

PG No. 21 C_6 6 [hexagonal] (lg basis)

bra: = $\langle s |$
ket: = $|s\rangle$

Table 1: (s,s) block.

| No. | multipole | matrix |
|-----|----------------|-----------------------------------|
| 1 | symmetry | 1 |
| | $Q_0^{(a)}(A)$ | $\begin{bmatrix} 1 \end{bmatrix}$ |

bra: = $\langle s |$
ket: = $|p_x\rangle, |p_y\rangle, |p_z\rangle$

Table 2: (s,p) block.

| No. | multipole | matrix |
|-----|----------------------|---|
| 2 | symmetry | z |
| | $Q_1^{(a)}(A)$ | $\begin{bmatrix} 0 & 0 & \frac{\sqrt{2}}{2} \end{bmatrix}$ |
| 3 | symmetry | x |
| | $Q_{1,1}^{(a)}(E_1)$ | $\begin{bmatrix} \frac{\sqrt{2}}{2} & 0 & 0 \end{bmatrix}$ |
| 4 | symmetry | y |
| | $Q_{1,2}^{(a)}(E_1)$ | $\begin{bmatrix} 0 & \frac{\sqrt{2}}{2} & 0 \end{bmatrix}$ |
| 5 | symmetry | z |
| | $T_1^{(a)}(A)$ | $\begin{bmatrix} 0 & 0 & \frac{\sqrt{2}i}{2} \end{bmatrix}$ |
| 6 | symmetry | x |
| | $T_{1,1}^{(a)}(E_1)$ | $\begin{bmatrix} \frac{\sqrt{2}i}{2} & 0 & 0 \end{bmatrix}$ |
| 7 | symmetry | y |
| | $T_{1,2}^{(a)}(E_1)$ | $\begin{bmatrix} 0 & \frac{\sqrt{2}i}{2} & 0 \end{bmatrix}$ |

bra: = $\langle s |$
ket: = $|d_v\rangle, |d_{xy}\rangle, |d_{xz}\rangle, |d_{yz}\rangle, |d_u\rangle$

Table 3: (s,d) block.

| No. | multipole | matrix |
|-----|-------------------------------|--|
| 8 | symmetry | $-\frac{x^2}{2} - \frac{y^2}{2} + z^2$ |
| | $\mathbb{Q}_2^{(a)}(A)$ | $\begin{bmatrix} 0 & 0 & 0 & 0 & \frac{\sqrt{2}}{2} \end{bmatrix}$ |
| 9 | symmetry | $\sqrt{3}yz$ |
| | $\mathbb{Q}_{2,1}^{(a)}(E_1)$ | $\begin{bmatrix} 0 & 0 & 0 & \frac{\sqrt{2}}{2} & 0 \end{bmatrix}$ |
| 10 | symmetry | $-\sqrt{3}xz$ |
| | $\mathbb{Q}_{2,2}^{(a)}(E_1)$ | $\begin{bmatrix} 0 & 0 & -\frac{\sqrt{2}}{2} & 0 & 0 \end{bmatrix}$ |
| 11 | symmetry | $\frac{\sqrt{3}(x-y)(x+y)}{2}$ |
| | $\mathbb{Q}_{2,1}^{(a)}(E_2)$ | $\begin{bmatrix} \frac{\sqrt{2}}{2} & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| 12 | symmetry | $-\sqrt{3}xy$ |
| | $\mathbb{Q}_{2,2}^{(a)}(E_2)$ | $\begin{bmatrix} 0 & -\frac{\sqrt{2}}{2} & 0 & 0 & 0 \end{bmatrix}$ |
| 13 | symmetry | $-\frac{x^2}{2} - \frac{y^2}{2} + z^2$ |
| | $\mathbb{T}_2^{(a)}(A)$ | $\begin{bmatrix} 0 & 0 & 0 & 0 & \frac{\sqrt{2}i}{2} \end{bmatrix}$ |
| 14 | symmetry | $\sqrt{3}yz$ |
| | $\mathbb{T}_{2,1}^{(a)}(E_1)$ | $\begin{bmatrix} 0 & 0 & 0 & \frac{\sqrt{2}i}{2} & 0 \end{bmatrix}$ |
| 15 | symmetry | $-\sqrt{3}xz$ |
| | $\mathbb{T}_{2,2}^{(a)}(E_1)$ | $\begin{bmatrix} 0 & 0 & -\frac{\sqrt{2}i}{2} & 0 & 0 \end{bmatrix}$ |
| 16 | symmetry | $\frac{\sqrt{3}(x-y)(x+y)}{2}$ |
| | $\mathbb{T}_{2,1}^{(a)}(E_2)$ | $\begin{bmatrix} \frac{\sqrt{2}i}{2} & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| 17 | symmetry | $-\sqrt{3}xy$ |
| | $\mathbb{T}_{2,2}^{(a)}(E_2)$ | $\begin{bmatrix} 0 & -\frac{\sqrt{2}i}{2} & 0 & 0 & 0 \end{bmatrix}$ |

bra: = $\langle s|$ ket: = $|f_2\rangle, |f_1\rangle, |f_{bz}\rangle, |f_3\rangle, |f_{3x}\rangle, |f_{3y}\rangle, |f_{az}\rangle$

Table 4: (s,f) block.

