

PG No. 32 O_h $m\bar{3}m$ [cubic]

Table 1 Harmonics for rank 0.

| No. | multipole | expression |
|-----|------------------------|------------|
| 1 | $\mathbb{G}_0(A_{1u})$ | 1 |

Table 2 Harmonics for rank 1.

| No. | multipole | expression |
|-----|----------------------------|------------|
| 2 | $\mathbb{G}_{1,1}(T_{1g})$ | x |
| 3 | $\mathbb{G}_{1,2}(T_{1g})$ | y |
| 4 | $\mathbb{G}_{1,3}(T_{1g})$ | z |

Table 3 Harmonics for rank 2.

| No. | multipole | expression |
|-----|----------------------------|--|
| 5 | $\mathbb{G}_{2,1}(E_u)$ | $-\frac{x^2}{2} - \frac{y^2}{2} + z^2$ |
| 6 | $\mathbb{G}_{2,2}(E_u)$ | $\frac{\sqrt{3}(x-y)(x+y)}{2}$ |
| 7 | $\mathbb{G}_{2,1}(T_{2u})$ | $\sqrt{3}yz$ |
| 8 | $\mathbb{G}_{2,2}(T_{2u})$ | $\sqrt{3}xz$ |
| 9 | $\mathbb{G}_{2,3}(T_{2u})$ | $\sqrt{3}xy$ |

Table 4 Harmonics for rank 3.

| No. | multipole | expression |
|-----|----------------------------|-----------------------------------|
| 10 | $\mathbb{G}_3(A_{2g})$ | $\sqrt{15}xyz$ |
| 11 | $\mathbb{G}_{3,1}(T_{1g})$ | $\frac{x(2x^2-3y^2-3z^2)}{2}$ |
| 12 | $\mathbb{G}_{3,2}(T_{1g})$ | $-\frac{y(3x^2-2y^2+3z^2)}{2}$ |
| 13 | $\mathbb{G}_{3,3}(T_{1g})$ | $-\frac{z(3x^2+3y^2-2z^2)}{2}$ |
| 14 | $\mathbb{G}_{3,1}(T_{2g})$ | $\frac{\sqrt{15}x(y-z)(y+z)}{2}$ |
| 15 | $\mathbb{G}_{3,2}(T_{2g})$ | $-\frac{\sqrt{15}y(x-z)(x+z)}{2}$ |
| 16 | $\mathbb{G}_{3,3}(T_{2g})$ | $\frac{\sqrt{15}z(x-y)(x+y)}{2}$ |

Table 5 Harmonics for rank 4.

| No. | multipole | expression |
|-----|----------------------------|--|
| 17 | $\mathbb{G}_4(A_{1u})$ | $\frac{\sqrt{21}(x^4 - 3x^2y^2 - 3x^2z^2 + y^4 - 3y^2z^2 + z^4)}{6}$ |
| 18 | $\mathbb{G}_{4,1}(E_u)$ | $-\frac{\sqrt{15}(x^4 - 12x^2y^2 + 6x^2z^2 + y^4 + 6y^2z^2 - 2z^4)}{12}$ |
| 19 | $\mathbb{G}_{4,2}(E_u)$ | $\frac{\sqrt{5}(x-y)(x+y)(x^2 + y^2 - 6z^2)}{4}$ |
| 20 | $\mathbb{G}_{4,1}(T_{1u})$ | $\frac{\sqrt{35}yz(y-z)(y+z)}{2}$ |
| 21 | $\mathbb{G}_{4,2}(T_{1u})$ | $-\frac{\sqrt{35}xz(x-z)(x+z)}{2}$ |
| 22 | $\mathbb{G}_{4,3}(T_{1u})$ | $\frac{\sqrt{35}xy(x-y)(x+y)}{2}$ |
| 23 | $\mathbb{G}_{4,1}(T_{2u})$ | $\frac{\sqrt{5}yz(6x^2 - y^2 - z^2)}{2}$ |
| 24 | $\mathbb{G}_{4,2}(T_{2u})$ | $-\frac{\sqrt{5}xz(x^2 - 6y^2 + z^2)}{2}$ |
| 25 | $\mathbb{G}_{4,3}(T_{2u})$ | $-\frac{\sqrt{5}xy(x^2 + y^2 - 6z^2)}{2}$ |

Table 6 Harmonics for rank 5.

| No. | multipole | expression |
|-----|-------------------------------|--|
| 26 | $\mathbb{G}_{5,1}(E_g)$ | $\frac{3\sqrt{35}xyz(x-y)(x+y)}{2}$ |
| 27 | $\mathbb{G}_{5,2}(E_g)$ | $\frac{\sqrt{105}xyz(x^2 + y^2 - 2z^2)}{2}$ |
| 28 | $\mathbb{G}_{5,1}(T_{1g}, 1)$ | $\frac{x(8x^4 - 40x^2y^2 - 40x^2z^2 + 15y^4 + 30y^2z^2 + 15z^4)}{8}$ |
| 29 | $\mathbb{G}_{5,2}(T_{1g}, 1)$ | $\frac{y(15x^4 - 40x^2y^2 + 30x^2z^2 + 8y^4 - 40y^2z^2 + 15z^4)}{8}$ |
| 30 | $\mathbb{G}_{5,3}(T_{1g}, 1)$ | $\frac{z(15x^4 + 30x^2y^2 - 40x^2z^2 + 15y^4 - 40y^2z^2 + 8z^4)}{8}$ |
| 31 | $\mathbb{G}_{5,1}(T_{1g}, 2)$ | $\frac{3\sqrt{35}x(y^2 - 2yz - z^2)(y^2 + 2yz - z^2)}{8}$ |
| 32 | $\mathbb{G}_{5,2}(T_{1g}, 2)$ | $\frac{3\sqrt{35}y(x^2 - 2xz - z^2)(x^2 + 2xz - z^2)}{8}$ |
| 33 | $\mathbb{G}_{5,3}(T_{1g}, 2)$ | $\frac{3\sqrt{35}z(x^2 - 2xy - y^2)(x^2 + 2xy - y^2)}{8}$ |
| 34 | $\mathbb{G}_{5,1}(T_{2g})$ | $\frac{\sqrt{105}x(y-z)(y+z)(2x^2 - y^2 - z^2)}{4}$ |
| 35 | $\mathbb{G}_{5,2}(T_{2g})$ | $\frac{\sqrt{105}y(x-z)(x+z)(x^2 - 2y^2 + z^2)}{4}$ |
| 36 | $\mathbb{G}_{5,3}(T_{2g})$ | $-\frac{\sqrt{105}z(x-y)(x+y)(x^2 + y^2 - 2z^2)}{4}$ |

