

PG No. 15 D_{4h} $4/mmm$ [tetragonal] (polar, internal polar quadrupole)

* Harmonics for rank 0

$$\bar{Q}_0^{(2,2)}[q](A_{1g})$$

** symmetry

$$1$$

** expression

$$-\frac{\sqrt{5}Q_u(x^2+y^2-2z^2)}{10} + \frac{\sqrt{15}Q_v(x-y)(x+y)}{10} + \frac{\sqrt{15}Q_{xy}xy}{5} + \frac{\sqrt{15}Q_{xz}xz}{5} + \frac{\sqrt{15}Q_{yz}yz}{5}$$

* Harmonics for rank 1

$$\bar{Q}_1^{(2,0)}[q](A_{2u})$$

** symmetry

$$z$$

** expression

$$\frac{\sqrt{10}Q_u z}{5} + \frac{\sqrt{30}Q_{xz}x}{10} + \frac{\sqrt{30}Q_{yz}y}{10}$$

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

** symmetry

$$z$$

** expression

$$-\frac{3\sqrt{35}Q_u z(3x^2+3y^2-2z^2)}{70} + \frac{\sqrt{105}Q_v z(x-y)(x+y)}{14} + \frac{\sqrt{105}Q_{xy}xyz}{7} - \frac{\sqrt{105}Q_{xz}x(x^2+y^2-4z^2)}{35} - \frac{\sqrt{105}Q_{yz}y(x^2+y^2-4z^2)}{35}$$

$$\bar{Q}_{1,1}^{(2,0)}[q](E_u), \bar{Q}_{1,2}^{(2,0)}[q](E_u)$$

** symmetry

$$x$$

$$y$$

** expression

$$-\frac{\sqrt{10}Q_u x}{10} + \frac{\sqrt{30}Q_v x}{10} + \frac{\sqrt{30}Q_{xy}y}{10} + \frac{\sqrt{30}Q_{xz}z}{10}$$

$$-\frac{\sqrt{10}Q_u y}{10} - \frac{\sqrt{30}Q_v y}{10} + \frac{\sqrt{30}Q_{xy}x}{10} + \frac{\sqrt{30}Q_{yz}z}{10}$$

$$\bar{Q}_{1,1}^{(2,2)}[q](E_u), \bar{Q}_{1,2}^{(2,2)}[q](E_u)$$

** symmetry

$$x$$

$$y$$

** expression

$$-\frac{3\sqrt{35}Q_u x(x^2+y^2-4z^2)}{70} + \frac{\sqrt{105}Q_v x(3x^2-7y^2-2z^2)}{70} + \frac{\sqrt{105}Q_{xy}y(4x^2-y^2-z^2)}{35} + \frac{\sqrt{105}Q_{xz}z(4x^2-y^2-z^2)}{35} + \frac{\sqrt{105}Q_{yz}xyz}{7}$$

$$-\frac{3\sqrt{35}Q_u y(x^2+y^2-4z^2)}{70} + \frac{\sqrt{105}Q_v y(7x^2-3y^2+2z^2)}{70} - \frac{\sqrt{105}Q_{xy}x(x^2-4y^2+z^2)}{35} + \frac{\sqrt{105}Q_{xz}xyz}{7} - \frac{\sqrt{105}Q_{yz}z(x^2-4y^2+z^2)}{35}$$

* Harmonics for rank 2

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

** symmetry

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

** expression

$$Q_u$$

$$\bar{Q}_2^{(2,0)}[q](A_{1g})$$

** symmetry

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

** expression

$$-\frac{\sqrt{14}Q_u(x^2+y^2-2z^2)}{14}-\frac{\sqrt{42}Q_v(x-y)(x+y)}{14}-\frac{\sqrt{42}Q_{xy}xy}{7}+\frac{\sqrt{42}Q_{xz}xz}{14}+\frac{\sqrt{42}Q_{yz}yz}{14}$$

$\tilde{\mathbb{Q}}_2^{(2,2)}[q](A_{1g})$

** symmetry

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

** expression

$$\frac{\sqrt{14}Q_u(3x^4+6x^2y^2-24x^2z^2+3y^4-24y^2z^2+8z^4)}{56}-\frac{5\sqrt{42}Q_v(x-y)(x+y)(x^2+y^2-6z^2)}{168}-\frac{5\sqrt{42}Q_{xy}xy(x^2+y^2-6z^2)}{84}-\frac{5\sqrt{42}Q_{xz}xz(3x^2+3y^2-4z^2)}{84}-\frac{5\sqrt{42}Q_{yz}yz(3x^2+3y^2-4z^2)}{84}$$

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

** symmetry

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

** expression

$$Q_v$$

$\tilde{\mathbb{Q}}_2^{(2,0)}[q](B_{1g})$

** symmetry

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

** expression

$$-\frac{\sqrt{42}Q_u(x-y)(x+y)}{14}+\frac{\sqrt{14}Q_v(x^2+y^2-2z^2)}{14}+\frac{3\sqrt{14}Q_{xz}xz}{14}-\frac{3\sqrt{14}Q_{yz}yz}{14}$$

