

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

\* Harmonics for rank 0

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

\*\* 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

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

\*\* symmetry

$z$

\*\* expression

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

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

\*\* symmetry

$z$

\*\* expression

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

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

\*\* symmetry

$x$

$y$

\*\* expression

$$-\frac{\sqrt{10}Q_ux}{10} + \frac{\sqrt{30}Q_vx}{10} + \frac{\sqrt{30}Q_{xy}y}{10} + \frac{\sqrt{30}Q_{xz}z}{10}$$

$$-\frac{\sqrt{10}Q_uy}{10} - \frac{\sqrt{30}Q_vy}{10} + \frac{\sqrt{30}Q_{xy}x}{10} + \frac{\sqrt{30}Q_{yz}z}{10}$$

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

\*\* symmetry

$x$

$y$

\*\* expression

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

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

\* Harmonics for rank 2

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

\*\* symmetry

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

\*\* expression

$Q_u$

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

\*\* 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

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

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

\*\* 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

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

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

\*\* 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

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

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

\*\* symmetry

$$\sqrt{3}yz$$

$$\sqrt{3}xz$$

\*\* expression

$$Q_{yz}$$

$$Q_{xz}$$

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

\*\* symmetry

$$\sqrt{3}yz$$

$$\sqrt{3}xz$$

\*\* expression

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

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

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

\*\* symmetry

$$\sqrt{3}yz$$

$$\sqrt{3}xz$$

\*\* expression

$$-\frac{5\sqrt{42}Q_uyz(3x^2 + 3y^2 - 4z^2)}{84} + \frac{5\sqrt{14}Q_vyz(9x^2 - 5y^2 + 2z^2)}{84} - \frac{5\sqrt{14}Q_{xy}xz(x^2 - 6y^2 + z^2)}{42} \\ - \frac{5\sqrt{14}Q_{xz}xy(x^2 + y^2 - 6z^2)}{42} + \frac{\sqrt{14}Q_{yz}(x^4 - 3x^2y^2 - 3x^2z^2 - 4y^4 + 27y^2z^2 - 4z^4)}{42}$$

$$-\frac{5\sqrt{42}Q_uxz(3x^2 + 3y^2 - 4z^2)}{84} + \frac{5\sqrt{14}Q_vxz(5x^2 - 9y^2 - 2z^2)}{84} + \frac{5\sqrt{14}Q_{xy}yz(6x^2 - y^2 - z^2)}{42} \\ - \frac{\sqrt{14}Q_{xz}(4x^4 + 3x^2y^2 - 27x^2z^2 - y^4 + 3y^2z^2 + 4z^4)}{42} - \frac{5\sqrt{14}Q_{yz}xy(x^2 + y^2 - 6z^2)}{42}$$

\* Harmonics for rank 3

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

\*\* symmetry

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

\*\* expression

$$\frac{\sqrt{15}Q_uz}{5} - \frac{\sqrt{5}Q_{xz}x}{5} - \frac{\sqrt{5}Q_{yz}y}{5}$$

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

\*\* symmetry

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

\*\* expression

$$-\frac{\sqrt{15}Q_uz(3x^2 + 3y^2 - 2z^2)}{15} - \frac{\sqrt{5}Q_vz(x - y)(x + y)}{2} - \sqrt{5}Q_{xy}xyz - \frac{\sqrt{5}Q_{xz}x(x^2 + y^2 - 4z^2)}{20} - \frac{\sqrt{5}Q_{yz}y(x^2 + y^2 - 4z^2)}{20}$$

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

\*\* symmetry

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

\*\* expression

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

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

\*\* symmetry

$$\sqrt{15}xyz$$

\*\* expression

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

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

\*\* symmetry

$$\sqrt{15}xyz$$

\*\* expression

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

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

\*\* symmetry

$$\sqrt{15}xyz$$

\*\* expression

$$\begin{aligned} & -\frac{21\sqrt{22}Q_{uxyz}(x^2 + y^2 - 2z^2)}{44} + \frac{21\sqrt{66}Q_{vxyz}(x-y)(x+y)}{44} - \frac{\sqrt{66}Q_{xy}z(6x^4 - 51x^2y^2 + 5x^2z^2 + 6y^4 + 5y^2z^2 - z^4)}{66} \\ & - \frac{\sqrt{66}Q_{xz}y(6x^4 + 5x^2y^2 - 51x^2z^2 - y^4 + 5y^2z^2 + 6z^4)}{66} + \frac{\sqrt{66}Q_{yz}x(x^4 - 5x^2y^2 - 5x^2z^2 - 6y^4 + 51y^2z^2 - 6z^4)}{66} \end{aligned}$$

