,1)}[q](B_{3g}, 1)$

** symmetry

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

** expression

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

$\bar{Q}_4^{(1,1)}[q](B_{3g}, 2)$

** symmetry

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

** expression

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