Table 7 Harmonics for rank 6.

| No. | multipole | expression |
|-----|-------------------------------|---|
| 37 | $\mathbb{G}_6(A_{1u})$ | $\frac{\sqrt{2}(2x^6 - 15x^4y^2 - 15x^4z^2 - 15x^2y^4 + 180x^2y^2z^2 - 15x^2z^4 + 2y^6 - 15y^4z^2 - 15y^2z^4 + 2z^6)}{8}$ |
| 38 | $\mathbb{G}_6(A_{2u})$ | $-\frac{\sqrt{2310}(x-y)(x+y)(x-z)(x+z)(y-z)(y+z)}{8}$ |
| 39 | $\mathbb{G}_{6,1}(E_u)$ | $-\frac{\sqrt{14}(x^6 - 15x^4z^2 + 15x^2z^4 + y^6 - 15y^4z^2 + 15y^2z^4 - 2z^6)}{8}$ |
| 40 | $\mathbb{G}_{6,2}(E_u)$ | $\frac{\sqrt{42}(x-y)(x+y)(x^4 - 9x^2y^2 - 5x^2z^2 + y^4 - 5y^2z^2 + 5z^4)}{8}$ |
| 41 | $\mathbb{G}_{6,1}(T_{1u})$ | $\frac{3\sqrt{7}yz(y-z)(y+z)(10x^2 - y^2 - z^2)}{4}$ |
| 42 | $\mathbb{G}_{6,2}(T_{1u})$ | $\frac{3\sqrt{7}xz(x-z)(x+z)(x^2 - 10y^2 + z^2)}{4}$ |
| 43 | $\mathbb{G}_{6,3}(T_{1u})$ | $-\frac{3\sqrt{7}xy(x-y)(x+y)(x^2 + y^2 - 10z^2)}{4}$ |
| 44 | $\mathbb{G}_{6,1}(T_{2u}, 1)$ | $\frac{\sqrt{462}yz(y^2 - 3z^2)(3y^2 - z^2)}{16}$ |
| 45 | $\mathbb{G}_{6,2}(T_{2u}, 1)$ | $\frac{\sqrt{462}xz(x^2 - 3z^2)(3x^2 - z^2)}{16}$ |
| 46 | $\mathbb{G}_{6,3}(T_{2u}, 1)$ | $\frac{\sqrt{462}xy(x^2 - 3y^2)(3x^2 - y^2)}{16}$ |
| 47 | $\mathbb{G}_{6,1}(T_{2u}, 2)$ | $\frac{\sqrt{210}yz(16x^4 - 16x^2y^2 - 16x^2z^2 + y^4 + 2y^2z^2 + z^4)}{16}$ |
| 48 | $\mathbb{G}_{6,2}(T_{2u}, 2)$ | $\frac{\sqrt{210}xz(x^4 - 16x^2y^2 + 2x^2z^2 + 16y^4 - 16y^2z^2 + z^4)}{16}$ |
| 49 | $\mathbb{G}_{6,3}(T_{2u}, 2)$ | $\frac{\sqrt{210}xy(x^4 + 2x^2y^2 - 16x^2z^2 + y^4 - 16y^2z^2 + 16z^4)}{16}$ |

Table 8 Harmonics for rank 7.