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

\*\* symmetry

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

\*\* expression

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

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

\*\* symmetry

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

\*\* expression

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

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

\*\* symmetry

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

\*\* expression

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

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

\*\* symmetry

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

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

\*\* expression

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

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

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

\*\* symmetry

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

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

\*\* expression

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

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

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

\*\* symmetry

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

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

\*\* expression

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

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

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

\*\* symmetry

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

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

\*\* expression

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

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

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

\*\* symmetry

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

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

\*\* expression

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

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

$$\begin{aligned} & \frac{\sqrt{330}Q_{uy}(3x^4 - x^2y^2 - 15x^2z^2 - 4y^4 + 41y^2z^2 - 18z^4)}{264} - \frac{\sqrt{110}Q_vy(11x^4 - 27x^2y^2 + 15x^2z^2 + 4y^4 - 13y^2z^2 + 4z^4)}{88} \\ & + \frac{\sqrt{110}Q_{xy}x(x^4 - 12x^2y^2 + 2x^2z^2 + 8y^4 - 12y^2z^2 + z^4)}{44} - \frac{7\sqrt{110}Q_{xz}xyz(x^2 - 2y^2 + z^2)}{44} + \frac{\sqrt{110}Q_{yz}z(x^4 - 12x^2y^2 + 2x^2z^2 + 8y^4 - 12y^2z^2 + z^4)}{44} \end{aligned}$$

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

\*\* symmetry

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

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

\*\* expression

$$\begin{aligned} & -\frac{\sqrt{22}Q_{ux}(2x^4 + 11x^2y^2 - 31x^2z^2 + 9y^4 - 87y^2z^2 + 30z^4)}{88} - \frac{\sqrt{66}Q_vx(2x^4 - 73x^2y^2 + 53x^2z^2 + 51y^4 - 87y^2z^2 - 12z^4)}{264} \\ & - \frac{\sqrt{66}Q_{xy}y(12x^4 - 46x^2y^2 + 66x^2z^2 + 5y^4 - 4y^2z^2 - 9z^4)}{132} \\ & + \frac{\sqrt{66}Q_{xz}z(12x^4 + 66x^2y^2 - 46x^2z^2 - 9y^4 - 4y^2z^2 + 5z^4)}{132} + \frac{21\sqrt{66}Q_{yz}xyz(y-z)(y+z)}{44} \end{aligned}$$

$$\begin{aligned} & -\frac{\sqrt{22}Q_{uy}(9x^4 + 11x^2y^2 - 87x^2z^2 + 2y^4 - 31y^2z^2 + 30z^4)}{88} + \frac{\sqrt{66}Q_vy(51x^4 - 73x^2y^2 - 87x^2z^2 + 2y^4 + 53y^2z^2 - 12z^4)}{264} \\ & - \frac{\sqrt{66}Q_{xy}x(5x^4 - 46x^2y^2 - 4x^2z^2 + 12y^4 + 66y^2z^2 - 9z^4)}{132} + \frac{21\sqrt{66}Q_{xz}xyz(x-z)(x+z)}{44} \\ & - \frac{\sqrt{66}Q_{yz}z(9x^4 - 66x^2y^2 + 4x^2z^2 - 12y^4 + 46y^2z^2 - 5z^4)}{132} \end{aligned}$$

\* Harmonics for rank 4

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

\*\* symmetry

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

\*\* expression

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

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

\*\* symmetry

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

\*\* expression

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

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

\*\* symmetry

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

\*\* expression

$$\begin{aligned} & -\frac{\sqrt{165}Q_u(x^4 - 12x^2y^2 + 6x^2z^2 + y^4 + 6y^2z^2 - 2z^4)}{66} + \frac{\sqrt{55}Q_v(x-y)(x+y)(x^2 + y^2 - 6z^2)}{22} \\ & + \frac{\sqrt{55}Q_{xy}xy(x^2 + y^2 - 6z^2)}{22} + \frac{\sqrt{55}Q_{xz}xz(x^2 - 6y^2 + z^2)}{22} - \frac{\sqrt{55}Q_{yz}yz(6x^2 - y^2 - z^2)}{22} \end{aligned}$$

