

PG No. 27  $D_{6h}$  6/mmm [ hexagonal ] (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

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

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

\*\* symmetry

$x$

$y$

\*\* expression

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

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

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

\*\* 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

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

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

\*\* symmetry

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

\*\* expression

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

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

\*\* symmetry

$$\sqrt{3}yz$$

$$-\sqrt{3}xz$$

\*\* expression

$$Q_{yz}$$

$$-Q_{xz}$$

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

\*\* symmetry

$$\sqrt{3}yz$$

$$-\sqrt{3}xz$$

\*\* expression

$$\begin{aligned} & \frac{\sqrt{42}Q_{uyz}}{14} - \frac{3\sqrt{14}Q_{vyz}}{14} + \frac{3\sqrt{14}Q_{xyxz}}{14} + \frac{3\sqrt{14}Q_{xzxy}}{14} - \frac{\sqrt{14}Q_{yz}(2x^2 - y^2 - z^2)}{14} \\ & - \frac{\sqrt{42}Q_{uxz}}{14} - \frac{3\sqrt{14}Q_{vxz}}{14} - \frac{3\sqrt{14}Q_{xyyz}}{14} - \frac{\sqrt{14}Q_{xz}(x^2 - 2y^2 + z^2)}{14} - \frac{3\sqrt{14}Q_{yzxy}}{14} \end{aligned}$$

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

\*\* symmetry

$$\sqrt{3}yz$$

$$-\sqrt{3}xz$$

\*\* expression

$$\begin{aligned} & -\frac{5\sqrt{42}Q_{uyz}(3x^2 + 3y^2 - 4z^2)}{84} + \frac{5\sqrt{14}Q_{vyz}(9x^2 - 5y^2 + 2z^2)}{84} - \frac{5\sqrt{14}Q_{xyxz}(x^2 - 6y^2 + z^2)}{42} \\ & - \frac{5\sqrt{14}Q_{xzxy}(x^2 + y^2 - 6z^2)}{42} + \frac{\sqrt{14}Q_{yz}(x^4 - 3x^2y^2 - 3x^2z^2 - 4y^4 + 27y^2z^2 - 4z^4)}{42} \\ & \frac{5\sqrt{42}Q_{uxz}(3x^2 + 3y^2 - 4z^2)}{84} - \frac{5\sqrt{14}Q_{vxz}(5x^2 - 9y^2 - 2z^2)}{84} - \frac{5\sqrt{14}Q_{xyyz}(6x^2 - y^2 - z^2)}{42} \\ & + \frac{\sqrt{14}Q_{xz}(4x^4 + 3x^2y^2 - 27x^2z^2 - y^4 + 3y^2z^2 + 4z^4)}{42} + \frac{5\sqrt{14}Q_{yzxy}(x^2 + y^2 - 6z^2)}{42} \end{aligned}$$

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

\*\* symmetry

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

$$-\sqrt{3}xy$$

\*\* expression

$$Q_v$$

$$-Q_{xy}$$

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

\*\* symmetry

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

$$-\sqrt{3}xy$$

\*\* expression

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

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

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

\*\* symmetry

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

$$-\sqrt{3}xy$$

\*\* expression

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

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

\* Harmonics for rank 3

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

\*\* symmetry

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

\*\* expression

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

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

\*\* symmetry

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

\*\* expression

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

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

\*\* symmetry

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

\*\* expression

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

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

\*\* symmetry

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

\*\* expression

$$\frac{\sqrt{2}Q_vy}{2} + \frac{\sqrt{2}Q_{xy}x}{2}$$

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

\*\* symmetry

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

\*\* expression

$$-\frac{5\sqrt{6}Q_uy(3x^2 - y^2)}{24} + \frac{\sqrt{2}Q_vy(x^2 + y^2 - 4z^2)}{8} + \frac{\sqrt{2}Q_{xy}x(x^2 + y^2 - 4z^2)}{8} + \frac{5\sqrt{2}Q_{xz}xyz}{4} + \frac{5\sqrt{2}Q_{yz}z(x - y)(x + y)}{8}$$