| No. | multipole | expression |
|-----|-------------------------------|---|
| 50 | $\mathbb{G}_7(A_{2g})$ | $\frac{\sqrt{91}xyz(3x^4 - 5x^2y^2 - 5x^2z^2 + 3y^4 - 5y^2z^2 + 3z^4)}{2}$ |
| 51 | $\mathbb{G}_{7,1}(E_g)$ | $-\frac{\sqrt{231}xyz(x-y)(x+y)(3x^2 + 3y^2 - 10z^2)}{4}$ |
| 52 | $\mathbb{G}_{7,2}(E_g)$ | $-\frac{\sqrt{77}xyz(3x^4 - 20x^2y^2 + 10x^2z^2 + 3y^4 + 10y^2z^2 - 6z^4)}{4}$ |
| 53 | $\mathbb{G}_{7,1}(T_{1g}, 1)$ | $\frac{x(16x^6 - 168x^4y^2 - 168x^4z^2 + 210x^2y^4 + 420x^2y^2z^2 + 210x^2z^4 - 35y^6 - 105y^4z^2 - 105y^2z^4 - 35z^6)}{16}$ |
| 54 | $\mathbb{G}_{7,2}(T_{1g}, 1)$ | $-\frac{y(35x^6 - 210x^4y^2 + 105x^4z^2 + 168x^2y^4 - 420x^2y^2z^2 + 105x^2z^4 - 16y^6 + 168y^4z^2 - 210y^2z^4 + 35z^6)}{16}$ |
| 55 | $\mathbb{G}_{7,3}(T_{1g}, 1)$ | $-\frac{z(35x^6 + 105x^4y^2 - 210x^4z^2 + 105x^2y^4 - 420x^2y^2z^2 + 168x^2z^4 + 35y^6 - 210y^4z^2 + 168y^2z^4 - 16z^6)}{16}$ |
| 56 | $\mathbb{G}_{7,1}(T_{1g}, 2)$ | $\frac{\sqrt{231}x(10x^2 - 3y^2 - 3z^2)(y^2 - 2yz - z^2)(y^2 + 2yz - z^2)}{16}$ |
| 57 | $\mathbb{G}_{7,2}(T_{1g}, 2)$ | $-\frac{\sqrt{231}y(x^2 - 2xz - z^2)(x^2 + 2xz - z^2)(3x^2 - 10y^2 + 3z^2)}{16}$ |
| 58 | $\mathbb{G}_{7,3}(T_{1g}, 2)$ | $-\frac{\sqrt{231}z(x^2 - 2xy - y^2)(x^2 + 2xy - y^2)(3x^2 + 3y^2 - 10z^2)}{16}$ |
| 59 | $\mathbb{G}_{7,1}(T_{2g}, 1)$ | $\frac{\sqrt{6006}x(y-z)(y+z)(y^2 - 4yz + z^2)(y^2 + 4yz + z^2)}{32}$ |
| 60 | $\mathbb{G}_{7,2}(T_{2g}, 1)$ | $-\frac{\sqrt{6006}y(x-z)(x+z)(x^2 - 4xz + z^2)(x^2 + 4xz + z^2)}{32}$ |
| 61 | $\mathbb{G}_{7,3}(T_{2g}, 1)$ | $\frac{\sqrt{6006}z(x-y)(x+y)(x^2 - 4xy + y^2)(x^2 + 4xy + y^2)}{32}$ |
| 62 | $\mathbb{G}_{7,1}(T_{2g}, 2)$ | $\frac{\sqrt{42}x(y-z)(y+z)(48x^4 - 80x^2y^2 - 80x^2z^2 + 15y^4 + 30y^2z^2 + 15z^4)}{32}$ |
| 63 | $\mathbb{G}_{7,2}(T_{2g}, 2)$ | $-\frac{\sqrt{42}y(x-z)(x+z)(15x^4 - 80x^2y^2 + 30x^2z^2 + 48y^4 - 80y^2z^2 + 15z^4)}{32}$ |
| 64 | $\mathbb{G}_{7,3}(T_{2g}, 2)$ | $\frac{\sqrt{42}z(x-y)(x+y)(15x^4 + 30x^2y^2 - 80x^2z^2 + 15y^4 - 80y^2z^2 + 48z^4)}{32}$ |

Table 9 Harmonics for rank 8.

