

PG No. 2 $C_i \bar{1}$ [triclinic] (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

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

** symmetry

x

** expression

$$Q_x$$

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

** symmetry

y

** expression

$$Q_y$$

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

** symmetry

z

** expression

$$Q_z$$

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

** symmetry

x

** expression

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

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

** symmetry

y

** expression

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

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

** symmetry

z

** expression

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

* 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

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

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

** symmetry

$$\sqrt{3}yz$$

** expression

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

$$\bar{Q}_2^{(1,-1)}[q](A_g, 4)$$

** symmetry

$$\sqrt{3}xz$$

** expression

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

$$\bar{Q}_2^{(1,-1)}[q](A_g, 5)$$

** symmetry

$$\sqrt{3}xy$$

** expression

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

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

** 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

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

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

** symmetry

$$\sqrt{3}yz$$

** expression

$$\frac{5\sqrt{7}Q_{xyz}}{7} - \frac{\sqrt{7}Q_{yz}(x^2-4y^2+z^2)}{7} - \frac{\sqrt{7}Q_{zy}(x^2+y^2-4z^2)}{7}$$

$$\bar{Q}_2^{(1,1)}[q](A_g, 4)$$

** symmetry

$$\sqrt{3}xz$$

** expression

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

$$\bar{Q}_2^{(1,1)}[q](A_g, 5)$$

** symmetry

$$\sqrt{3}xy$$

** expression

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

* Harmonics for rank 3

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

** symmetry

$$\sqrt{15}xyz$$

** expression

$$Q_xyz + Q_yxz + Q_zxy$$

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

** symmetry

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

** expression

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

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

** symmetry

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

** expression

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

$$\bar{Q}_3^{(1,-1)}[q](A_u, 4)$$

** symmetry

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

** expression

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

$$\bar{Q}_3^{(1,-1)}[q](A_u, 5)$$

** symmetry

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

** expression

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

$$\bar{Q}_3^{(1,-1)}[q](A_u, 6)$$

** symmetry

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

** expression

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

$$\bar{Q}_3^{(1,-1)}[q](A_u, 7)$$

** symmetry

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

** expression

$$Q_x xz - Q_y yz + \frac{Q_z (x - y)(x + y)}{2}$$

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

** symmetry

$$\sqrt{15}xyz$$

** expression

$$\frac{\sqrt{15}Q_x yz (6x^2 - y^2 - z^2)}{6} - \frac{\sqrt{15}Q_y xz (x^2 - 6y^2 + z^2)}{6} - \frac{\sqrt{15}Q_z xy (x^2 + y^2 - 6z^2)}{6}$$

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

** symmetry

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

** expression

$$\frac{Q_x (8x^4 - 24x^2y^2 - 24x^2z^2 + 3y^4 + 6y^2z^2 + 3z^4)}{12} + \frac{5Q_y xy (4x^2 - 3y^2 - 3z^2)}{12} + \frac{5Q_z xz (4x^2 - 3y^2 - 3z^2)}{12}$$

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

** symmetry

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

** expression

$$-\frac{5Q_x xy (3x^2 - 4y^2 + 3z^2)}{12} + \frac{Q_y (3x^4 - 24x^2y^2 + 6x^2z^2 + 8y^4 - 24y^2z^2 + 3z^4)}{12} - \frac{5Q_z yz (3x^2 - 4y^2 + 3z^2)}{12}$$

$$\bar{Q}_3^{(1,1)}[q](A_u, 4)$$

** symmetry

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

** expression

$$-\frac{5Q_x xz (3x^2 + 3y^2 - 4z^2)}{12} - \frac{5Q_y yz (3x^2 + 3y^2 - 4z^2)}{12} + \frac{Q_z (3x^4 + 6x^2y^2 - 24x^2z^2 + 3y^4 - 24y^2z^2 + 8z^4)}{12}$$

$$\bar{Q}_3^{(1,1)}[q](A_u, 5)$$

** symmetry

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

** expression

$$\frac{\sqrt{15}Q_x (y - z)(y + z)(6x^2 - y^2 - z^2)}{12} - \frac{\sqrt{15}Q_y xy (2x^2 - 5y^2 + 9z^2)}{12} + \frac{\sqrt{15}Q_z xz (2x^2 + 9y^2 - 5z^2)}{12}$$