| No. | multipole | matrix |
|-----|-------------------------------|---|
| 18 | symmetry | $-\frac{z(3x^2+3y^2-2z^2)}{2}$ |
| | $\mathbb{Q}_3^{(a)}(A)$ | $\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{2}}{2} \end{bmatrix}$ |
| 19 | symmetry | $\frac{\sqrt{10}y(3x^2-y^2)}{4}$ |
| | $\mathbb{Q}_3^{(a)}(B, 1)$ | $\begin{bmatrix} 0 & \frac{\sqrt{2}}{2} & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| 20 | symmetry | $\frac{\sqrt{10}x(x^2-3y^2)}{4}$ |
| | $\mathbb{Q}_3^{(a)}(B, 2)$ | $\begin{bmatrix} \frac{\sqrt{2}}{2} & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| 21 | symmetry | $-\frac{\sqrt{6}x(x^2+y^2-4z^2)}{4}$ |
| | $\mathbb{Q}_{3,1}^{(a)}(E_1)$ | $\begin{bmatrix} 0 & 0 & 0 & 0 & \frac{\sqrt{2}}{2} & 0 & 0 \end{bmatrix}$ |
| 22 | symmetry | $-\frac{\sqrt{6}y(x^2+y^2-4z^2)}{4}$ |
| | $\mathbb{Q}_{3,2}^{(a)}(E_1)$ | $\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{2}}{2} & 0 \end{bmatrix}$ |
| 23 | symmetry | $\sqrt{15}xyz$ |
| | $\mathbb{Q}_{3,1}^{(a)}(E_2)$ | $\begin{bmatrix} 0 & 0 & 0 & \frac{\sqrt{2}}{2} & 0 & 0 & 0 \end{bmatrix}$ |
| 24 | symmetry | $\frac{\sqrt{15}z(x-y)(x+y)}{2}$ |
| | $\mathbb{Q}_{3,2}^{(a)}(E_2)$ | $\begin{bmatrix} 0 & 0 & \frac{\sqrt{2}}{2} & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| 25 | symmetry | $-\frac{z(3x^2+3y^2-2z^2)}{2}$ |
| | $\mathbb{T}_3^{(a)}(A)$ | $\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{2}i}{2} \end{bmatrix}$ |
| 26 | symmetry | $\frac{\sqrt{10}y(3x^2-y^2)}{4}$ |
| | $\mathbb{T}_3^{(a)}(B, 1)$ | $\begin{bmatrix} 0 & \frac{\sqrt{2}i}{2} & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| 27 | symmetry | $\frac{\sqrt{10}x(x^2-3y^2)}{4}$ |
| | $\mathbb{T}_3^{(a)}(B, 2)$ | $\begin{bmatrix} \frac{\sqrt{2}i}{2} & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| 28 | symmetry | $-\frac{\sqrt{6}x(x^2+y^2-4z^2)}{4}$ |
| | $\mathbb{T}_{3,1}^{(a)}(E_1)$ | $\begin{bmatrix} 0 & 0 & 0 & 0 & \frac{\sqrt{2}i}{2} & 0 & 0 \end{bmatrix}$ |
| 29 | symmetry | $-\frac{\sqrt{6}y(x^2+y^2-4z^2)}{4}$ |
| | $\mathbb{T}_{3,2}^{(a)}(E_1)$ | $\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{2}i}{2} & 0 \end{bmatrix}$ |
| 30 | symmetry | $\sqrt{15}xyz$ |
| | $\mathbb{T}_{3,1}^{(a)}(E_2)$ | $\begin{bmatrix} 0 & 0 & 0 & \frac{\sqrt{2}i}{2} & 0 & 0 & 0 \end{bmatrix}$ |
| 31 | symmetry | $\frac{\sqrt{15}z(x-y)(x+y)}{2}$ |

continued ...

Table 4

| No. | multipole | matrix |
|-----|-------------------------------|---|
| | $\mathbb{T}_{3,2}^{(a)}(E_2)$ | $\begin{bmatrix} 0 & 0 & \frac{\sqrt{2}i}{2} & 0 & 0 & 0 & 0 \end{bmatrix}$ |

bra: = $\langle p_x |, \langle p_y |, \langle p_z |$
ket: = $|p_x\rangle, |p_y\rangle, |p_z\rangle$

Table 5: (p,p) block.

| No. | multipole | matrix |
|-----|-------------------------------|--|
| 32 | symmetry | 1 |
| | $\mathbb{Q}_0^{(a)}(A)$ | $\begin{bmatrix} \frac{\sqrt{3}}{3} & 0 & 0 \\ 0 & \frac{\sqrt{3}}{3} & 0 \\ 0 & 0 & \frac{\sqrt{3}}{3} \end{bmatrix}$ |
| 33 | symmetry | $-\frac{x^2}{2} - \frac{y^2}{2} + z^2$ |
| | $\mathbb{Q}_2^{(a)}(A)$ | $\begin{bmatrix} -\frac{\sqrt{6}}{6} & 0 & 0 \\ 0 & -\frac{\sqrt{6}}{6} & 0 \\ 0 & 0 & \frac{\sqrt{6}}{3} \end{bmatrix}$ |
| 34 | symmetry | $\sqrt{3}yz$ |
| | $\mathbb{Q}_{2,1}^{(a)}(E_1)$ | $\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{2}}{2} \\ 0 & \frac{\sqrt{2}}{2} & 0 \end{bmatrix}$ |
| 35 | symmetry | $-\sqrt{3}xz$ |
| | $\mathbb{Q}_{2,2}^{(a)}(E_1)$ | $\begin{bmatrix} 0 & 0 & -\frac{\sqrt{2}}{2} \\ 0 & 0 & 0 \\ -\frac{\sqrt{2}}{2} & 0 & 0 \end{bmatrix}$ |
| 36 | symmetry | $\frac{\sqrt{3}(x-y)(x+y)}{2}$ |
| | $\mathbb{Q}_{2,1}^{(a)}(E_2)$ | $\begin{bmatrix} \frac{\sqrt{2}}{2} & 0 & 0 \\ 0 & -\frac{\sqrt{2}}{2} & 0 \\ 0 & 0 & 0 \end{bmatrix}$ |

continued ...