| No. | multipole | expression |
|-----|-------------------------------|---|
| 65 | $\mathbb{G}_8(A_{1u})$ | $\frac{\sqrt{33}(x^8 - 14x^6y^2 - 14x^6z^2 + 35x^4y^4 + 35x^4z^4 - 14x^2y^6 - 14x^2z^6 + y^8 - 14y^6z^2 + 35y^4z^4 - 14y^2z^6 + z^8)}{8}$ |
| 66 | $\mathbb{G}_{8,1}(E_u, 1)$ | $\frac{\sqrt{286}(x^8 - 14x^6y^2 - 14x^6z^2 + 210x^4y^2z^2 - 14x^2y^6 + 210x^2y^4z^2 - 420x^2y^2z^4 + 28x^2z^6 + y^8 - 14y^6z^2 + 28y^2z^6 - 2z^8)}{64}$ |
| 67 | $\mathbb{G}_{8,2}(E_u, 1)$ | $-\frac{\sqrt{858}(x-y)(x+y)(x^2+y^2-14z^2)(x^2-4xy+y^2)(x^2+4xy+y^2)}{64}$ |
| 68 | $\mathbb{G}_{8,1}(E_u, 2)$ | $\frac{\sqrt{210}(x^8 - 62x^6y^2 + 34x^6z^2 + 160x^4y^4 - 30x^4y^2z^2 - 80x^4z^4 - 62x^2y^6 - 30x^2y^4z^2 + 60x^2y^2z^4 + 28x^2z^6 + y^8 + 34y^6z^2 - 80y^4z^4 + 28y^2z^6 - 2z^8)}{64}$ |
| 69 | $\mathbb{G}_{8,2}(E_u, 2)$ | $-\frac{3\sqrt{70}(x-y)(x+y)(x^6 + 3x^4y^2 - 30x^4z^2 + 3x^2y^4 - 60x^2y^2z^2 + 80x^2z^4 + y^6 - 30y^4z^2 + 80y^2z^4 - 32z^6)}{64}$ |
| 70 | $\mathbb{G}_{8,1}(T_{1u}, 1)$ | $\frac{3\sqrt{715}yz(y-z)(y+z)(y^2-2yz-z^2)(y^2+2yz-z^2)}{16}$ |
| 71 | $\mathbb{G}_{8,2}(T_{1u}, 1)$ | $-\frac{3\sqrt{715}xz(x-z)(x+z)(x^2-2xz-z^2)(x^2+2xz-z^2)}{16}$ |
| 72 | $\mathbb{G}_{8,3}(T_{1u}, 1)$ | $\frac{3\sqrt{715}xy(x-y)(x+y)(x^2-2xy-y^2)(x^2+2xy-y^2)}{16}$ |
| 73 | $\mathbb{G}_{8,1}(T_{1u}, 2)$ | $\frac{3\sqrt{77}yz(y-z)(y+z)(40x^4 - 24x^2y^2 - 24x^2z^2 + y^4 + 2y^2z^2 + z^4)}{16}$ |
| 74 | $\mathbb{G}_{8,2}(T_{1u}, 2)$ | $-\frac{3\sqrt{77}xz(x-z)(x+z)(x^4 - 24x^2y^2 + 2x^2z^2 + 40y^4 - 24y^2z^2 + z^4)}{16}$ |
| 75 | $\mathbb{G}_{8,3}(T_{1u}, 2)$ | $\frac{3\sqrt{77}xy(x-y)(x+y)(x^4 + 2x^2y^2 - 24x^2z^2 + y^4 - 24y^2z^2 + 40z^4)}{16}$ |
| 76 | $\mathbb{G}_{8,1}(T_{2u}, 1)$ | $\frac{\sqrt{858}yz(y^2-3z^2)(3y^2-z^2)(14x^2-y^2-z^2)}{32}$ |
| 77 | $\mathbb{G}_{8,2}(T_{2u}, 1)$ | $-\frac{\sqrt{858}xz(x^2-3z^2)(3x^2-z^2)(x^2-14y^2+z^2)}{32}$ |
| 78 | $\mathbb{G}_{8,3}(T_{2u}, 1)$ | $-\frac{\sqrt{858}xy(x^2-3y^2)(3x^2-y^2)(x^2+y^2-14z^2)}{32}$ |
| 79 | $\mathbb{G}_{8,1}(T_{2u}, 2)$ | $\frac{3\sqrt{70}yz(32x^6 - 80x^4y^2 - 80x^4z^2 + 30x^2y^4 + 60x^2y^2z^2 + 30x^2z^4 - y^6 - 3y^4z^2 - 3y^2z^4 - z^6)}{32}$ |
| 80 | $\mathbb{G}_{8,2}(T_{2u}, 2)$ | $-\frac{3\sqrt{70}xz(x^6 - 30x^4y^2 + 3x^4z^2 + 80x^2y^4 - 60x^2y^2z^2 + 3x^2z^4 - 32y^6 + 80y^4z^2 - 30y^2z^4 + z^6)}{32}$ |
| 81 | $\mathbb{G}_{8,3}(T_{2u}, 2)$ | $-\frac{3\sqrt{70}xy(x^6 + 3x^4y^2 - 30x^4z^2 + 3x^2y^4 - 60x^2y^2z^2 + 80x^2z^4 + y^6 - 30y^4z^2 + 80y^2z^4 - 32z^6)}{32}$ |

Table 10 Harmonics for rank 9.