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

** symmetry

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

** expression

$$-\frac{5\sqrt{42}Q_u(x-y)(x+y)(x^2+y^2-6z^2)}{168}+\frac{\sqrt{14}Q_v(19x^4-102x^2y^2-12x^2z^2+19y^4-12y^2z^2+4z^4)}{168}+\frac{5\sqrt{14}Q_{xy}xy(x-y)(x+y)}{12}+\frac{5\sqrt{14}Q_{xz}xz(5x^2-9y^2-2z^2)}{84}+\frac{5\sqrt{14}Q_{yz}yz(9x^2-5y^2+2z^2)}{84}$$

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

** symmetry

$$\sqrt{3}xy$$

** expression

$$Q_{xy}$$

$\tilde{\mathbb{Q}}_2^{(2,0)}[q](B_{2g})$

** symmetry

$$\sqrt{3}xy$$

** expression

$$-\frac{\sqrt{42}Q_uxy}{7}+\frac{\sqrt{14}Q_{xy}(x^2+y^2-2z^2)}{14}+\frac{3\sqrt{14}Q_{xz}yz}{14}+\frac{3\sqrt{14}Q_{yz}xz}{14}$$

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

** symmetry

$$\sqrt{3}xy$$

** expression

$$-\frac{5\sqrt{42}Q_uxy(x^2+y^2-6z^2)}{84}+\frac{5\sqrt{14}Q_vxy(x-y)(x+y)}{12}-\frac{\sqrt{14}Q_{xy}(4x^4-27x^2y^2+3x^2z^2+4y^4+3y^2z^2-z^4)}{42}+\frac{5\sqrt{14}Q_{xz}yz(6x^2-y^2-z^2)}{42}-\frac{5\sqrt{14}Q_{yz}xz(x^2-6y^2+z^2)}{42}$$

$$\tilde{Q}_{2,1}^{(2,-2)}[q](E_g), \tilde{Q}_{2,2}^{(2,-2)}[q](E_g)$$

** symmetry

$$\sqrt{3}yz$$

$$\sqrt{3}xz$$

** expression

$$Q_{yz}$$

$$Q_{xz}$$

$$\tilde{Q}_{2,1}^{(2,0)}[q](E_g), \tilde{Q}_{2,2}^{(2,0)}[q](E_g)$$

** symmetry

$$\sqrt{3}yz$$

$$\sqrt{3}xz$$

** expression

$$\frac{\sqrt{42}Q_{uyz}}{14} - \frac{3\sqrt{14}Q_{vyz}}{14} + \frac{3\sqrt{14}Q_{xyxz}}{14} + \frac{3\sqrt{14}Q_{xzy}}{14} - \frac{\sqrt{14}Q_{yz}(2x^2 - y^2 - z^2)}{14}$$

$$\frac{\sqrt{42}Q_{uxz}}{14} + \frac{3\sqrt{14}Q_{vzx}}{14} + \frac{3\sqrt{14}Q_{xyyz}}{14} + \frac{\sqrt{14}Q_{xz}(x^2 - 2y^2 + z^2)}{14} + \frac{3\sqrt{14}Q_{yzxy}}{14}$$

$$\tilde{Q}_{2,1}^{(2,2)}[q](E_g), \tilde{Q}_{2,2}^{(2,2)}[q](E_g)$$

** symmetry

$$\sqrt{3}yz$$

$$\sqrt{3}xz$$

** expression

$$-\frac{5\sqrt{42}Q_{uyz}(3x^2 + 3y^2 - 4z^2)}{84} + \frac{5\sqrt{14}Q_{vyz}(9x^2 - 5y^2 + 2z^2)}{84} - \frac{5\sqrt{14}Q_{xyxz}(x^2 - 6y^2 + z^2)}{42} \\ - \frac{5\sqrt{14}Q_{xzy}(x^2 + y^2 - 6z^2)}{42} + \frac{\sqrt{14}Q_{yz}(x^4 - 3x^2y^2 - 3x^2z^2 - 4y^4 + 27y^2z^2 - 4z^4)}{42}$$

$$-\frac{5\sqrt{42}Q_{uxz}(3x^2 + 3y^2 - 4z^2)}{84} + \frac{5\sqrt{14}Q_{vzx}(5x^2 - 9y^2 - 2z^2)}{84} + \frac{5\sqrt{14}Q_{xyyz}(6x^2 - y^2 - z^2)}{42} \\ - \frac{\sqrt{14}Q_{xz}(4x^4 + 3x^2y^2 - 27x^2z^2 - y^4 + 3y^2z^2 + 4z^4)}{42} - \frac{5\sqrt{14}Q_{yzxy}(x^2 + y^2 - 6z^2)}{42}$$