Table 5

| No. | multipole | matrix |
|-----|----------------------|--|
| 37 | symmetry | $-\sqrt{3}xy$ |
| | $Q_{2,2}^{(a)}(E_2)$ | $\begin{bmatrix} 0 & -\frac{\sqrt{2}}{2} & 0 \\ -\frac{\sqrt{2}}{2} & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$ |
| 38 | symmetry | z |
| | $M_1^{(a)}(A)$ | $\begin{bmatrix} 0 & -\frac{\sqrt{2}i}{2} & 0 \\ \frac{\sqrt{2}i}{2} & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$ |
| 39 | symmetry | x |
| | $M_{1,1}^{(a)}(E_1)$ | $\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{2}i}{2} \\ 0 & \frac{\sqrt{2}i}{2} & 0 \end{bmatrix}$ |
| 40 | symmetry | y |
| | $M_{1,2}^{(a)}(E_1)$ | $\begin{bmatrix} 0 & 0 & \frac{\sqrt{2}i}{2} \\ 0 & 0 & 0 \\ -\frac{\sqrt{2}i}{2} & 0 & 0 \end{bmatrix}$ |

bra: = $\langle p_x |, \langle p_y |, \langle p_z |$
ket: = $|d_v\rangle, |d_{xy}\rangle, |d_{xz}\rangle, |d_{yz}\rangle, |d_u\rangle$

Table 6: (p,d) block.

| No. | multipole | matrix |
|-----|----------------|--|
| 41 | symmetry | z |
| | $Q_1^{(a)}(A)$ | $\begin{bmatrix} 0 & 0 & \frac{\sqrt{15}}{10} & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{15}}{10} & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{5}}{5} \end{bmatrix}$ |
| 42 | symmetry | x |

continued ...

Table 6

| No. | multipole | matrix |
|-----|-------------------------------|--|
| | $\mathbb{Q}_{1,1}^{(a)}(E_1)$ | $\begin{bmatrix} \frac{\sqrt{15}}{10} & 0 & 0 & 0 & -\frac{\sqrt{5}}{10} \\ 0 & \frac{\sqrt{15}}{10} & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{15}}{10} & 0 & 0 \end{bmatrix}$ |
| 43 | symmetry | y |
| | $\mathbb{Q}_{1,2}^{(a)}(E_1)$ | $\begin{bmatrix} 0 & \frac{\sqrt{15}}{10} & 0 & 0 & 0 \\ -\frac{\sqrt{15}}{10} & 0 & 0 & 0 & -\frac{\sqrt{5}}{10} \\ 0 & 0 & 0 & \frac{\sqrt{15}}{10} & 0 \end{bmatrix}$ |
| 44 | symmetry | $-\frac{z(3x^2+3y^2-2z^2)}{2}$ |
| | $\mathbb{Q}_3^{(a)}(A)$ | $\begin{bmatrix} 0 & 0 & -\frac{\sqrt{10}}{10} & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{10}}{10} & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{30}}{10} \end{bmatrix}$ |
| 45 | symmetry | $\frac{\sqrt{10}y(3x^2-y^2)}{4}$ |
| | $\mathbb{Q}_3^{(a)}(B, 1)$ | $\begin{bmatrix} 0 & \frac{1}{2} & 0 & 0 & 0 \\ \frac{1}{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| 46 | symmetry | $\frac{\sqrt{10}x(x^2-3y^2)}{4}$ |
| | $\mathbb{Q}_3^{(a)}(B, 2)$ | $\begin{bmatrix} \frac{1}{2} & 0 & 0 & 0 & 0 \\ 0 & -\frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| 47 | symmetry | $-\frac{\sqrt{6}x(x^2+y^2-4z^2)}{4}$ |
| | $\mathbb{Q}_{3,1}^{(a)}(E_1)$ | $\begin{bmatrix} -\frac{\sqrt{15}}{30} & 0 & 0 & 0 & \frac{\sqrt{5}}{5} \\ 0 & -\frac{\sqrt{15}}{30} & 0 & 0 & 0 \\ 0 & 0 & \frac{2\sqrt{15}}{15} & 0 & 0 \end{bmatrix}$ |
| 48 | symmetry | $-\frac{\sqrt{6}y(x^2+y^2-4z^2)}{4}$ |
| | $\mathbb{Q}_{3,2}^{(a)}(E_1)$ | $\begin{bmatrix} 0 & -\frac{\sqrt{15}}{30} & 0 & 0 & 0 \\ \frac{\sqrt{15}}{30} & 0 & 0 & 0 & \frac{\sqrt{5}}{5} \\ 0 & 0 & 0 & \frac{2\sqrt{15}}{15} & 0 \end{bmatrix}$ |
| 49 | symmetry | $\sqrt{15}xyz$ |

continued ...

Table 6

| No. | multipole | matrix |
|-----|-------------------------------|---|
| | $\mathbb{Q}_{3,1}^{(a)}(E_2)$ | $\begin{bmatrix} 0 & 0 & 0 & \frac{\sqrt{6}}{6} & 0 \\ 0 & 0 & \frac{\sqrt{6}}{6} & 0 & 0 \\ 0 & \frac{\sqrt{6}}{6} & 0 & 0 & 0 \end{bmatrix}$ |
| 50 | symmetry | $\frac{\sqrt{15}z(x-y)(x+y)}{2}$ |
| | $\mathbb{Q}_{3,2}^{(a)}(E_2)$ | $\begin{bmatrix} 0 & 0 & \frac{\sqrt{6}}{6} & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{6}}{6} & 0 \\ \frac{\sqrt{6}}{6} & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| 51 | symmetry | $-\frac{x^2}{2} - \frac{y^2}{2} + z^2$ |
| | $\mathbb{G}_2^{(a)}(A)$ | $\begin{bmatrix} 0 & 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & -\frac{1}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| 52 | symmetry | $\sqrt{3}yz$ |
| | $\mathbb{G}_{2,1}^{(a)}(E_1)$ | $\begin{bmatrix} -\frac{\sqrt{3}}{6} & 0 & 0 & 0 & -\frac{1}{2} \\ 0 & -\frac{\sqrt{3}}{6} & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{3}}{6} & 0 & 0 \end{bmatrix}$ |
| 53 | symmetry | $-\sqrt{3}xz$ |
| | $\mathbb{G}_{2,2}^{(a)}(E_1)$ | $\begin{bmatrix} 0 & -\frac{\sqrt{3}}{6} & 0 & 0 & 0 \\ \frac{\sqrt{3}}{6} & 0 & 0 & 0 & -\frac{1}{2} \\ 0 & 0 & 0 & \frac{\sqrt{3}}{6} & 0 \end{bmatrix}$ |
| 54 | symmetry | $\frac{\sqrt{3}(x-y)(x+y)}{2}$ |
| | $\mathbb{G}_{2,1}^{(a)}(E_2)$ | $\begin{bmatrix} 0 & 0 & 0 & \frac{\sqrt{3}}{6} & 0 \\ 0 & 0 & \frac{\sqrt{3}}{6} & 0 & 0 \\ 0 & -\frac{\sqrt{3}}{3} & 0 & 0 & 0 \end{bmatrix}$ |
| 55 | symmetry | $-\sqrt{3}xy$ |
| | $\mathbb{G}_{2,2}^{(a)}(E_2)$ | $\begin{bmatrix} 0 & 0 & \frac{\sqrt{3}}{6} & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{3}}{6} & 0 \\ -\frac{\sqrt{3}}{3} & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| 56 | symmetry | z |