| No. | multipole | expression |
|-----|-------------------------------|---|
| 82 | $\mathbb{G}_9(A_{1g})$ | $-\frac{\sqrt{5}10510xyz(x-y)(x+y)(x-z)(x+z)(y-z)(y+z)}{8}$ |
| 83 | $\mathbb{G}_9(A_{2g})$ | $\frac{\sqrt{330}xyz(6x^6-21x^4y^2-21x^4z^2-21x^2y^4+140x^2y^2z^2-21x^2z^4+6y^6-21y^4z^2-21y^2z^4+6z^6)}{8}$ |
| 84 | $\mathbb{G}_{9,1}(E_g)$ | $\frac{\sqrt{4290}xyz(x-y)(x+y)(3x^4-11x^2y^2-7x^2z^2+3y^4-7y^2z^2+7z^4)}{8}$ |
| 85 | $\mathbb{G}_{9,2}(E_g)$ | $\frac{3\sqrt{1430}xyz(x^6-7x^4z^2+7x^2z^4+y^6-7y^4z^2+7y^2z^4-2z^6)}{8}$ |
| 86 | $\mathbb{G}_{9,1}(T_{1g}, 1)$ | $\frac{x(128x^8-2304x^6y^2-2304x^6z^2+6048x^4y^4+12096x^4y^2z^2+6048x^4z^4-3360x^2y^6-10080x^2y^4z^2-10080x^2y^2z^4-3360x^2z^6+315y^8+1260y^6z^2+1890y^4z^4+1260y^2z^6+315z^8)}{128}$ |
| 87 | $\mathbb{G}_{9,2}(T_{1g}, 1)$ | $\frac{y(315x^8-3360x^6y^2+1260x^6z^2+6048x^4y^4-10080x^4y^2z^2+1890x^4z^4-2304x^2y^6+12096x^2y^4z^2-10080x^2y^2z^4+1260x^2z^6+128y^8-2304y^6z^2+6048y^4z^4-3360y^2z^6+315z^8)}{128}$ |
| 88 | $\mathbb{G}_{9,3}(T_{1g}, 1)$ | $\frac{z(315x^8+1260x^6y^2-3360x^6z^2+1890x^4y^4-10080x^4y^2z^2+6048x^4z^4+1260x^2y^6-10080x^2y^4z^2+12096x^2y^2z^4-2304x^2z^6+315y^8-3360y^6z^2+6048y^4z^4-2304y^2z^6+128z^8)}{128}$ |
| 89 | $\mathbb{G}_{9,1}(T_{1g}, 2)$ | $\frac{3\sqrt{12155}x(y^4-4y^3z-6y^2z^2+4yz^3+z^4)(y^4+4y^3z-6y^2z^2-4yz^3+z^4)}{128}$ |
| 90 | $\mathbb{G}_{9,2}(T_{1g}, 2)$ | $\frac{3\sqrt{12155}y(x^4-4x^3z-6x^2z^2+4xz^3+z^4)(x^4+4x^3z-6x^2z^2-4xz^3+z^4)}{128}$ |
| 91 | $\mathbb{G}_{9,3}(T_{1g}, 2)$ | $\frac{3\sqrt{12155}z(x^4-4x^3y-6x^2y^2+4xy^3+y^4)(x^4+4x^3y-6x^2y^2-4xy^3+y^4)}{128}$ |
| 92 | $\mathbb{G}_{9,1}(T_{1g}, 3)$ | $\frac{3\sqrt{5005}x(y^2-2yz-z^2)(y^2+2yz-z^2)(8x^4-8x^2y^2-8x^2z^2+y^4+2y^2z^2+z^4)}{64}$ |
| 93 | $\mathbb{G}_{9,2}(T_{1g}, 3)$ | $\frac{3\sqrt{5005}y(x^2-2xz-z^2)(x^2+2xz-z^2)(x^4-8x^2y^2+2x^2z^2+8y^4-8y^2z^2+z^4)}{64}$ |
| 94 | $\mathbb{G}_{9,3}(T_{1g}, 3)$ | $\frac{3\sqrt{5005}z(x^2-2xy-y^2)(x^2+2xy-y^2)(x^4+2x^2y^2-8x^2z^2+y^4-8y^2z^2+z^4)}{64}$ |
| 95 | $\mathbb{G}_{9,1}(T_{2g}, 1)$ | $\frac{\sqrt{4290}x(y-z)(y+z)(14x^2-3y^2-3z^2)(y^2-4yz+z^2)(y^2+4yz+z^2)}{64}$ |
| 96 | $\mathbb{G}_{9,2}(T_{2g}, 1)$ | $\frac{\sqrt{4290}y(x-z)(x+z)(x^2-4xz+z^2)(x^2+4xz+z^2)(3x^2-14y^2+3z^2)}{64}$ |
| 97 | $\mathbb{G}_{9,3}(T_{2g}, 1)$ | $-\frac{\sqrt{4290}z(x-y)(x+y)(x^2-4xy+y^2)(x^2+4xy+y^2)(3x^2+3y^2-14z^2)}{64}$ |
| 98 | $\mathbb{G}_{9,1}(T_{2g}, 2)$ | $\frac{3\sqrt{110}x(y-z)(y+z)(32x^6-112x^4y^2-112x^4z^2+70x^2y^4+140x^2y^2z^2+70x^2z^4-7y^6-21y^4z^2-21y^2z^4-7z^6)}{64}$ |
| 99 | $\mathbb{G}_{9,2}(T_{2g}, 2)$ | $\frac{3\sqrt{110}y(x-z)(x+z)(7x^6-70x^4y^2+21x^4z^2+112x^2y^4-140x^2y^2z^2+21x^2z^4-32y^6+112y^4z^2-70y^2z^4+7z^6)}{64}$ |
| 100 | $\mathbb{G}_{9,3}(T_{2g}, 2)$ | $-\frac{3\sqrt{110}z(x-y)(x+y)(7x^6+21x^4y^2-70x^4z^2+21x^2y^4-140x^2y^2z^2+112x^2z^4+7y^6-70y^4z^2+112y^2z^4-32z^6)}{64}$ |

Table 11 Harmonics for rank 10.