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

\*\* symmetry

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

\*\* expression

$$-\frac{7\sqrt{33}Q_uy(3x^2 - y^2)(x^2 + y^2 - 8z^2)}{264} + \frac{\sqrt{11}Q_vy(53x^4 - 104x^2y^2 - 6x^2z^2 + 11y^4 - 6y^2z^2 + 4z^4)}{88} \\ - \frac{\sqrt{11}Q_{xy}x(5x^4 - 53x^2y^2 + 3x^2z^2 + 26y^4 + 3y^2z^2 - 2z^4)}{44} + \frac{7\sqrt{11}Q_{xz}xyz(7x^2 - 5y^2 - 2z^2)}{44} - \frac{7\sqrt{11}Q_{yz}z(x^4 - 9x^2y^2 + x^2z^2 + 2y^4 - y^2z^2)}{44}$$

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

\*\* symmetry

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

\*\* expression

$$\frac{\sqrt{2}Q_vx}{2} - \frac{\sqrt{2}Q_{xy}y}{2}$$

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

\*\* symmetry

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

\*\* expression

$$-\frac{5\sqrt{6}Q_ux(x^2 - 3y^2)}{24} + \frac{\sqrt{2}Q_vx(x^2 + y^2 - 4z^2)}{8} - \frac{\sqrt{2}Q_{xy}y(x^2 + y^2 - 4z^2)}{8} + \frac{5\sqrt{2}Q_{xz}z(x - y)(x + y)}{8} - \frac{5\sqrt{2}Q_{yz}xyz}{4}$$

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

\*\* symmetry

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

\*\* expression

$$-\frac{7\sqrt{33}Q_ux(x^2 - 3y^2)(x^2 + y^2 - 8z^2)}{264} + \frac{\sqrt{11}Q_vx(11x^4 - 104x^2y^2 - 6x^2z^2 + 53y^4 - 6y^2z^2 + 4z^4)}{88} \\ + \frac{\sqrt{11}Q_{xy}y(26x^4 - 53x^2y^2 + 3x^2z^2 + 5y^4 + 3y^2z^2 - 2z^4)}{44} + \frac{7\sqrt{11}Q_{xz}z(2x^4 - 9x^2y^2 - x^2z^2 + y^4 + y^2z^2)}{44} + \frac{7\sqrt{11}Q_{yz}xyz(5x^2 - 7y^2 + 2z^2)}{44}$$

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

\*\* symmetry

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

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

\*\* expression

$$\frac{\sqrt{10}Q_{ux}}{5} - \frac{\sqrt{30}Q_{vx}}{30} - \frac{\sqrt{30}Q_{xy}y}{30} + \frac{2\sqrt{30}Q_{xz}z}{15}$$

$$\frac{\sqrt{10}Q_{uy}}{5} + \frac{\sqrt{30}Q_{vy}}{30} - \frac{\sqrt{30}Q_{xy}x}{30} + \frac{2\sqrt{30}Q_{yz}z}{15}$$

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

\*\* symmetry

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

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

\*\* expression

$$-\frac{3\sqrt{10}Q_{ux}(x^2 + y^2 - 4z^2)}{40} - \frac{\sqrt{30}Q_{vx}(11x^2 - 9y^2 - 24z^2)}{120} - \frac{\sqrt{30}Q_{xy}y(21x^2 + y^2 - 24z^2)}{120} + \frac{\sqrt{30}Q_{xz}z(9x^2 - 21y^2 + 4z^2)}{120} + \frac{\sqrt{30}Q_{yz}xyz}{4}$$

$$-\frac{3\sqrt{10}Q_{uy}(x^2 + y^2 - 4z^2)}{40} - \frac{\sqrt{30}Q_{vy}(9x^2 - 11y^2 + 24z^2)}{120} - \frac{\sqrt{30}Q_{xy}x(x^2 + 21y^2 - 24z^2)}{120} + \frac{\sqrt{30}Q_{xz}xyz}{4} - \frac{\sqrt{30}Q_{yz}z(21x^2 - 9y^2 - 4z^2)}{120}$$