continued ...

Table 6

| No. | multipole | matrix |
|-----|-------------------------------|--|
| | $\mathbb{T}_1^{(a)}(A)$ | $\begin{bmatrix} 0 & 0 & \frac{\sqrt{15}i}{10} & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{15}i}{10} & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{5}i}{5} \end{bmatrix}$ |
| 57 | symmetry | x |
| | $\mathbb{T}_{1,1}^{(a)}(E_1)$ | $\begin{bmatrix} \frac{\sqrt{15}i}{10} & 0 & 0 & 0 & -\frac{\sqrt{5}i}{10} \\ 0 & \frac{\sqrt{15}i}{10} & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{15}i}{10} & 0 & 0 \end{bmatrix}$ |
| 58 | symmetry | y |
| | $\mathbb{T}_{1,2}^{(a)}(E_1)$ | $\begin{bmatrix} 0 & \frac{\sqrt{15}i}{10} & 0 & 0 & 0 \\ -\frac{\sqrt{15}i}{10} & 0 & 0 & 0 & -\frac{\sqrt{5}i}{10} \\ 0 & 0 & 0 & \frac{\sqrt{15}i}{10} & 0 \end{bmatrix}$ |
| 59 | symmetry | $-\frac{z(3x^2+3y^2-2z^2)}{2}$ |
| | $\mathbb{T}_3^{(a)}(A)$ | $\begin{bmatrix} 0 & 0 & -\frac{\sqrt{10}i}{10} & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{10}i}{10} & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{30}i}{10} \end{bmatrix}$ |
| 60 | symmetry | $\frac{\sqrt{10}y(3x^2-y^2)}{4}$ |
| | $\mathbb{T}_3^{(a)}(B, 1)$ | $\begin{bmatrix} 0 & \frac{i}{2} & 0 & 0 & 0 \\ \frac{i}{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| 61 | symmetry | $\frac{\sqrt{10}x(x^2-3y^2)}{4}$ |
| | $\mathbb{T}_3^{(a)}(B, 2)$ | $\begin{bmatrix} \frac{i}{2} & 0 & 0 & 0 & 0 \\ 0 & -\frac{i}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| 62 | symmetry | $-\frac{\sqrt{6}x(x^2+y^2-4z^2)}{4}$ |
| | $\mathbb{T}_{3,1}^{(a)}(E_1)$ | $\begin{bmatrix} -\frac{\sqrt{15}i}{30} & 0 & 0 & 0 & \frac{\sqrt{5}i}{5} \\ 0 & -\frac{\sqrt{15}i}{30} & 0 & 0 & 0 \\ 0 & 0 & \frac{2\sqrt{15}i}{15} & 0 & 0 \end{bmatrix}$ |
| 63 | symmetry | $-\frac{\sqrt{6}y(x^2+y^2-4z^2)}{4}$ |

continued ...

Table 6

| No. | multipole | matrix |
|-----|-------------------------------|---|
| | $\mathbb{T}_{3,2}^{(a)}(E_1)$ | $\begin{bmatrix} 0 & -\frac{\sqrt{15}i}{30} & 0 & 0 & 0 \\ \frac{\sqrt{15}i}{30} & 0 & 0 & 0 & \frac{\sqrt{5}i}{5} \\ 0 & 0 & 0 & \frac{2\sqrt{15}i}{15} & 0 \end{bmatrix}$ |
| 64 | symmetry | $\sqrt{15}xyz$ |
| | $\mathbb{T}_{3,1}^{(a)}(E_2)$ | $\begin{bmatrix} 0 & 0 & 0 & \frac{\sqrt{6}i}{6} & 0 \\ 0 & 0 & \frac{\sqrt{6}i}{6} & 0 & 0 \\ 0 & \frac{\sqrt{6}i}{6} & 0 & 0 & 0 \end{bmatrix}$ |
| 65 | symmetry | $\frac{\sqrt{15}z(x-y)(x+y)}{2}$ |
| | $\mathbb{T}_{3,2}^{(a)}(E_2)$ | $\begin{bmatrix} 0 & 0 & \frac{\sqrt{6}i}{6} & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{6}i}{6} & 0 \\ \frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| 66 | symmetry | $-\frac{x^2}{2} - \frac{y^2}{2} + z^2$ |
| | $\mathbb{M}_2^{(a)}(A)$ | $\begin{bmatrix} 0 & 0 & 0 & -\frac{i}{2} & 0 \\ 0 & 0 & \frac{i}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| 67 | symmetry | $\sqrt{3}yz$ |
| | $\mathbb{M}_{2,1}^{(a)}(E_1)$ | $\begin{bmatrix} \frac{\sqrt{3}i}{6} & 0 & 0 & 0 & \frac{i}{2} \\ 0 & \frac{\sqrt{3}i}{6} & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{3}i}{6} & 0 & 0 \end{bmatrix}$ |
| 68 | symmetry | $-\sqrt{3}xz$ |
| | $\mathbb{M}_{2,2}^{(a)}(E_1)$ | $\begin{bmatrix} 0 & \frac{\sqrt{3}i}{6} & 0 & 0 & 0 \\ -\frac{\sqrt{3}i}{6} & 0 & 0 & 0 & \frac{i}{2} \\ 0 & 0 & 0 & -\frac{\sqrt{3}i}{6} & 0 \end{bmatrix}$ |
| 69 | symmetry | $\frac{\sqrt{3}(x-y)(x+y)}{2}$ |
| | $\mathbb{M}_{2,1}^{(a)}(E_2)$ | $\begin{bmatrix} 0 & 0 & 0 & -\frac{\sqrt{3}i}{6} & 0 \\ 0 & 0 & -\frac{\sqrt{3}i}{6} & 0 & 0 \\ 0 & \frac{\sqrt{3}i}{3} & 0 & 0 & 0 \end{bmatrix}$ |
| 70 | symmetry | $-\sqrt{3}xy$ |