| No. | multipole | expression |
|-----|--------------------------------|--|
| 101 | $\mathbb{G}_{10}(A_{1u})$ | $\frac{\sqrt{390}(2x^{10}-45x^8y^2-45x^8z^2+42x^6y^4+1008x^6y^2z^2+42x^6z^4+42x^4y^6-1260x^4y^4z^2-1260x^4y^2z^4+42x^4z^6-45x^2y^8+1008x^2y^6z^2-1260x^2y^4z^4+1008x^2y^2z^6-45x^2z^8+2y^{10}-45y^8z^2+42y^6z^4-45y^2z^8+2z^{10})}{96}$ |
| 102 | $\mathbb{G}_{10}(A_{2u})$ | $-\frac{\sqrt{27170}(x-y)(x+y)(x-z)(x+z)(y-z)(y+z)(3x^4-11x^2y^2-11x^2z^2+3y^4-11y^2z^2+3z^4)}{32}$ |
| 103 | $\mathbb{G}_{10,1}(E_u, 1)$ | $-\frac{\sqrt{420189}(22x^{10}+45x^8y^2-1035x^8z^2-105x^6y^4-630x^6y^2z^2+4935x^6z^4-105x^4y^6+3150x^4y^4z^2-1575x^4y^2z^4-4830x^4z^6+45x^2y^8-630x^2y^6z^2-1575x^2y^4z^4+1260x^2y^2z^6+990x^2z^8+22y^{10}-1035y^8z^2+4935y^6z^4-4830y^4z^6+990y^2z^8-44z^{10})}{35952}$ |
| 104 | $\mathbb{G}_{10,2}(E_u, 1)$ | $\frac{\sqrt{140063}(x-y)(x+y)(22x^8-653x^6y^2-315x^6z^2+2602x^4y^4-945x^4y^2z^2+1575x^4z^4-653x^2y^6-945x^2y^4z^2+3150x^2y^2z^4-1680x^2z^6+22y^8-315y^6z^2+1575y^4z^4-1680y^2z^6+360z^8)}{11984}$ |
| 105 | $\mathbb{G}_{10,1}(E_u, 2)$ | $-\frac{\sqrt{3213210}(3x^{10}-96x^8y^2-39x^8z^2+224x^6y^4+1344x^6y^2z^2-42x^6z^4+224x^4y^6-6720x^4y^4z^2+3360x^4y^2z^4-182x^4z^6-96x^2y^8+1344x^2y^6z^2+3360x^2y^4z^4-2688x^2y^2z^6+135x^2z^8+3y^{10}-39y^8z^2-42y^6z^4-182y^4z^6+135y^2z^8-6z^{10})}{23968}$ |
| 106 | $\mathbb{G}_{10,2}(E_u, 2)$ | $\frac{\sqrt{1071070}(x-y)(x+y)(9x^8-165x^6y^2-231x^6z^2-25x^4y^4+3801x^4y^2z^2+406x^4z^4-165x^2y^6+3801x^2y^4z^2-9674x^2y^2z^4+266x^2z^6+9y^8-231y^6z^2+406y^4z^4+266y^2z^6-57z^8)}{23968}$ |
| 107 | $\mathbb{G}_{10,1}(T_{1u}, 1)$ | $\frac{\sqrt{12155}yz(y-z)(y+z)(18x^2-y^2-z^2)(y^2-2yz-z^2)(y^2+2yz-z^2)}{32}$ |
| 108 | $\mathbb{G}_{10,2}(T_{1u}, 1)$ | $\frac{\sqrt{12155}xz(x-z)(x+z)(x^2-18y^2+z^2)(x^2-2xz-z^2)(x^2+2xz-z^2)}{32}$ |
| 109 | $\mathbb{G}_{10,3}(T_{1u}, 1)$ | $-\frac{\sqrt{12155}xy(x-y)(x+y)(x^2+y^2-18z^2)(x^2-2xy-y^2)(x^2+2xy-y^2)}{32}$ |
| 110 | $\mathbb{G}_{10,1}(T_{1u}, 2)$ | $\frac{\sqrt{2145}yz(y-z)(y+z)(112x^6-168x^4y^2-168x^4z^2+42x^2y^4+84x^2y^2z^2+42x^2z^4-y^6-3y^4z^2-3y^2z^4-z^6)}{32}$ |
| 111 | $\mathbb{G}_{10,2}(T_{1u}, 2)$ | $\frac{\sqrt{2145}xz(x-z)(x+z)(x^6-42x^4y^2+3x^4z^2+168x^2y^4-84x^2y^2z^2+3x^2z^4-112y^6+168y^4z^2-42y^2z^4+z^6)}{32}$ |
| 112 | $\mathbb{G}_{10,3}(T_{1u}, 2)$ | $-\frac{\sqrt{2145}xy(x-y)(x+y)(x^6+3x^4y^2-42x^4z^2+3x^2y^4-84x^2y^2z^2+168x^2z^4+y^6-42y^4z^2+168y^2z^4-112z^6)}{32}$ |
| 113 | $\mathbb{G}_{10,1}(T_{2u}, 1)$ | $\frac{\sqrt{92378}yz(y^4-10y^2z^2+5z^4)(5y^4-10y^2z^2+z^4)}{256}$ |
| 114 | $\mathbb{G}_{10,2}(T_{2u}, 1)$ | $\frac{\sqrt{92378}xz(x^4-10x^2z^2+5z^4)(5x^4-10x^2z^2+z^4)}{256}$ |
| 115 | $\mathbb{G}_{10,3}(T_{2u}, 1)$ | $\frac{\sqrt{92378}xy(x^4-10x^2y^2+5y^4)(5x^4-10x^2y^2+y^4)}{256}$ |
| 116 | $\mathbb{G}_{10,1}(T_{2u}, 2)$ | $\frac{\sqrt{4290}yz(y^2-3z^2)(3y^2-z^2)(224x^4-96x^2y^2-96x^2z^2+3y^4+6y^2z^2+3z^4)}{256}$ |
| 117 | $\mathbb{G}_{10,2}(T_{2u}, 2)$ | $\frac{\sqrt{4290}xz(x^2-3z^2)(3x^2-z^2)(3x^4-96x^2y^2+6x^2z^2+224y^4-96y^2z^2+3z^4)}{256}$ |
| 118 | $\mathbb{G}_{10,3}(T_{2u}, 2)$ | $\frac{\sqrt{4290}xy(x^2-3y^2)(3x^2-y^2)(3x^4+6x^2y^2-96x^2z^2+3y^4-96y^2z^2+224z^4)}{256}$ |
| 119 | $\mathbb{G}_{10,1}(T_{2u}, 3)$ | $\frac{\sqrt{165}yz(384x^8-1792x^6y^2-1792x^6z^2+1680x^4y^4+3360x^4y^2z^2+1680x^4z^4-336x^2y^6-1008x^2y^4z^2-1008x^2y^2z^4-336x^2z^6+7y^8+28y^6z^2+42y^4z^4+28y^2z^6+7z^8)}{128}$ |
| 120 | $\mathbb{G}_{10,2}(T_{2u}, 3)$ | $\frac{\sqrt{165}xz(7x^8-336x^6y^2+28x^6z^2+1680x^4y^4-1008x^4y^2z^2+42x^4z^4-1792x^2y^6+3360x^2y^4z^2-1008x^2y^2z^4+28x^2z^6+384y^8-1792y^6z^2+1680y^4z^4-336y^2z^6+7z^8)}{128}$ |
| 121 | $\mathbb{G}_{10,3}(T_{2u}, 3)$ | $\frac{\sqrt{165}xy(7x^8+28x^6y^2-336x^6z^2+42x^4y^4-1008x^4y^2z^2+1680x^4z^4+28x^2y^6-1008x^2y^4z^2+3360x^2y^2z^4-1792x^2z^6+7y^8-336y^6z^2+1680y^4z^4-1792y^2z^6+384z^8)}{128}$ |