* Harmonics for rank 3

$$\tilde{Q}_3^{(2,-2)}[q](A_{2u})$$

** symmetry

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

** expression

$$\frac{\sqrt{15}Q_{uz}}{5} - \frac{\sqrt{5}Q_{zx}}{5} - \frac{\sqrt{5}Q_{yz}}{5}$$

$$\tilde{Q}_3^{(2,0)}[q](A_{2u})$$

** symmetry

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

** expression

$$-\frac{\sqrt{15}Q_{uz}(3x^2 + 3y^2 - 2z^2)}{15} - \frac{\sqrt{5}Q_{vz}(x - y)(x + y)}{2} - \sqrt{5}Q_{xyyz} - \frac{\sqrt{5}Q_{zx}(x^2 + y^2 - 4z^2)}{20} - \frac{\sqrt{5}Q_{yz}(x^2 + y^2 - 4z^2)}{20}$$

$$\tilde{Q}_3^{(2,2)}[q](A_{2u})$$

** symmetry

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

** expression

$$\frac{\sqrt{330}Q_u z (15x^4 + 30x^2y^2 - 40x^2z^2 + 15y^4 - 40y^2z^2 + 8z^4)}{264} - \frac{7\sqrt{110}Q_v z (x-y)(x+y)(x^2+y^2-2z^2)}{88} - \frac{7\sqrt{110}Q_{xy}xyz(x^2+y^2-2z^2)}{44} \\ + \frac{\sqrt{110}Q_{xz}x(x^4+2x^2y^2-12x^2z^2+y^4-12y^2z^2+8z^4)}{44} + \frac{\sqrt{110}Q_{yz}y(x^4+2x^2y^2-12x^2z^2+y^4-12y^2z^2+8z^4)}{44}$$

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

** symmetry

$$\sqrt{15}xyz$$

** expression

$$\frac{\sqrt{3}Q_{xy}z}{3} + \frac{\sqrt{3}Q_{xz}y}{3} + \frac{\sqrt{3}Q_{yz}x}{3}$$

$$\tilde{Q}_3^{(2,0)}[q](B_{1u})$$

** symmetry

$$\sqrt{15}xyz$$

** expression

$$\frac{\sqrt{3}Q_{xy}z(3x^2+3y^2-2z^2)}{6} + \frac{\sqrt{3}Q_{xz}y(3x^2-2y^2+3z^2)}{6} - \frac{\sqrt{3}Q_{yz}x(2x^2-3y^2-3z^2)}{6}$$

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

** symmetry

$$\sqrt{15}xyz$$

** expression

$$-\frac{21\sqrt{22}Q_uxyz(x^2+y^2-2z^2)}{44} + \frac{21\sqrt{66}Q_vxyz(x-y)(x+y)}{44} - \frac{\sqrt{66}Q_{xy}z(6x^4-51x^2y^2+5x^2z^2+6y^4+5y^2z^2-z^4)}{66} \\ - \frac{\sqrt{66}Q_{xz}y(6x^4+5x^2y^2-51x^2z^2-y^4+5y^2z^2+6z^4)}{66} + \frac{\sqrt{66}Q_{yz}x(x^4-5x^2y^2-5x^2z^2-6y^4+51y^2z^2-6z^4)}{66}$$

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

** symmetry

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

** expression

$$\frac{\sqrt{3}Q_vz}{3} + \frac{\sqrt{3}Q_{xz}x}{3} - \frac{\sqrt{3}Q_{yz}y}{3}$$

$$\tilde{Q}_3^{(2,0)}[q](B_{2u})$$

** symmetry

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

** expression

$$\frac{\sqrt{3}Q_vz(3x^2+3y^2-2z^2)}{6} + \frac{\sqrt{3}Q_{xz}x(x^2-9y^2+6z^2)}{12} + \frac{\sqrt{3}Q_{yz}y(9x^2-y^2-6z^2)}{12}$$

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

** symmetry

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

** expression

$$-\frac{21\sqrt{22}Q_u z (x-y)(x+y)(x^2+y^2-2z^2)}{88} + \frac{\sqrt{66}Q_v z (39x^4-174x^2y^2-20x^2z^2+39y^4-20y^2z^2+4z^4)}{264} + \frac{21\sqrt{66}Q_{xy}xyz(x-y)(x+y)}{44} \\ - \frac{\sqrt{66}Q_{xz}x(5x^4-4x^2y^2-46x^2z^2-9y^4+66y^2z^2+12z^4)}{132} - \frac{\sqrt{66}Q_{yz}y(9x^4+4x^2y^2-66x^2z^2-5y^4+46y^2z^2-12z^4)}{132}$$

$$\tilde{Q}_{3,1}^{(2,-2)}[q](E_u, 1), \tilde{Q}_{3,2}^{(2,-2)}[q](E_u, 1)$$

** symmetry

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

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

** expression

$$-\frac{\sqrt{15}Q_u x}{10} + \frac{3\sqrt{5}Q_v x}{10} - \frac{\sqrt{5}Q_{xy} y}{5} - \frac{\sqrt{5}Q_{xz} z}{5}$$

$$-\frac{\sqrt{15}Q_u y}{10} - \frac{3\sqrt{5}Q_v y}{10} - \frac{\sqrt{5}Q_{xy} x}{5} - \frac{\sqrt{5}Q_{yz} z}{5}$$

$$\tilde{Q}_{3,1}^{(2,-2)}[q](E_u, 2), \tilde{Q}_{3,2}^{(2,-2)}[q](E_u, 2)$$

** symmetry

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

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

** expression

$$-\frac{Q_u x}{2} - \frac{\sqrt{3}Q_v x}{6} + \frac{\sqrt{3}Q_{xy} y}{3} - \frac{\sqrt{3}Q_{xz} z}{3}$$