continued ...

Table 6

| No. | multipole | matrix |
|-----|----------------------|--|
| | $M_{2,2}^{(a)}(E_2)$ | $\begin{bmatrix} 0 & 0 & -\frac{\sqrt{3}i}{6} & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{3}i}{6} & 0 \\ \frac{\sqrt{3}i}{3} & 0 & 0 & 0 & 0 \end{bmatrix}$ |

bra: = $\langle p_x |, \langle p_y |, \langle p_z |$

ket: = $|f_2\rangle, |f_1\rangle, |f_{bz}\rangle, |f_3\rangle, |f_{3x}\rangle, |f_{3y}\rangle, |f_{az}\rangle$

Table 7: (p,f) block.

| No. | multipole | matrix |
|-----|----------------------|--|
| 71 | symmetry | $-\frac{x^2}{2} - \frac{y^2}{2} + z^2$ |
| | $Q_2^{(a)}(A)$ | $\begin{bmatrix} 0 & 0 & 0 & 0 & \frac{\sqrt{7}}{7} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{7}}{7} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{42}}{14} \end{bmatrix}$ |
| 72 | symmetry | $\sqrt{3}yz$ |
| | $Q_{2,1}^{(a)}(E_1)$ | $\begin{bmatrix} 0 & 0 & 0 & \frac{\sqrt{210}}{42} & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{210}}{42} & 0 & 0 & 0 & -\frac{\sqrt{14}}{14} \\ 0 & 0 & 0 & 0 & 0 & \frac{2\sqrt{21}}{21} & 0 \end{bmatrix}$ |
| 73 | symmetry | $-\sqrt{3}xz$ |
| | $Q_{2,2}^{(a)}(E_1)$ | $\begin{bmatrix} 0 & 0 & -\frac{\sqrt{210}}{42} & 0 & 0 & 0 & \frac{\sqrt{14}}{14} \\ 0 & 0 & 0 & -\frac{\sqrt{210}}{42} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{2\sqrt{21}}{21} & 0 & 0 \end{bmatrix}$ |
| 74 | symmetry | $\frac{\sqrt{3}(x-y)(x+y)}{2}$ |
| | $Q_{2,1}^{(a)}(E_2)$ | $\begin{bmatrix} \frac{\sqrt{35}}{14} & 0 & 0 & 0 & -\frac{\sqrt{21}}{42} & 0 & 0 \\ 0 & \frac{\sqrt{35}}{14} & 0 & 0 & 0 & \frac{\sqrt{21}}{42} & 0 \\ 0 & 0 & \frac{\sqrt{210}}{42} & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| 75 | symmetry | $-\sqrt{3}xy$ |

continued ...

Table 7

| No. | multipole | matrix |
|-----|----------------------------------|---|
| | $\mathbb{Q}_{2,2}^{(a)}(E_2)$ | $\begin{bmatrix} 0 & -\frac{\sqrt{35}}{14} & 0 & 0 & 0 & \frac{\sqrt{21}}{42} & 0 \\ \frac{\sqrt{35}}{14} & 0 & 0 & 0 & 0 & \frac{\sqrt{21}}{42} & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{210}}{42} & 0 & 0 & 0 \end{bmatrix}$ |
| 76 | symmetry | $\frac{3x^4}{8} + \frac{3x^2y^2}{4} - 3x^2z^2 + \frac{3y^4}{8} - 3y^2z^2 + z^4$ |
| | $\mathbb{Q}_4^{(a)}(A)$ | $\begin{bmatrix} 0 & 0 & 0 & 0 & -\frac{\sqrt{21}}{14} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{21}}{14} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{14}}{7} \end{bmatrix}$ |
| 77 | symmetry | $\frac{\sqrt{70}xz(x^2-3y^2)}{4}$ |
| | $\mathbb{Q}_4^{(a)}(B, 1)$ | $\begin{bmatrix} 0 & 0 & \frac{\sqrt{3}}{4} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{3}}{4} & 0 & 0 & 0 \\ \frac{\sqrt{2}}{4} & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| 78 | symmetry | $\frac{\sqrt{70}yz(3x^2-y^2)}{4}$ |
| | $\mathbb{Q}_4^{(a)}(B, 2)$ | $\begin{bmatrix} 0 & 0 & 0 & \frac{\sqrt{3}}{4} & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{3}}{4} & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{2}}{4} & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| 79 | symmetry | $-\frac{\sqrt{10}yz(3x^2+3y^2-4z^2)}{4}$ |
| | $\mathbb{Q}_{4,1}^{(a)}(E_1)$ | $\begin{bmatrix} 0 & 0 & 0 & -\frac{\sqrt{21}}{28} & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{21}}{28} & 0 & 0 & 0 & \frac{\sqrt{35}}{14} \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{210}}{28} & 0 \end{bmatrix}$ |
| 80 | symmetry | $\frac{\sqrt{10}xz(3x^2+3y^2-4z^2)}{4}$ |
| | $\mathbb{Q}_{4,2}^{(a)}(E_1)$ | $\begin{bmatrix} 0 & 0 & \frac{\sqrt{21}}{28} & 0 & 0 & 0 & -\frac{\sqrt{35}}{14} \\ 0 & 0 & 0 & \frac{\sqrt{21}}{28} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{210}}{28} & 0 & 0 \end{bmatrix}$ |
| 81 | symmetry | $\frac{\sqrt{35}(x^2-2xy-y^2)(x^2+2xy-y^2)}{8}$ |
| | $\mathbb{Q}_{4,1}^{(a)}(E_2, 1)$ | $\begin{bmatrix} \frac{1}{2} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{1}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| 82 | symmetry | $\frac{\sqrt{35}xy(x-y)(x+y)}{2}$ |