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

\*\* symmetry

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

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

\*\* expression

$$\begin{aligned} & \frac{3\sqrt{55}Q_{ux}(x^4 + 2x^2y^2 - 12x^2z^2 + y^4 - 12y^2z^2 + 8z^4)}{88} - \frac{\sqrt{165}Q_{vx}(5x^4 - 4x^2y^2 - 46x^2z^2 - 9y^4 + 66y^2z^2 + 12z^4)}{264} \\ & - \frac{\sqrt{165}Q_{xy}y(6x^4 + 5x^2y^2 - 51x^2z^2 - y^4 + 5y^2z^2 + 6z^4)}{132} \\ & - \frac{\sqrt{165}Q_{xz}z(18x^4 + 15x^2y^2 - 41x^2z^2 - 3y^4 + y^2z^2 + 4z^4)}{132} - \frac{7\sqrt{165}Q_{yz}xyz(x^2 + y^2 - 2z^2)}{44} \end{aligned}$$

$$\begin{aligned} & \frac{3\sqrt{55}Q_{uy}(x^4 + 2x^2y^2 - 12x^2z^2 + y^4 - 12y^2z^2 + 8z^4)}{88} - \frac{\sqrt{165}Q_{vy}(9x^4 + 4x^2y^2 - 66x^2z^2 - 5y^4 + 46y^2z^2 - 12z^4)}{264} \\ & + \frac{\sqrt{165}Q_{xy}x(x^4 - 5x^2y^2 - 5x^2z^2 - 6y^4 + 51y^2z^2 - 6z^4)}{132} - \frac{7\sqrt{165}Q_{xz}xyz(x^2 + y^2 - 2z^2)}{44} \\ & + \frac{\sqrt{165}Q_{yz}z(3x^4 - 15x^2y^2 - x^2z^2 - 18y^4 + 41y^2z^2 - 4z^4)}{132} \end{aligned}$$

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

\*\* symmetry

$$\sqrt{15}xyz$$

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

\*\* expression

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

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

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

\*\* symmetry

$$\sqrt{15}xyz$$

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

\*\* expression

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

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

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

\*\* symmetry

$$\sqrt{15}xyz$$

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

\*\* expression

$$\begin{aligned} & -\frac{21\sqrt{22}Q_uxyz(x^2 + y^2 - 2z^2)}{44} + \frac{21\sqrt{66}Q_vxyz(x-y)(x+y)}{44} - \frac{\sqrt{66}Q_{xyz}(6x^4 - 51x^2y^2 + 5x^2z^2 + 6y^4 + 5y^2z^2 - z^4)}{66} \\ & - \frac{\sqrt{66}Q_{xz}y(6x^4 + 5x^2y^2 - 51x^2z^2 - y^4 + 5y^2z^2 + 6z^4)}{66} + \frac{\sqrt{66}Q_{yz}x(x^4 - 5x^2y^2 - 5x^2z^2 - 6y^4 + 51y^2z^2 - 6z^4)}{66} \\ & - \frac{21\sqrt{22}Q_uz(x-y)(x+y)(x^2 + y^2 - 2z^2)}{88} + \frac{\sqrt{66}Q_vz(39x^4 - 174x^2y^2 - 20x^2z^2 + 39y^4 - 20y^2z^2 + 4z^4)}{264} + \frac{21\sqrt{66}Q_{xy}xyz(x-y)(x+y)}{44} \\ & - \frac{\sqrt{66}Q_{xz}x(5x^4 - 4x^2y^2 - 46x^2z^2 - 9y^4 + 66y^2z^2 + 12z^4)}{132} - \frac{\sqrt{66}Q_{yz}y(9x^4 + 4x^2y^2 - 66x^2z^2 - 5y^4 + 46y^2z^2 - 12z^4)}{132} \end{aligned}$$