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

\*\* symmetry

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

\*\* expression

$$\begin{aligned} & \frac{\sqrt{231}Q_u(8x^4 - 33x^2y^2 - 15x^2z^2 + 8y^4 - 15y^2z^2 + 5z^4)}{231} + \frac{\sqrt{77}Q_v(x-y)(x+y)(x^2 + y^2 - 6z^2)}{77} \\ & + \frac{\sqrt{77}Q_{xy}xy(x^2 + y^2 - 6z^2)}{14} - \frac{\sqrt{77}Q_{xz}xz(16x^2 - 33y^2 - 5z^2)}{154} + \frac{\sqrt{77}Q_{yz}yz(33x^2 - 16y^2 + 5z^2)}{154} \end{aligned}$$

$\tilde{\mathbb{Q}}_4^{(2,2)}[q](A_{1g}, 1)$   
\*\* symmetry

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

\*\* expression

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

$\tilde{\mathbb{Q}}_4^{(2,2)}[q](A_{1g}, 2)$   
\*\* symmetry

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

\*\* expression

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

$\tilde{\mathbb{Q}}_4^{(2,-2)}[q](A_{2g})$   
\*\* symmetry

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

\*\* expression

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

$\tilde{\mathbb{Q}}_4^{(2,0)}[q](A_{2g})$   
\*\* symmetry

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

\*\* expression

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

$\tilde{\mathbb{Q}}_4^{(2,2)}[q](A_{2g})$   
\*\* symmetry

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

\*\* expression

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

$\tilde{\mathbb{Q}}_4^{(2,-2)}[q](B_{1g})$   
\*\* symmetry

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

\*\* expression

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

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

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

\*\* expression

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

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

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

\*\* expression

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

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

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

\*\* expression

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

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

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

\*\* expression

$$\begin{aligned} & -\frac{2\sqrt{77}Q_{uxy}(x^2+y^2-6z^2)}{77} - \frac{\sqrt{231}Q_{vxy}(x-y)(x+y)}{22} - \frac{\sqrt{231}Q_{xy}(x^4+30x^2y^2-36x^2z^2+y^4-36y^2z^2+12z^4)}{308} \\ & + \frac{\sqrt{231}Q_{xz}yz(39x^2-31y^2+18z^2)}{308} - \frac{\sqrt{231}Q_{yz}xz(31x^2-39y^2-18z^2)}{308} \end{aligned}$$

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

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

\*\* expression

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

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

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

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

\*\* expression

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

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

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

\*\* symmetry

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

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

\*\* expression

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

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

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

\*\* symmetry

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

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

\*\* expression

$$\begin{aligned} & \frac{\sqrt{11}Q_{uyz}(18x^2 + 11y^2 - 17z^2)}{44} + \frac{\sqrt{33}Q_{vyz}(6x^2 - 15y^2 + 13z^2)}{44} + \frac{7\sqrt{33}Q_{xy}xz(3y^2 - z^2)}{44} \\ & + \frac{7\sqrt{33}Q_{xz}xy(y^2 - 3z^2)}{44} - \frac{\sqrt{33}Q_{yz}(y-z)(y+z)(6x^2 - y^2 - z^2)}{44} \end{aligned}$$

$$\begin{aligned} & \frac{\sqrt{11}Q_{uxz}(11x^2 + 18y^2 - 17z^2)}{44} + \frac{\sqrt{33}Q_{vzx}(15x^2 - 6y^2 - 13z^2)}{44} + \frac{7\sqrt{33}Q_{xy}yz(3x^2 - z^2)}{44} \\ & + \frac{\sqrt{33}Q_{xz}(x-z)(x+z)(x^2 - 6y^2 + z^2)}{44} + \frac{7\sqrt{33}Q_{yz}xy(x^2 - 3z^2)}{44} \end{aligned}$$

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

\*\* symmetry

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

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

\*\* expression

$$\begin{aligned} & -\frac{\sqrt{77}Q_{uyz}(24x^2 - 25y^2 + 17z^2)}{308} + \frac{\sqrt{231}Q_{vyz}(24x^2 + 3y^2 - 11z^2)}{308} + \frac{\sqrt{231}Q_{xy}xz(18x^2 + 39y^2 - 31z^2)}{308} \\ & + \frac{\sqrt{231}Q_{xz}xy(18x^2 - 31y^2 + 39z^2)}{308} - \frac{\sqrt{231}Q_{yz}(12x^4 - 36x^2y^2 - 36x^2z^2 + y^4 + 30y^2z^2 + z^4)}{308} \end{aligned}$$

$$\begin{aligned} & -\frac{\sqrt{77}Q_{uxz}(25x^2 - 24y^2 - 17z^2)}{308} - \frac{\sqrt{231}Q_{vzx}(3x^2 + 24y^2 - 11z^2)}{308} + \frac{\sqrt{231}Q_{xy}yz(39x^2 + 18y^2 - 31z^2)}{308} \\ & - \frac{\sqrt{231}Q_{xz}(x^4 - 36x^2y^2 + 30x^2z^2 + 12y^4 - 36y^2z^2 + z^4)}{308} - \frac{\sqrt{231}Q_{yz}xy(31x^2 - 18y^2 - 39z^2)}{308} \end{aligned}$$