$$-\frac{Q_u y}{2} + \frac{\sqrt{3}Q_v y}{6} + \frac{\sqrt{3}Q_{xy} x}{3} - \frac{\sqrt{3}Q_{yz} z}{3}$$

$$\tilde{Q}_{3,1}^{(2,0)}[q](E_u, 1), \tilde{Q}_{3,2}^{(2,0)}[q](E_u, 1)$$

** symmetry

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

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

** expression

$$-\frac{\sqrt{15}Q_u x(4x^2 - 21y^2 + 9z^2)}{60} + \frac{\sqrt{5}Q_v x(4x^2 - y^2 - 11z^2)}{20} + \frac{\sqrt{5}Q_{xy} y(4x^2 - y^2 - z^2)}{20} + \frac{\sqrt{5}Q_{xz} z(4x^2 - y^2 - z^2)}{20} - \sqrt{5}Q_{yz} x y z$$

$$\frac{\sqrt{15}Q_u y(21x^2 - 4y^2 - 9z^2)}{60} + \frac{\sqrt{5}Q_v y(x^2 - 4y^2 + 11z^2)}{20} - \frac{\sqrt{5}Q_{xy} x(x^2 - 4y^2 + z^2)}{20} - \sqrt{5}Q_{xz} x y z - \frac{\sqrt{5}Q_{yz} z(x^2 - 4y^2 + z^2)}{20}$$

$$\tilde{Q}_{3,1}^{(2,0)}[q](E_u, 2), \tilde{Q}_{3,2}^{(2,0)}[q](E_u, 2)$$

** symmetry

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

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

** expression

$$\frac{Q_u x(2x^2 - 3y^2 - 3z^2)}{4} + \frac{\sqrt{3}Q_v x(2x^2 - 3y^2 - 3z^2)}{12} + \frac{\sqrt{3}Q_{xy} y(6x^2 + y^2 - 9z^2)}{12} - \frac{\sqrt{3}Q_{xz} z(6x^2 - 9y^2 + z^2)}{12}$$

$$-\frac{Q_u y(3x^2 - 2y^2 + 3z^2)}{4} + \frac{\sqrt{3}Q_v y(3x^2 - 2y^2 + 3z^2)}{12} + \frac{\sqrt{3}Q_{xy} x(x^2 + 6y^2 - 9z^2)}{12} + \frac{\sqrt{3}Q_{yz} z(9x^2 - 6y^2 - z^2)}{12}$$

$$\tilde{Q}_{3,1}^{(2,2)}[q](E_u, 1), \tilde{Q}_{3,2}^{(2,2)}[q](E_u, 1)$$

** symmetry

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

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

** expression

$$-\frac{\sqrt{330}Q_u x(4x^4 + x^2 y^2 - 41x^2 z^2 - 3y^4 + 15y^2 z^2 + 18z^4)}{264} + \frac{\sqrt{110}Q_v x(4x^4 - 27x^2 y^2 - 13x^2 z^2 + 11y^4 + 15y^2 z^2 + 4z^4)}{88} \\ + \frac{\sqrt{110}Q_{xy} y(8x^4 - 12x^2 y^2 - 12x^2 z^2 + y^4 + 2y^2 z^2 + z^4)}{44} + \frac{\sqrt{110}Q_{xz} z(8x^4 - 12x^2 y^2 - 12x^2 z^2 + y^4 + 2y^2 z^2 + z^4)}{44} + \frac{7\sqrt{110}Q_{yz} x y z(2x^2 - y^2 - z^2)}{44}$$

$$\frac{\sqrt{330}Q_u y (3x^4 - x^2 y^2 - 15x^2 z^2 - 4y^4 + 41y^2 z^2 - 18z^4)}{264} - \frac{\sqrt{110}Q_v y (11x^4 - 27x^2 y^2 + 15x^2 z^2 + 4y^4 - 13y^2 z^2 + 4z^4)}{88}$$

$$+ \frac{\sqrt{110}Q_{xy} x (x^4 - 12x^2 y^2 + 2x^2 z^2 + 8y^4 - 12y^2 z^2 + z^4)}{44} - \frac{7\sqrt{110}Q_{xz} x y z (x^2 - 2y^2 + z^2)}{44} + \frac{\sqrt{110}Q_{yz} z (x^4 - 12x^2 y^2 + 2x^2 z^2 + 8y^4 - 12y^2 z^2 + z^4)}{44}$$

$$\bar{Q}_{3,1}^{(2,2)}[q](E_u, 2), \bar{Q}_{3,2}^{(2,2)}[q](E_u, 2)$$

** symmetry

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

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

** expression

$$- \frac{\sqrt{22}Q_u x (2x^4 + 11x^2 y^2 - 31x^2 z^2 + 9y^4 - 87y^2 z^2 + 30z^4)}{88} - \frac{\sqrt{66}Q_v x (2x^4 - 73x^2 y^2 + 53x^2 z^2 + 51y^4 - 87y^2 z^2 - 12z^4)}{264}$$