$$\bar{Q}_3^{(1,1)}[q](A_u, 6)$$

** symmetry

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

** expression

$$-\frac{\sqrt{15}Q_x xy (5x^2 - 2y^2 - 9z^2)}{12} + \frac{\sqrt{15}Q_y (x - z)(x + z)(x^2 - 6y^2 + z^2)}{12} - \frac{\sqrt{15}Q_z yz (9x^2 + 2y^2 - 5z^2)}{12}$$

$$\bar{Q}_3^{(1,1)}[q](A_u, 7)$$

** symmetry

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

** expression

$$\frac{\sqrt{15}Q_x xz (5x^2 - 9y^2 - 2z^2)}{12} + \frac{\sqrt{15}Q_y yz (9x^2 - 5y^2 + 2z^2)}{12} - \frac{\sqrt{15}Q_z (x - y)(x + y)(x^2 + y^2 - 6z^2)}{12}$$

* Harmonics for rank 4

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

** 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

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

$$\bar{Q}_4^{(1,-1)}[q](A_g, 4)$$

** symmetry

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

** expression

$$\frac{\sqrt{5}Q_{yz} (3y^2 - z^2)}{4} + \frac{\sqrt{5}Q_{zy} (y^2 - 3z^2)}{4}$$

$$\bar{Q}_4^{(1,-1)}[q](A_g, 5)$$

** symmetry

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

** expression

$$-\frac{\sqrt{5}Q_{xz} (3x^2 - z^2)}{4} - \frac{\sqrt{5}Q_{zx} (x^2 - 3z^2)}{4}$$

$$\bar{Q}_4^{(1,-1)}[q](A_g, 6)$$

** symmetry

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

** expression

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

$$\bar{Q}_4^{(1,-1)}[q](A_g, 7)$$

** symmetry

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

** expression

$$\frac{3\sqrt{35}Q_{xyz}}{7} + \frac{\sqrt{35}Q_{yz} (6x^2 - 3y^2 - z^2)}{28} + \frac{\sqrt{35}Q_{zy} (6x^2 - y^2 - 3z^2)}{28}$$

$$\bar{Q}_4^{(1,-1)}[q](A_g, 8)$$

** symmetry

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

** expression

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

$$\bar{Q}_4^{(1,-1)}[q](A_g, 9)$$

** symmetry

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

** expression

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

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

** symmetry

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

** expression

$$\frac{\sqrt{1155}Q_x x (x^4 - 5x^2 y^2 - 5x^2 z^2 + 3y^4 - 3y^2 z^2 + 3z^4)}{66} + \frac{\sqrt{1155}Q_y y (3x^4 - 5x^2 y^2 - 3x^2 z^2 + y^4 - 5y^2 z^2 + 3z^4)}{66} + \frac{\sqrt{1155}Q_z z (3x^4 - 3x^2 y^2 - 5x^2 z^2 + 3y^4 - 5y^2 z^2 + z^4)}{66}$$

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

** symmetry

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

** expression

$$-\frac{\sqrt{33}Q_x x (5x^4 - 88x^2 y^2 + 38x^2 z^2 + 33y^4 + 66y^2 z^2 - 30z^4)}{132} - \frac{\sqrt{33}Q_y y (33x^4 - 88x^2 y^2 + 66x^2 z^2 + 5y^4 + 38y^2 z^2 - 30z^4)}{132} + \frac{\sqrt{33}Q_z z (3x^4 + 132x^2 y^2 - 50x^2 z^2 + 3y^4 - 50y^2 z^2 + 10z^4)}{132}$$

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

** symmetry

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

** expression

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

$$\bar{Q}_4^{(1,1)}[q](A_g, 4)$$

** symmetry

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

** expression

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

$$\bar{Q}_4^{(1,1)}[q](A_g, 5)$$

** symmetry

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

** expression

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

$$\bar{Q}_4^{(1,1)}[q](A_g, 6)$$

** symmetry

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

** expression

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

$\bar{Q}_4^{(1,1)}[q](A_g, 7)$

** symmetry

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

** expression

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

$\bar{Q}_4^{(1,1)}[q](A_g, 8)$

** symmetry

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

** expression

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

$\bar{Q}_4^{(1,1)}[q](A_g, 9)$

** symmetry

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

** expression

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