continued ...

Table 7

| No. | multipole | matrix |
|-----|----------------------------------|--|
| | $\mathbb{Q}_{4,2}^{(a)}(E_2, 1)$ | $\begin{bmatrix} 0 & \frac{1}{2} & 0 & 0 & 0 & 0 & 0 \\ \frac{1}{2} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| 83 | symmetry | $-\frac{\sqrt{5}(x-y)(x+y)(x^2+y^2-6z^2)}{4}$ |
| | $\mathbb{Q}_{4,1}^{(a)}(E_2, 2)$ | $\begin{bmatrix} -\frac{\sqrt{7}}{28} & 0 & 0 & 0 & \frac{\sqrt{105}}{28} & 0 & 0 \\ 0 & -\frac{\sqrt{7}}{28} & 0 & 0 & 0 & -\frac{\sqrt{105}}{28} & 0 \\ 0 & 0 & \frac{\sqrt{42}}{14} & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| 84 | symmetry | $\frac{\sqrt{5}xy(x^2+y^2-6z^2)}{2}$ |
| | $\mathbb{Q}_{4,2}^{(a)}(E_2, 2)$ | $\begin{bmatrix} 0 & \frac{\sqrt{7}}{28} & 0 & 0 & 0 & -\frac{\sqrt{105}}{28} & 0 \\ -\frac{\sqrt{7}}{28} & 0 & 0 & 0 & -\frac{\sqrt{105}}{28} & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{42}}{14} & 0 & 0 & 0 \end{bmatrix}$ |
| 85 | symmetry | $-\frac{z(3x^2+3y^2-2z^2)}{2}$ |
| | $\mathbb{G}_3^{(a)}(A)$ | $\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & 0 & -\frac{1}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| 86 | symmetry | $\frac{\sqrt{10}y(3x^2-y^2)}{4}$ |
| | $\mathbb{G}_3^{(a)}(B, 1)$ | $\begin{bmatrix} 0 & 0 & -\frac{1}{4} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{4} & 0 & 0 & 0 \\ \frac{\sqrt{6}}{4} & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| 87 | symmetry | $\frac{\sqrt{10}x(x^2-3y^2)}{4}$ |
| | $\mathbb{G}_3^{(a)}(B, 2)$ | $\begin{bmatrix} 0 & 0 & 0 & \frac{1}{4} & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{4} & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{6}}{4} & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| 88 | symmetry | $-\frac{\sqrt{6}x(x^2+y^2-4z^2)}{4}$ |
| | $\mathbb{G}_{3,1}^{(a)}(E_1)$ | $\begin{bmatrix} 0 & 0 & 0 & \frac{\sqrt{15}}{12} & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{15}}{12} & 0 & 0 & 0 & \frac{1}{2} \\ 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{6}}{12} & 0 \end{bmatrix}$ |
| 89 | symmetry | $-\frac{\sqrt{6}y(x^2+y^2-4z^2)}{4}$ |

continued ...

Table 7

| No. | multipole | matrix |
|-----|-------------------------------|---|
| | $\mathbb{G}_{3,2}^{(a)}(E_1)$ | $\begin{bmatrix} 0 & 0 & -\frac{\sqrt{15}}{12} & 0 & 0 & 0 & -\frac{1}{2} \\ 0 & 0 & 0 & -\frac{\sqrt{15}}{12} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{6}}{12} & 0 & 0 \end{bmatrix}$ |
| 90 | symmetry | $\sqrt{15}xyz$ |
| | $\mathbb{G}_{3,1}^{(a)}(E_2)$ | $\begin{bmatrix} -\frac{1}{4} & 0 & 0 & 0 & -\frac{\sqrt{15}}{12} & 0 & 0 \\ 0 & -\frac{1}{4} & 0 & 0 & 0 & \frac{\sqrt{15}}{12} & 0 \\ 0 & 0 & \frac{\sqrt{6}}{6} & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| 91 | symmetry | $\frac{\sqrt{15}z(x-y)(x+y)}{2}$ |
| | $\mathbb{G}_{3,2}^{(a)}(E_2)$ | $\begin{bmatrix} 0 & \frac{1}{4} & 0 & 0 & 0 & \frac{\sqrt{15}}{12} & 0 \\ -\frac{1}{4} & 0 & 0 & 0 & \frac{\sqrt{15}}{12} & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{6}}{6} & 0 & 0 & 0 \end{bmatrix}$ |
| 92 | symmetry | $-\frac{x^2}{2} - \frac{y^2}{2} + z^2$ |
| | $\mathbb{T}_2^{(a)}(A)$ | $\begin{bmatrix} 0 & 0 & 0 & 0 & \frac{\sqrt{7}i}{7} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{7}i}{7} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{42}i}{14} \end{bmatrix}$ |
| 93 | symmetry | $\sqrt{3}yz$ |
| | $\mathbb{T}_{2,1}^{(a)}(E_1)$ | $\begin{bmatrix} 0 & 0 & 0 & \frac{\sqrt{210}i}{42} & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{210}i}{42} & 0 & 0 & 0 & -\frac{\sqrt{14}i}{14} \\ 0 & 0 & 0 & 0 & 0 & \frac{2\sqrt{21}i}{21} & 0 \end{bmatrix}$ |
| 94 | symmetry | $-\sqrt{3}xz$ |
| | $\mathbb{T}_{2,2}^{(a)}(E_1)$ | $\begin{bmatrix} 0 & 0 & -\frac{\sqrt{210}i}{42} & 0 & 0 & 0 & \frac{\sqrt{14}i}{14} \\ 0 & 0 & 0 & -\frac{\sqrt{210}i}{42} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{2\sqrt{21}i}{21} & 0 & 0 \end{bmatrix}$ |
| 95 | symmetry | $\frac{\sqrt{3}(x-y)(x+y)}{2}$ |
| | $\mathbb{T}_{2,1}^{(a)}(E_2)$ | $\begin{bmatrix} \frac{\sqrt{35}i}{14} & 0 & 0 & 0 & -\frac{\sqrt{21}i}{42} & 0 & 0 \\ 0 & \frac{\sqrt{35}i}{14} & 0 & 0 & 0 & \frac{\sqrt{21}i}{42} & 0 \\ 0 & 0 & \frac{\sqrt{210}i}{42} & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| 96 | symmetry | $-\sqrt{3}xy$ |