Table 12 Harmonics for rank 11.

| No. | multipole | expression |
|-----|--------------------------------|---|
| 122 | $\mathbb{G}_{11}(A_{2g})$ | $\frac{\sqrt{243}xyz(5x^8 - 30x^6y^2 - 30x^6z^2 + 63x^4y^4 + 63x^4z^4 - 30x^2y^6 - 30x^2z^6 + 5y^8 - 30y^6z^2 + 63y^4z^4 - 30y^2z^6 + 5z^8)}{8}$ |
| 123 | $\mathbb{G}_{11,1}(E_g, 1)$ | $-\frac{\sqrt{692835}xyz(x-y)(x+y)(x^2+y^2-6z^2)(x^2-2xy-y^2)(x^2+2xy-y^2)}{32}$ |
| 124 | $\mathbb{G}_{11,2}(E_g, 1)$ | $-\frac{\sqrt{230945}xyz(x^8 - 6x^6y^2 - 6x^6z^2 + 42x^4y^2z^2 - 6x^2y^6 + 42x^2y^4z^2 - 84x^2y^2z^4 + 12x^2z^6 + y^8 - 6y^6z^2 + 12y^2z^6 - 2z^8)}{32}$ |
| 125 | $\mathbb{G}_{11,1}(E_g, 2)$ | $-\frac{3\sqrt{1001}xyz(x-y)(x+y)(5x^6 + 15x^4y^2 - 70x^4z^2 + 15x^2y^4 - 140x^2y^2z^2 + 168x^2z^4 + 5y^6 - 70y^4z^2 + 168y^2z^4 - 80z^6)}{32}$ |
| 126 | $\mathbb{G}_{11,2}(E_g, 2)$ | $-\frac{\sqrt{3003}xyz(5x^8 - 150x^6y^2 + 90x^6z^2 + 336x^4y^4 - 70x^4y^2z^2 - 168x^4z^4 - 150x^2y^6 - 70x^2y^4z^2 + 140x^2y^2z^4 + 60x^2z^6 + 5y^8 + 90y^6z^2 - 168y^4z^4 + 60y^2z^6 - 10z^8)}{32}$ |
| 127 | $\mathbb{G}_{11,1}(T_{1g}, 1)$ | $\frac{x(256x^{10} - 7040x^8y^2 - 7040x^8z^2 + 31680x^6y^4 + 63360x^6y^2z^2 + 31680x^6z^4 - 36960x^4y^6 - 110880x^4y^2z^4 - 36960x^4z^6 + 11550x^2y^8 + 46200x^2y^6z^2 + 69300x^2y^4z^4 + 46200x^2y^2z^6 + 11550x^2z^8 - 693y^{10} - 3465y^8z^2 - 6930y^6z^4 - 6930y^4z^6 - 3465y^2z^8 - 693z^{10})}{256}$ |
| 128 | $\mathbb{G}_{11,2}(T_{1g}, 1)$ | $-\frac{y(693x^{10} - 11550x^8y^2 + 3465x^8z^2 + 36960x^6y^4 - 46200x^6y^2z^2 + 6930x^6z^4 - 31680x^4y^6 + 110880x^4y^2z^4 - 69300x^4z^6 + 7040x^2y^8 - 63360x^2y^6z^2 + 110880x^2y^4z^4 - 46200x^2y^2z^6 + 3465x^2z^8 - 256y^{10} + 7040y^8z^2 - 31680y^6z^4 - 36960y^4z^6 - 11550y^2z^8 + 693z^{10})}{256}$ |
| 129 | $\mathbb{G}_{11,3}(T_{1g}, 1)$ | $-\frac{z(693x^{10} + 3465x^8y^2 - 11550x^8z^2 + 6930x^6y^4 - 46200x^6y^2z^2 + 36960x^6z^4 + 6930x^4y^6 - 69300x^4y^2z^4 + 110880x^4y^2z^4 - 31680x^4z^6 + 3465x^2y^8 - 46200x^2y^6z^2 + 110880x^2y^4z^4 - 63360x^2y^2z^6 + 7040x^2z^8 + 693y^{10} - 11550y^8z^2 + 36960y^6z^4 - 31680y^4z^6 + 7040y^2z^8 - 256z^{10})}{256}$ |
| 130 | $\mathbb{G}_{11,1}(T_{1g}, 2)$ | $\frac{\sqrt{692835}x(6x^2 - y^2 - z^2)(y^4 - 4y^3z - 6y^2z^2 + 4yz^3 + z^4)(y^4 + 4y^3z - 6y^2z^2 - 4yz^3 + z^4)}{256}$ |
| 131 | $\mathbb{G}_{11,2}(T_{1g}, 2)$ | $-\frac{\sqrt{692835}y(x^2 - 6y^2 + z^2)(x^4 - 4x^3z - 6x^2z^2 + 4xz^3 + z^4)(x^4 + 4x^3z - 6x^2z^2 - 4xz^3 + z^4)}{256}$ |