$$- \frac{\sqrt{66}Q_{xy} y (12x^4 - 46x^2 y^2 + 66x^2 z^2 + 5y^4 - 4y^2 z^2 - 9z^4)}{132}$$

$$+ \frac{\sqrt{66}Q_{xz} z (12x^4 + 66x^2 y^2 - 46x^2 z^2 - 9y^4 - 4y^2 z^2 + 5z^4)}{132} + \frac{21\sqrt{66}Q_{yz} x y z (y-z)(y+z)}{44}$$

$$- \frac{\sqrt{22}Q_u y (9x^4 + 11x^2 y^2 - 87x^2 z^2 + 2y^4 - 31y^2 z^2 + 30z^4)}{88} + \frac{\sqrt{66}Q_v y (51x^4 - 73x^2 y^2 - 87x^2 z^2 + 2y^4 + 53y^2 z^2 - 12z^4)}{264}$$

$$- \frac{\sqrt{66}Q_{xy} x (5x^4 - 46x^2 y^2 - 4x^2 z^2 + 12y^4 + 66y^2 z^2 - 9z^4)}{132} + \frac{21\sqrt{66}Q_{xz} x y z (x-z)(x+z)}{44}$$

$$- \frac{\sqrt{66}Q_{yz} z (9x^4 - 66x^2 y^2 + 4x^2 z^2 - 12y^4 + 46y^2 z^2 - 5z^4)}{132}$$

* Harmonics for rank 4

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

** symmetry

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

** expression

$$- \frac{\sqrt{30}Q_u (x^2 + y^2 - 2z^2)}{20} + \frac{3\sqrt{10}Q_v (x-y)(x+y)}{20} - \frac{\sqrt{10}Q_{xy} xy}{5} - \frac{\sqrt{10}Q_{xz} xz}{5} - \frac{\sqrt{10}Q_{yz} yz}{5}$$

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

** symmetry

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

** expression

$$- \frac{\sqrt{42}Q_u (x^2 + y^2 - 2z^2)}{28} - \frac{3\sqrt{14}Q_v (x-y)(x+y)}{28} + \frac{2\sqrt{14}Q_{xy} xy}{7} - \frac{\sqrt{14}Q_{xz} xz}{7} - \frac{\sqrt{14}Q_{yz} yz}{7}$$

$$\bar{Q}_4^{(2,0)}[q](A_{1g}, 1)$$

** symmetry

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

** expression

$$- \frac{\sqrt{165}Q_u (x^4 - 12x^2 y^2 + 6x^2 z^2 + y^4 + 6y^2 z^2 - 2z^4)}{66} + \frac{\sqrt{55}Q_v (x-y)(x+y)(x^2 + y^2 - 6z^2)}{22}$$

$$+ \frac{\sqrt{55}Q_{xy} xy (x^2 + y^2 - 6z^2)}{22} + \frac{\sqrt{55}Q_{xz} xz (x^2 - 6y^2 + z^2)}{22} - \frac{\sqrt{55}Q_{yz} yz (6x^2 - y^2 - z^2)}{22}$$

$$\bar{Q}_4^{(2,0)}[q](A_{1g}, 2)$$

** symmetry

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

** expression

$$\frac{\sqrt{231}Q_u (8x^4 - 33x^2 y^2 - 15x^2 z^2 + 8y^4 - 15y^2 z^2 + 5z^4)}{231} + \frac{\sqrt{77}Q_v (x-y)(x+y)(x^2 + y^2 - 6z^2)}{77}$$

$$+ \frac{\sqrt{77}Q_{xy} xy (x^2 + y^2 - 6z^2)}{14} - \frac{\sqrt{77}Q_{xz} xz (16x^2 - 33y^2 - 5z^2)}{154} + \frac{\sqrt{77}Q_{yz} yz (33x^2 - 16y^2 + 5z^2)}{154}$$

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

** symmetry

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

** expression

$$\begin{aligned} & - \frac{\sqrt{15015}Q_u (x^6 - 15x^4z^2 + 15x^2z^4 + y^6 - 15y^4z^2 + 15y^2z^4 - 2z^6)}{572} \\ & + \frac{3\sqrt{5005}Q_v (x-y)(x+y)(x^4 - 9x^2y^2 - 5x^2z^2 + y^4 - 5y^2z^2 + 5z^4)}{572} + \frac{\sqrt{5005}Q_{xy}xy (7x^4 - 19x^2y^2 - 13x^2z^2 + 7y^4 - 13y^2z^2 + 13z^4)}{286} \\ & + \frac{\sqrt{5005}Q_{xz}xz (7x^4 - 13x^2y^2 - 19x^2z^2 + 13y^4 - 13y^2z^2 + 7z^4)}{286} + \frac{\sqrt{5005}Q_{yz}yz (13x^4 - 13x^2y^2 - 13x^2z^2 + 7y^4 - 19y^2z^2 + 7z^4)}{286} \end{aligned}$$