\* Harmonics for rank 4

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

\*\* symmetry

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

\*\* expression

$$-\frac{3\sqrt{70}Q_u(x^2 + y^2 - 2z^2)}{70} + \frac{\sqrt{210}Q_v(x-y)(x+y)}{140} + \frac{\sqrt{210}Q_{xy}xy}{70} - \frac{2\sqrt{210}Q_{xz}xz}{35} - \frac{2\sqrt{210}Q_{yz}yz}{35}$$

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

\*\* symmetry

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

\*\* expression

$$\begin{aligned} & \frac{\sqrt{385}Q_u(3x^4 + 6x^2y^2 - 24x^2z^2 + 3y^4 - 24y^2z^2 + 8z^4)}{308} + \frac{3\sqrt{1155}Q_v(x-y)(x+y)(x^2 + y^2 - 6z^2)}{308} \\ & + \frac{3\sqrt{1155}Q_{xy}xy(x^2 + y^2 - 6z^2)}{154} - \frac{\sqrt{1155}Q_{xz}xz(3x^2 + 3y^2 - 4z^2)}{308} - \frac{\sqrt{1155}Q_{yz}yz(3x^2 + 3y^2 - 4z^2)}{308} \end{aligned}$$

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

\*\* symmetry

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

\*\* expression

$$\begin{aligned} & -\frac{3\sqrt{715}Q_u(5x^6 + 15x^4y^2 - 90x^4z^2 + 15x^2y^4 - 180x^2y^2z^2 + 120x^2z^4 + 5y^6 - 90y^4z^2 + 120y^2z^4 - 16z^6)}{2288} \\ & + \frac{7\sqrt{2145}Q_v(x-y)(x+y)(x^4 + 2x^2y^2 - 16x^2z^2 + y^4 - 16y^2z^2 + 16z^4)}{2288} + \frac{7\sqrt{2145}Q_{xy}xy(x^4 + 2x^2y^2 - 16x^2z^2 + y^4 - 16y^2z^2 + 16z^4)}{1144} \\ & + \frac{7\sqrt{2145}Q_{xz}xz(5x^4 + 10x^2y^2 - 20x^2z^2 + 5y^4 - 20y^2z^2 + 8z^4)}{1144} + \frac{7\sqrt{2145}Q_{yz}yz(5x^4 + 10x^2y^2 - 20x^2z^2 + 5y^4 - 20y^2z^2 + 8z^4)}{1144} \end{aligned}$$

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

\*\* symmetry

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

\*\* expression

$$\frac{\sqrt{3}Q_vxz}{2} - \frac{\sqrt{3}Q_{xy}yz}{2} + \frac{\sqrt{3}Q_{xz}(x-y)(x+y)}{4} - \frac{\sqrt{3}Q_{yz}xy}{2}$$

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

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

\*\* expression

$$-\frac{7\sqrt{22}Q_uxz(x^2 - 3y^2)}{88} + \frac{3\sqrt{66}Q_vxz(3x^2 + 3y^2 - 4z^2)}{88} - \frac{3\sqrt{66}Q_{xy}yz(3x^2 + 3y^2 - 4z^2)}{88} \\ + \frac{\sqrt{66}Q_{xz}(x^4 - 21x^2y^2 + 15x^2z^2 + 6y^4 - 15y^2z^2)}{88} + \frac{\sqrt{66}Q_{yz}xy(19x^2 - 9y^2 - 30z^2)}{88}$$

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

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

\*\* expression

$$-\frac{9\sqrt{2002}Q_uxz(x^2 - 3y^2)(3x^2 + 3y^2 - 8z^2)}{1144} + \frac{\sqrt{6006}Q_vxz(19x^4 - 160x^2y^2 - 10x^2z^2 + 85y^4 - 10y^2z^2 + 4z^4)}{1144} \\ + \frac{\sqrt{6006}Q_{xy}yz(40x^4 - 85x^2y^2 + 5x^2z^2 + 7y^4 + 5y^2z^2 - 2z^4)}{572} \\ - \frac{\sqrt{6006}Q_{xz}(2x^6 - 7x^4y^2 - 23x^4z^2 - 8x^2y^4 + 90x^2y^2z^2 + 8x^2z^4 + y^6 - 7y^4z^2 - 8y^2z^4)}{572} \\ - \frac{\sqrt{6006}Q_{yz}xy(5x^4 - 2x^2y^2 - 44x^2z^2 - 7y^4 + 76y^2z^2 - 16z^4)}{572}$$