continued ...

Table 7

| No. | multipole | matrix |
|-----|----------------------------------|--|
| | $\mathbb{T}_{2,2}^{(a)}(E_2)$ | $\begin{bmatrix} 0 & -\frac{\sqrt{35}i}{14} & 0 & 0 & 0 & \frac{\sqrt{21}i}{42} & 0 \\ \frac{\sqrt{35}i}{14} & 0 & 0 & 0 & \frac{\sqrt{21}i}{42} & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{210}i}{42} & 0 & 0 & 0 \end{bmatrix}$ |
| 97 | symmetry | $\frac{3x^4}{8} + \frac{3x^2y^2}{4} - 3x^2z^2 + \frac{3y^4}{8} - 3y^2z^2 + z^4$ |
| | $\mathbb{T}_4^{(a)}(A)$ | $\begin{bmatrix} 0 & 0 & 0 & 0 & -\frac{\sqrt{21}i}{14} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{21}i}{14} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{14}i}{7} \end{bmatrix}$ |
| 98 | symmetry | $\frac{\sqrt{70}xz(x^2-3y^2)}{4}$ |
| | $\mathbb{T}_4^{(a)}(B, 1)$ | $\begin{bmatrix} 0 & 0 & \frac{\sqrt{3}i}{4} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{3}i}{4} & 0 & 0 & 0 \\ \frac{\sqrt{2}i}{4} & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| 99 | symmetry | $\frac{\sqrt{70}yz(3x^2-y^2)}{4}$ |
| | $\mathbb{T}_4^{(a)}(B, 2)$ | $\begin{bmatrix} 0 & 0 & 0 & \frac{\sqrt{3}i}{4} & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{3}i}{4} & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{2}i}{4} & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| 100 | symmetry | $-\frac{\sqrt{10}yz(3x^2+3y^2-4z^2)}{4}$ |
| | $\mathbb{T}_{4,1}^{(a)}(E_1)$ | $\begin{bmatrix} 0 & 0 & 0 & -\frac{\sqrt{21}i}{28} & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{21}i}{28} & 0 & 0 & 0 & \frac{\sqrt{35}i}{14} \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{210}i}{28} & 0 \end{bmatrix}$ |
| 101 | symmetry | $\frac{\sqrt{10}xz(3x^2+3y^2-4z^2)}{4}$ |
| | $\mathbb{T}_{4,2}^{(a)}(E_1)$ | $\begin{bmatrix} 0 & 0 & \frac{\sqrt{21}i}{28} & 0 & 0 & 0 & -\frac{\sqrt{35}i}{14} \\ 0 & 0 & 0 & \frac{\sqrt{21}i}{28} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{210}i}{28} & 0 & 0 \end{bmatrix}$ |
| 102 | symmetry | $\frac{\sqrt{35}(x^2-2xy-y^2)(x^2+2xy-y^2)}{8}$ |
| | $\mathbb{T}_{4,1}^{(a)}(E_2, 1)$ | $\begin{bmatrix} \frac{i}{2} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{i}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| 103 | symmetry | $\frac{\sqrt{35}xy(x-y)(x+y)}{2}$ |

continued ...