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

\*\* symmetry

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

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

\*\* expression

$$\begin{aligned}
& - \frac{3\sqrt{1001}Q_{uyz}(2x^4 + 13x^2y^2 - 17x^2z^2 + 11y^4 - 41y^2z^2 + 14z^4)}{572} - \frac{\sqrt{3003}Q_{vyz}(2x^4 - 47x^2y^2 + 43x^2z^2 + 17y^4 - 41y^2z^2 + 8z^4)}{572} \\
& - \frac{3\sqrt{3003}Q_{xyxz}(3x^2y^2 - x^2z^2 - 8y^4 + 13y^2z^2 - z^4)}{286} - \frac{3\sqrt{3003}Q_{xzxy}(x^2y^2 - 3x^2z^2 + y^4 - 13y^2z^2 + 8z^4)}{286} \\
& + \frac{\sqrt{3003}Q_{yz}(y-z)(y+z)(x^4 - x^2y^2 - x^2z^2 - 2y^4 + 29y^2z^2 - 2z^4)}{286} \\
& - \frac{3\sqrt{1001}Q_{uxz}(11x^4 + 13x^2y^2 - 41x^2z^2 + 2y^4 - 17y^2z^2 + 14z^4)}{572} \\
& + \frac{\sqrt{3003}Q_{vxz}(17x^4 - 47x^2y^2 - 41x^2z^2 + 2y^4 + 43y^2z^2 + 8z^4)}{572} + \frac{3\sqrt{3003}Q_{xyyz}(8x^4 - 3x^2y^2 - 13x^2z^2 + y^2z^2 + z^4)}{286} \\
& - \frac{\sqrt{3003}Q_{xz}(x-z)(x+z)(2x^4 + x^2y^2 - 29x^2z^2 - y^4 + y^2z^2 + 2z^4)}{286} - \frac{3\sqrt{3003}Q_{yzxy}(x^4 + x^2y^2 - 13x^2z^2 - 3y^2z^2 + 8z^4)}{286}
\end{aligned}$$

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

\*\* 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

$$\begin{aligned}
& - \frac{21\sqrt{143}Q_{uyz}(8x^4 + 7x^2y^2 - 23x^2z^2 - y^4 + y^2z^2 + 2z^4)}{572} + \frac{21\sqrt{429}Q_{vyz}(8x^4 - 13x^2y^2 - 3x^2z^2 + y^4 + y^2z^2)}{572} \\
& - \frac{7\sqrt{429}Q_{xyxz}(2x^4 - 23x^2y^2 + x^2z^2 + 8y^4 + 7y^2z^2 - z^4)}{286} - \frac{7\sqrt{429}Q_{xzxy}(2x^4 + x^2y^2 - 23x^2z^2 - y^4 + 7y^2z^2 + 8z^4)}{286} \\
& + \frac{\sqrt{429}Q_{yz}(2x^6 - 15x^4y^2 - 15x^4z^2 - 15x^2y^4 + 180x^2y^2z^2 - 15x^2z^4 + 2y^6 - 15y^4z^2 - 15y^2z^4 + 2z^6)}{286} \\
& - \frac{21\sqrt{143}Q_{uxz}(x^4 - 7x^2y^2 - x^2z^2 - 8y^4 + 23y^2z^2 - 2z^4)}{572} - \frac{21\sqrt{429}Q_{vxz}(x^4 - 13x^2y^2 + x^2z^2 + 8y^4 - 3y^2z^2)}{572} \\
& - \frac{7\sqrt{429}Q_{xyyz}(8x^4 - 23x^2y^2 + 7x^2z^2 + 2y^4 + y^2z^2 - z^4)}{286} \\
& + \frac{\sqrt{429}Q_{xz}(2x^6 - 15x^4y^2 - 15x^4z^2 - 15x^2y^4 + 180x^2y^2z^2 - 15x^2z^4 + 2y^6 - 15y^4z^2 - 15y^2z^4 + 2z^6)}{286} \\
& + \frac{7\sqrt{429}Q_{yzxy}(x^4 - x^2y^2 - 7x^2z^2 - 2y^4 + 23y^2z^2 - 8z^4)}{286}
\end{aligned}$$