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

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

\*\* expression

$$\frac{\sqrt{3}Q_vyz}{2} + \frac{\sqrt{3}Q_{xy}xz}{2} + \frac{\sqrt{3}Q_{xz}xy}{2} + \frac{\sqrt{3}Q_{yz}(x - y)(x + y)}{4}$$

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

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

\*\* expression

$$-\frac{7\sqrt{22}Q_uyz(3x^2 - y^2)}{88} + \frac{3\sqrt{66}Q_vyz(3x^2 + 3y^2 - 4z^2)}{88} + \frac{3\sqrt{66}Q_{xy}xz(3x^2 + 3y^2 - 4z^2)}{88} \\ + \frac{\sqrt{66}Q_{xz}xy(9x^2 - 19y^2 + 30z^2)}{88} - \frac{\sqrt{66}Q_{yz}(6x^4 - 21x^2y^2 - 15x^2z^2 + y^4 + 15y^2z^2)}{88}$$

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

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

\*\* expression

$$-\frac{9\sqrt{2002}Q_uyz(3x^2 - y^2)(3x^2 + 3y^2 - 8z^2)}{1144} + \frac{\sqrt{6006}Q_vyz(85x^4 - 160x^2y^2 - 10x^2z^2 + 19y^4 - 10y^2z^2 + 4z^4)}{1144} \\ - \frac{\sqrt{6006}Q_{xy}xz(7x^4 - 85x^2y^2 + 5x^2z^2 + 40y^4 + 5y^2z^2 - 2z^4)}{572} - \frac{\sqrt{6006}Q_{xz}xy(7x^4 + 2x^2y^2 - 76x^2z^2 - 5y^4 + 44y^2z^2 + 16z^4)}{572} \\ + \frac{\sqrt{6006}Q_{yz}(x^6 - 8x^4y^2 - 7x^4z^2 - 7x^2y^4 + 90x^2y^2z^2 - 8x^2z^4 + 2y^6 - 23y^4z^2 + 8y^2z^4)}{572}$$

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

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

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

\*\* expression

$$\frac{3\sqrt{7}Q_{uyz}}{7} + \frac{\sqrt{21}Q_{vyz}}{14} - \frac{\sqrt{21}Q_{xyxz}}{14} - \frac{\sqrt{21}Q_{xzy}}{14} - \frac{\sqrt{21}Q_{yz}(x^2 + 3y^2 - 4z^2)}{28}$$

$$- \frac{3\sqrt{7}Q_{uxz}}{7} + \frac{\sqrt{21}Q_{vxy}}{14} + \frac{\sqrt{21}Q_{xyyz}}{14} + \frac{\sqrt{21}Q_{xz}(3x^2 + y^2 - 4z^2)}{28} + \frac{\sqrt{21}Q_{yzxy}}{14}$$

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

\*\* symmetry

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

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

\*\* expression

$$- \frac{17\sqrt{154}Q_{uyz}(3x^2 + 3y^2 - 4z^2)}{616} - \frac{\sqrt{462}Q_{vyz}(33x^2 - 51y^2 + 40z^2)}{616} - \frac{\sqrt{462}Q_{xyxz}(9x^2 + 93y^2 - 40z^2)}{616}$$

$$- \frac{9\sqrt{462}Q_{xzxy}(x^2 + y^2 - 6z^2)}{616} + \frac{\sqrt{462}Q_{yz}(6x^4 + 3x^2y^2 - 39x^2z^2 - 3y^4 + 15y^2z^2 + 4z^4)}{616}$$

$$\frac{17\sqrt{154}Q_{uxz}(3x^2 + 3y^2 - 4z^2)}{616} + \frac{\sqrt{462}Q_{vxx}(51x^2 - 33y^2 - 40z^2)}{616} + \frac{\sqrt{462}Q_{xyyz}(93x^2 + 9y^2 - 40z^2)}{616}$$

$$+ \frac{\sqrt{462}Q_{xz}(3x^4 - 3x^2y^2 - 15x^2z^2 - 6y^4 + 39y^2z^2 - 4z^4)}{616} + \frac{9\sqrt{462}Q_{yzxy}(x^2 + y^2 - 6z^2)}{616}$$