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

** symmetry

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

** expression

$$\begin{aligned} & - \frac{\sqrt{429}Q_u (x^6 + 45x^4y^2 - 60x^4z^2 + 45x^2y^4 - 540x^2y^2z^2 + 150x^2z^4 + y^6 - 60y^4z^2 + 150y^2z^4 - 20z^6)}{1144} \\ & - \frac{21\sqrt{143}Q_v (x-y)(x+y)(x^4 - 20x^2y^2 + 6x^2z^2 + y^4 + 6y^2z^2 - 6z^4)}{1144} - \frac{7\sqrt{143}Q_{xy}xy (x^4 - 4x^2y^2 + 2x^2z^2 + y^4 + 2y^2z^2 - 2z^4)}{52} \\ & + \frac{7\sqrt{143}Q_{xz}xz (x^4 + 56x^2y^2 - 22x^2z^2 - 11y^4 - 34y^2z^2 + 10z^4)}{572} - \frac{7\sqrt{143}Q_{yz}yz (11x^4 - 56x^2y^2 + 34x^2z^2 - y^4 + 22y^2z^2 - 10z^4)}{572} \end{aligned}$$

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

** symmetry

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

** expression

$$\frac{\sqrt{6}Q_vxy}{2} + \frac{\sqrt{6}Q_{xy}(x-y)(x+y)}{4}$$

$$\bar{Q}_4^{(2,0)}[q](A_{2g})$$

** symmetry

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

** expression

$$\begin{aligned} & - \frac{7\sqrt{11}Q_uxy (x-y)(x+y)}{11} + \frac{\sqrt{33}Q_vxy (x^2 + y^2 - 6z^2)}{22} \\ & + \frac{\sqrt{33}Q_{xy}(x-y)(x+y)(x^2 + y^2 - 6z^2)}{44} + \frac{7\sqrt{33}Q_{xz}yz (3x^2 - y^2)}{44} + \frac{7\sqrt{33}Q_{yz}xz (x^2 - 3y^2)}{44} \end{aligned}$$

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

** symmetry

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

** expression

$$\begin{aligned} & - \frac{9\sqrt{1001}Q_uxy (x-y)(x+y)(x^2 + y^2 - 10z^2)}{572} + \frac{\sqrt{3003}Q_vxy (25x^4 - 82x^2y^2 - 4x^2z^2 + 25y^4 - 4y^2z^2 + 4z^4)}{572} \\ & - \frac{\sqrt{3003}Q_{xy}(x-y)(x+y)(2x^4 - 29x^2y^2 + x^2z^2 + 2y^4 + y^2z^2 - z^4)}{286} \\ & + \frac{3\sqrt{3003}Q_{xz}yz (8x^4 - 13x^2y^2 - 3x^2z^2 + y^4 + y^2z^2)}{286} - \frac{3\sqrt{3003}Q_{yz}xz (x^4 - 13x^2y^2 + x^2z^2 + 8y^4 - 3y^2z^2)}{286} \end{aligned}$$

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

** symmetry

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

** expression

$$- \frac{3\sqrt{14}Q_u (x-y)(x+y)}{28} + \frac{\sqrt{42}Q_v (x^2 + y^2 - 2z^2)}{28} - \frac{\sqrt{42}Q_{xz}xz}{7} + \frac{\sqrt{42}Q_{yz}yz}{7}$$

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

** symmetry

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

** expression

$$\frac{\sqrt{77}Q_u(x-y)(x+y)(x^2+y^2-6z^2)}{77} + \frac{\sqrt{231}Q_v(2x^4-3x^2y^2-9x^2z^2+2y^4-9y^2z^2+3z^4)}{77} \\ + \frac{\sqrt{231}Q_{xy}xy(x-y)(x+y)}{22} - \frac{\sqrt{231}Q_{xz}xz(2x^2-3y^2+9z^2)}{154} - \frac{\sqrt{231}Q_{yz}yz(33x^2-2y^2-9z^2)}{154}$$

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

** symmetry

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

** expression

$$- \frac{21\sqrt{143}Q_u(x-y)(x+y)(x^4+2x^2y^2-16x^2z^2+y^4-16y^2z^2+16z^4)}{1144} \\ + \frac{\sqrt{429}Q_v(13x^6-45x^4y^2-150x^4z^2-45x^2y^4+540x^2y^2z^2+60x^2z^4+13y^6-150y^4z^2+60y^2z^4-8z^6)}{1144} \\ + \frac{21\sqrt{429}Q_{xy}xy(x-y)(x+y)(x^2+y^2-10z^2)}{572} + \frac{7\sqrt{429}Q_{xz}xz(7x^4-4x^2y^2-22x^2z^2-11y^4+26y^2z^2+4z^4)}{572} \\ + \frac{7\sqrt{429}Q_{yz}yz(11x^4+4x^2y^2-26x^2z^2-7y^4+22y^2z^2-4z^4)}{572}$$

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

** symmetry

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

** expression

$$\frac{3\sqrt{14}Q_uxy}{14} - \frac{\sqrt{42}Q_{xy}(x^2+y^2-2z^2)}{28} + \frac{\sqrt{42}Q_{xz}yz}{7} + \frac{\sqrt{42}Q_{yz}xz}{7}$$