| 132 | $\mathbb{G}_{11,3}(T_{1g}, 2)$ | $-\frac{\sqrt{692835}z(x^2 + y^2 - 6z^2)(x^4 - 4x^3y - 6x^2y^2 + 4xy^3 + y^4)(x^4 + 4x^3y - 6x^2y^2 - 4xy^3 + y^4)}{256}$ |
| 133 | $\mathbb{G}_{11,1}(T_{1g}, 3)$ | $3\sqrt{1001}x(y^2 - 2yz - z^2)(y^2 + 2yz - z^2)(80x^6 - 168x^4y^2 - 168x^4z^2 + 70x^2y^4 + 140x^2y^2z^2 + 70x^2z^4 - 5y^6 - 15y^4z^2 - 15y^2z^4 - 5z^6)$ |
| 134 | $\mathbb{G}_{11,2}(T_{1g}, 3)$ | $-\frac{3\sqrt{1001}y(x^2 - 2xz - z^2)(x^2 + 2xz - z^2)(5x^6 - 70x^4y^2 + 15x^4z^2 + 168x^2y^4 - 140x^2y^2z^2 + 15x^2z^4 - 80y^6 + 168y^4z^2 - 70y^2z^4 + 5z^6)}{128}$ |
| 135 | $\mathbb{G}_{11,3}(T_{1g}, 3)$ | $-\frac{3\sqrt{1001}z(x^2 - 2xy - y^2)(x^2 + 2xy - y^2)(5x^6 + 15x^4y^2 - 70x^4z^2 + 15x^2y^4 - 140x^2y^2z^2 + 168x^2z^4 + 5y^6 - 70y^4z^2 + 168y^2z^4 - 80z^6)}{128}$ |
| 136 | $\mathbb{G}_{11,1}(T_{2g}, 1)$ | $\frac{\sqrt{1939938}x(y-z)(y+z)(y^4 - 4y^3z - 14y^2z^2 - 4yz^3 + z^4)(y^4 + 4y^3z - 14y^2z^2 + 4yz^3 + z^4)}{512}$ |
| 137 | $\mathbb{G}_{11,2}(T_{2g}, 1)$ | $-\frac{\sqrt{1939938}y(x-z)(x+z)(x^4 - 4x^3z - 14x^2z^2 - 4xz^3 + z^4)(x^4 + 4x^3z - 14x^2z^2 + 4xz^3 + z^4)}{512}$ |
| 138 | $\mathbb{G}_{11,3}(T_{2g}, 1)$ | $\frac{\sqrt{1939938}z(x-y)(x+y)(x^4 - 4x^3y - 14x^2y^2 - 4xy^3 + y^4)(x^4 + 4x^3y - 14x^2y^2 + 4xy^3 + y^4)}{512}$ |
| 139 | $\mathbb{G}_{11,1}(T_{2g}, 2)$ | $\frac{\sqrt{14586}x(y-z)(y+z)(y^2 - 4yz + z^2)(y^2 + 4yz + z^2)(224x^4 - 160x^2y^2 - 160x^2z^2 + 15y^4 + 30y^2z^2 + 15z^4)}{512}$ |
| 140 | $\mathbb{G}_{11,2}(T_{2g}, 2)$ | $-\frac{\sqrt{14586}y(x-z)(x+z)(x^2 - 4xz + z^2)(x^2 + 4xz + z^2)(15x^4 - 160x^2y^2 + 30x^2z^2 + 224y^4 - 160y^2z^2 + 15z^4)}{512}$ |
| 141 | $\mathbb{G}_{11,3}(T_{2g}, 2)$ | $\frac{\sqrt{14586}z(x-y)(x+y)(x^2 - 4xy + y^2)(x^2 + 4xy + y^2)(15x^4 + 30x^2y^2 - 160x^2z^2 + 15y^4 - 160y^2z^2 + 224z^4)}{512}$ |
| 142 | $\mathbb{G}_{11,1}(T_{2g}, 3)$ | $\frac{\sqrt{2145}x(y-z)(y+z)(128x^8 - 768x^6y^2 - 768x^6z^2 + 1008x^4y^4 + 2016x^4y^2z^2 + 1008x^4z^4 - 336x^2y^6 - 1008x^2y^4z^2 - 336x^2z^6 + 21y^8 + 84y^6z^2 + 126y^4z^4 + 84y^2z^6 + 21z^8)}{256}$ |
| 143 | $\mathbb{G}_{11,2}(T_{2g}, 3)$ | $-\frac{\sqrt{2145}y(x-z)(x+z)(21x^8 - 336x^6y^2 + 84x^6z^2 + 1008x^4y^4 - 1008x^4y^2z^2 + 126x^4z^4 - 768x^2y^6 + 2016x^2y^4z^2 - 1008x^2y^2z^4 + 84x^2z^6 + 128y^8 - 768y^6z^2 + 1008y^4z^4 - 336y^2z^6 + 21z^8)}{256}$ |
| 144 | $\mathbb{G}_{11,3}(T_{2g}, 3)$ | $\frac{\sqrt{2145}z(x-y)(x+y)(21x^8 + 84x^6y^2 - 336x^6z^2 + 126x^4y^4 - 1008x^4y^2z^2 + 1008x^4z^4 + 84x^2y^6 - 1008x^2y^4z^2 + 2016x^2y^2z^4 - 768x^2z^6 + 21y^8 - 336y^6z^2 + 1008y^4z^4 - 768y^2z^6 + 128z^8)}{256}$ |