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

\*\* symmetry

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

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

\*\* expression

$$21\sqrt{286}Q_{uyz}(5x^4 + 10x^2y^2 - 20x^2z^2 + 5y^4 - 20y^2z^2 + 8z^4) - \frac{7\sqrt{858}Q_{vyz}(11x^4 + 4x^2y^2 - 26x^2z^2 - 7y^4 + 22y^2z^2 - 4z^4)}{1144}$$

$$+ \frac{7\sqrt{858}Q_{xyxz}(x^4 - 7x^2y^2 - x^2z^2 - 8y^4 + 23y^2z^2 - 2z^4)}{572} + \frac{7\sqrt{858}Q_{xzxy}(x^4 + 2x^2y^2 - 16x^2z^2 + y^4 - 16y^2z^2 + 16z^4)}{572}$$

$$- \frac{\sqrt{858}Q_{yz}(x^6 - 4x^4y^2 - 11x^4z^2 - 11x^2y^4 + 90x^2y^2z^2 - 4x^2z^4 - 6y^6 + 101y^4z^2 - 116y^2z^4 + 8z^6)}{572}$$

$$- \frac{21\sqrt{286}Q_{uxz}(5x^4 + 10x^2y^2 - 20x^2z^2 + 5y^4 - 20y^2z^2 + 8z^4)}{1144}$$

$$+ \frac{7\sqrt{858}Q_{vxx}(7x^4 - 4x^2y^2 - 22x^2z^2 - 11y^4 + 26y^2z^2 + 4z^4)}{1144} + \frac{7\sqrt{858}Q_{xyyz}(8x^4 + 7x^2y^2 - 23x^2z^2 - y^4 + y^2z^2 + 2z^4)}{572}$$

$$- \frac{\sqrt{858}Q_{xz}(6x^6 + 11x^4y^2 - 101x^4z^2 + 4x^2y^4 - 90x^2y^2z^2 + 116x^2z^4 - y^6 + 11y^4z^2 + 4y^2z^4 - 8z^6)}{572}$$

$$- \frac{7\sqrt{858}Q_{yzxy}(x^4 + 2x^2y^2 - 16x^2z^2 + y^4 - 16y^2z^2 + 16z^4)}{572}$$

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

\*\* symmetry

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

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

\*\* expression

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

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

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

\*\* symmetry

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

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

\*\* expression

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

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

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

\*\* symmetry

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

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

\*\* expression

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

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

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

\*\* symmetry

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

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

\*\* expression

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

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

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

\*\* symmetry

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

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

\*\* expression

$$\begin{aligned} & -\frac{9\sqrt{1001}Q_u(x^2+y^2-10z^2)(x^2-2xy-y^2)(x^2+2xy-y^2)}{2288} + \frac{\sqrt{3003}Q_v(x-y)(x+y)(17x^4-230x^2y^2-8x^2z^2+17y^4-8y^2z^2+8z^4)}{2288} \\ & + \frac{\sqrt{3003}Q_{xy}xy(49x^4-166x^2y^2+8x^2z^2+49y^4+8y^2z^2-8z^4)}{1144} \\ & + \frac{3\sqrt{3003}Q_{xz}xz(7x^4-58x^2y^2-4x^2z^2+23y^4+12y^2z^2)}{1144} + \frac{3\sqrt{3003}Q_{yz}yz(23x^4-58x^2y^2+12x^2z^2+7y^4-4y^2z^2)}{1144} \end{aligned}$$

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

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

\*\* symmetry

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

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

\*\* expression

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

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