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

** symmetry

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

** expression

$$- \frac{2\sqrt{77}Q_uxy(x^2+y^2-6z^2)}{77} - \frac{\sqrt{231}Q_vxy(x-y)(x+y)}{22} - \frac{\sqrt{231}Q_{xy}(x^4+30x^2y^2-36x^2z^2+y^4-36y^2z^2+12z^4)}{308} \\ + \frac{\sqrt{231}Q_{xz}yz(39x^2-31y^2+18z^2)}{308} - \frac{\sqrt{231}Q_{yz}xz(31x^2-39y^2-18z^2)}{308}$$

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

** symmetry

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

** expression

$$\frac{21\sqrt{143}Q_uxy(x^4+2x^2y^2-16x^2z^2+y^4-16y^2z^2+16z^4)}{572} - \frac{21\sqrt{429}Q_vxy(x-y)(x+y)(x^2+y^2-10z^2)}{572} \\ + \frac{\sqrt{429}Q_{xy}(2x^6-15x^4y^2-15x^4z^2-15x^2y^4+180x^2y^2z^2-15x^2z^4+2y^6-15y^4z^2-15y^2z^4+2z^6)}{286} \\ - \frac{7\sqrt{429}Q_{xz}yz(8x^4+7x^2y^2-23x^2z^2-y^4+y^2z^2+2z^4)}{286} + \frac{7\sqrt{429}Q_{yz}xz(x^4-7x^2y^2-x^2z^2-8y^4+23y^2z^2-2z^4)}{286}$$

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

** symmetry

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

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

** expression

$$-\frac{3\sqrt{2}Q_u yz}{4} - \frac{\sqrt{6}Q_v yz}{4} + \frac{\sqrt{6}Q_{yz}(y-z)(y+z)}{4}$$

$$-\frac{3\sqrt{2}Q_u xz}{4} + \frac{\sqrt{6}Q_v xz}{4} + \frac{\sqrt{6}Q_{xz}(x-z)(x+z)}{4}$$

$$\tilde{Q}_{4,1}^{(2,-2)}[q](E_g, 2), \tilde{Q}_{4,2}^{(2,-2)}[q](E_g, 2)$$

** symmetry

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

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

** expression

$$-\frac{3\sqrt{14}Q_u yz}{28} + \frac{3\sqrt{42}Q_v yz}{28} + \frac{\sqrt{42}Q_{xy}xz}{7} + \frac{\sqrt{42}Q_{xz}xy}{7} + \frac{\sqrt{42}Q_{yz}(2x^2 - y^2 - z^2)}{28}$$

$$-\frac{3\sqrt{14}Q_u xz}{28} - \frac{3\sqrt{42}Q_v xz}{28} + \frac{\sqrt{42}Q_{xy}yz}{7} - \frac{\sqrt{42}Q_{xz}(x^2 - 2y^2 + z^2)}{28} + \frac{\sqrt{42}Q_{yz}xy}{7}$$

$$\tilde{Q}_{4,1}^{(2,0)}[q](E_g, 1), \tilde{Q}_{4,2}^{(2,0)}[q](E_g, 1)$$

** symmetry

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

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

** expression

$$\frac{\sqrt{11}Q_u yz(18x^2 + 11y^2 - 17z^2)}{44} + \frac{\sqrt{33}Q_v yz(6x^2 - 15y^2 + 13z^2)}{44} + \frac{7\sqrt{33}Q_{xy}xz(3y^2 - z^2)}{44}$$

$$+ \frac{7\sqrt{33}Q_{xz}xy(y^2 - 3z^2)}{44} - \frac{\sqrt{33}Q_{yz}(y-z)(y+z)(6x^2 - y^2 - z^2)}{44}$$

$$\frac{\sqrt{11}Q_u xz(11x^2 + 18y^2 - 17z^2)}{44} + \frac{\sqrt{33}Q_v xz(15x^2 - 6y^2 - 13z^2)}{44} + \frac{7\sqrt{33}Q_{xy}yz(3x^2 - z^2)}{44}$$

$$+ \frac{\sqrt{33}Q_{xz}(x-z)(x+z)(x^2 - 6y^2 + z^2)}{44} + \frac{7\sqrt{33}Q_{yz}xy(x^2 - 3z^2)}{44}$$

$$\tilde{Q}_{4,1}^{(2,0)}[q](E_g, 2), \tilde{Q}_{4,2}^{(2,0)}[q](E_g, 2)$$

** symmetry

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

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

** expression

$$-\frac{\sqrt{77}Q_u yz(24x^2 - 25y^2 + 17z^2)}{308} + \frac{\sqrt{231}Q_v yz(24x^2 + 3y^2 - 11z^2)}{308} + \frac{\sqrt{231}Q_{xy}xz(18x^2 + 39y^2 - 31z^2)}{308}$$

$$+ \frac{\sqrt{231}Q_{xz}xy(18x^2 - 31y^2 + 39z^2)}{308} - \frac{\sqrt{231}Q_{yz}(12x^4 - 36x^2y^2 - 36x^2z^2 + y^4 + 30y^2z^2 + z^4)}{308}$$

$$\frac{\sqrt{77}Q_u xz(25x^2 - 24y^2 - 17z^2)}{308} - \frac{\sqrt{231}Q_v xz(3x^2 + 24y^2 - 11z^2)}{308} + \frac{\sqrt{231}Q_{xy}yz(39x^2 + 18y^2 - 31z^2)}{308}$$

$$- \frac{\sqrt{231}Q_{xz}(x^4 - 36x^2y^2 + 30x^2z^2 + 12y^4 - 36y^2z^2 + z^4)}{308} - \frac{\sqrt{231}Q_{yz}xy(31x^2 - 18y^2 - 39z^2)}{308}$$

$$\tilde{Q}_{4,1}^{(2,2)}[q](E_g, 1), \tilde{Q}_{4,2}^{(2,2)}[q](E_g, 1)$$

** symmetry

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

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

** expression

$$\begin{aligned}
& - \frac{3\sqrt{1001}Q_{u y z} (2x^4 + 13x^2y^2 - 17x^2z^2 + 11y^4 - 41y^2z^2 + 14z^4)}{572} - \frac{\sqrt{3003}Q_{v y z} (2x^4 - 47x^2y^2 + 43x^2z^2 + 17y^4 - 41y^2z^2 + 8z^4)}{572} \\
& - \frac{3\sqrt{3003}Q_{x y x z} (3x^2y^2 - x^2z^2 - 8y^4 + 13y^2z^2 - z^4)}{286} - \frac{3\sqrt{3003}Q_{x z x y} (x^2y^2 - 3x^2z^2 + y^4 - 13y^2z^2 + 8z^4)}{286} \\
& + \frac{\sqrt{3003}Q_{y z} (y - z) (y + z) (x^4 - x^2y^2 - x^2z^2 - 2y^4 + 29y^2z^2 - 2z^4)}{286} \\
& - \frac{3\sqrt{1001}Q_{u x z} (11x^4 + 13x^2y^2 - 41x^2z^2 + 2y^4 - 17y^2z^2 + 14z^4)}{572} \\
& + \frac{\sqrt{3003}Q_{v x z} (17x^4 - 47x^2y^2 - 41x^2z^2 + 2y^4 + 43y^2z^2 + 8z^4)}{572} + \frac{3\sqrt{3003}Q_{x y y z} (8x^4 - 3x^2y^2 - 13x^2z^2 + y^2z^2 + z^4)}{286} \\
& - \frac{\sqrt{3003}Q_{x z} (x - z) (x + z) (2x^4 + x^2y^2 - 29x^2z^2 - y^4 + y^2z^2 + 2z^4)}{286} - \frac{3\sqrt{3003}Q_{y z x y} (x^4 + x^2y^2 - 13x^2z^2 - 3y^2z^2 + 8z^4)}{286}
\end{aligned}$$

$$\tilde{Q}_{4,1}^{(2,2)}[q](E_g, 2), \tilde{Q}_{4,2}^{(2,2)}[q](E_g, 2)$$

** symmetry

$$\begin{aligned}
& \frac{\sqrt{5}yz (6x^2 - y^2 - z^2)}{2} \\
& - \frac{\sqrt{5}xz (x^2 - 6y^2 + z^2)}{2}
\end{aligned}$$

** expression

$$\begin{aligned}
& - \frac{21\sqrt{143}Q_{u y z} (8x^4 + 7x^2y^2 - 23x^2z^2 - y^4 + y^2z^2 + 2z^4)}{572} + \frac{21\sqrt{429}Q_{v y z} (8x^4 - 13x^2y^2 - 3x^2z^2 + y^4 + y^2z^2)}{572} \\
& - \frac{7\sqrt{429}Q_{x y x z} (2x^4 - 23x^2y^2 + x^2z^2 + 8y^4 + 7y^2z^2 - z^4)}{286} - \frac{7\sqrt{429}Q_{x z x y} (2x^4 + x^2y^2 - 23x^2z^2 - y^4 + 7y^2z^2 + 8z^4)}{286} \\
& + \frac{\sqrt{429}Q_{y z} (2x^6 - 15x^4y^2 - 15x^4z^2 - 15x^2y^4 + 180x^2y^2z^2 - 15x^2z^4 + 2y^6 - 15y^4z^2 - 15y^2z^4 + 2z^6)}{286} \\
& 21\sqrt{143}Q_{u x z} (x^4 - 7x^2y^2 - x^2z^2 - 8y^4 + 23y^2z^2 - 2z^4) - \frac{21\sqrt{429}Q_{v x z} (x^4 - 13x^2y^2 + x^2z^2 + 8y^4 - 3y^2z^2)}{572} \\
& - \frac{7\sqrt{429}Q_{x y y z} (8x^4 - 23x^2y^2 + 7x^2z^2 + 2y^4 + y^2z^2 - z^4)}{286} \\
& + \frac{\sqrt{429}Q_{x z} (2x^6 - 15x^4y^2 - 15x^4z^2 - 15x^2y^4 + 180x^2y^2z^2 - 15x^2z^4 + 2y^6 - 15y^4z^2 - 15y^2z^4 + 2z^6)}{286} \\
& + \frac{7\sqrt{429}Q_{y z x y} (x^4 - x^2y^2 - 7x^2z^2 - 2y^4 + 23y^2z^2 - 8z^4)}{286}
\end{aligned}$$