Table 7

| No. | multipole | matrix |
|-----|----------------------------------|---|
| | $\mathbb{T}_{4,2}^{(a)}(E_2, 1)$ | $\begin{bmatrix} 0 & \frac{i}{2} & 0 & 0 & 0 & 0 & 0 \\ \frac{i}{2} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| 104 | symmetry | $-\frac{\sqrt{5}(x-y)(x+y)(x^2+y^2-6z^2)}{4}$ |
| | $\mathbb{T}_{4,1}^{(a)}(E_2, 2)$ | $\begin{bmatrix} -\frac{\sqrt{7}i}{28} & 0 & 0 & 0 & \frac{\sqrt{105}i}{28} & 0 & 0 \\ 0 & -\frac{\sqrt{7}i}{28} & 0 & 0 & 0 & -\frac{\sqrt{105}i}{28} & 0 \\ 0 & 0 & \frac{\sqrt{42}i}{14} & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| 105 | symmetry | $\frac{\sqrt{5}xy(x^2+y^2-6z^2)}{2}$ |
| | $\mathbb{T}_{4,2}^{(a)}(E_2, 2)$ | $\begin{bmatrix} 0 & \frac{\sqrt{7}i}{28} & 0 & 0 & 0 & -\frac{\sqrt{105}i}{28} & 0 \\ -\frac{\sqrt{7}i}{28} & 0 & 0 & 0 & -\frac{\sqrt{105}i}{28} & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{42}i}{14} & 0 & 0 & 0 \end{bmatrix}$ |
| 106 | symmetry | $-\frac{z(3x^2+3y^2-2z^2)}{2}$ |
| | $\mathbb{M}_3^{(a)}(A)$ | $\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & -\frac{i}{2} & 0 \\ 0 & 0 & 0 & 0 & \frac{i}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| 107 | symmetry | $\frac{\sqrt{10}y(3x^2-y^2)}{4}$ |
| | $\mathbb{M}_3^{(a)}(B, 1)$ | $\begin{bmatrix} 0 & 0 & \frac{i}{4} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{i}{4} & 0 & 0 & 0 \\ -\frac{\sqrt{6}i}{4} & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| 108 | symmetry | $\frac{\sqrt{10}x(x^2-3y^2)}{4}$ |
| | $\mathbb{M}_3^{(a)}(B, 2)$ | $\begin{bmatrix} 0 & 0 & 0 & -\frac{i}{4} & 0 & 0 & 0 \\ 0 & 0 & -\frac{i}{4} & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{6}i}{4} & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| 109 | symmetry | $-\frac{\sqrt{6}x(x^2+y^2-4z^2)}{4}$ |
| | $\mathbb{M}_{3,1}^{(a)}(E_1)$ | $\begin{bmatrix} 0 & 0 & 0 & -\frac{\sqrt{15}i}{12} & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{15}i}{12} & 0 & 0 & 0 & -\frac{i}{2} \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{6}i}{12} & 0 \end{bmatrix}$ |
| 110 | symmetry | $-\frac{\sqrt{6}y(x^2+y^2-4z^2)}{4}$ |

continued ...

Table 7

| No. | multipole | matrix |
|-----|-------------------------------|--|
| | $\mathbb{M}_{3,2}^{(a)}(E_1)$ | $\begin{bmatrix} 0 & 0 & \frac{\sqrt{15}i}{12} & 0 & 0 & 0 & \frac{i}{2} \\ 0 & 0 & 0 & \frac{\sqrt{15}i}{12} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{6}i}{12} & 0 & 0 \end{bmatrix}$ |
| 111 | symmetry | $\sqrt{15}xyz$ |
| | $\mathbb{M}_{3,1}^{(a)}(E_2)$ | $\begin{bmatrix} \frac{i}{4} & 0 & 0 & 0 & \frac{\sqrt{15}i}{12} & 0 & 0 \\ 0 & \frac{i}{4} & 0 & 0 & 0 & -\frac{\sqrt{15}i}{12} & 0 \\ 0 & 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| 112 | symmetry | $\frac{\sqrt{15}z(x-y)(x+y)}{2}$ |
| | $\mathbb{M}_{3,2}^{(a)}(E_2)$ | $\begin{bmatrix} 0 & -\frac{i}{4} & 0 & 0 & 0 & -\frac{\sqrt{15}i}{12} & 0 \\ \frac{i}{4} & 0 & 0 & 0 & -\frac{\sqrt{15}i}{12} & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{6}i}{6} & 0 & 0 & 0 \end{bmatrix}$ |

bra: = $\langle d_v |, \langle d_{xy} |, \langle d_{xz} |, \langle d_{yz} |, \langle d_u |$
ket: = $|d_v\rangle, |d_{xy}\rangle, |d_{xz}\rangle, |d_{yz}\rangle, |d_u\rangle$

Table 8: (d,d) block.

| No. | multipole | matrix |
|-----|-------------------------|--|
| 113 | symmetry | 1 |
| | $\mathbb{Q}_0^{(a)}(A)$ | $\begin{bmatrix} \frac{\sqrt{5}}{5} & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{5}}{5} & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{5}}{5} & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{5}}{5} & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{5}}{5} \end{bmatrix}$ |
| 114 | symmetry | $-\frac{x^2}{2} - \frac{y^2}{2} + z^2$ |

continued ...

Table 8

| No. | multipole | matrix |
|-----|-------------------------------|---|
| | $\mathbb{Q}_2^{(a)}(A)$ | $\begin{bmatrix} -\frac{\sqrt{14}}{7} & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{14}}{7} & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{14}}{14} & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{14}}{14} & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{14}}{7} \end{bmatrix}$ |
| 115 | symmetry | $\sqrt{3}yz$ |
| | $\mathbb{Q}_{2,1}^{(a)}(E_1)$ | $\begin{bmatrix} 0 & 0 & 0 & -\frac{\sqrt{42}}{14} & 0 \\ 0 & 0 & \frac{\sqrt{42}}{14} & 0 & 0 \\ 0 & \frac{\sqrt{42}}{14} & 0 & 0 & 0 \\ -\frac{\sqrt{42}}{14} & 0 & 0 & 0 & \frac{\sqrt{14}}{14} \\ 0 & 0 & 0 & \frac{\sqrt{14}}{14} & 0 \end{bmatrix}$ |
| 116 | symmetry | $-\sqrt{3}xz$ |
| | $\mathbb{Q}_{2,2}^{(a)}(E_1)$ | $\begin{bmatrix} 0 & 0 & -\frac{\sqrt{42}}{14} & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{42}}{14} & 0 \\ -\frac{\sqrt{42}}{14} & 0 & 0 & 0 & -\frac{\sqrt{14}}{14} \\ 0 & -\frac{\sqrt{42}}{14} & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{14}}{14} & 0 & 0 \end{bmatrix}$ |
| 117 | symmetry | $\frac{\sqrt{3}(x-y)(x+y)}{2}$ |
| | $\mathbb{Q}_{2,1}^{(a)}(E_2)$ | $\begin{bmatrix} 0 & 0 & 0 & 0 & -\frac{\sqrt{14}}{7} \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{42}}{14} & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{42}}{14} & 0 \\ -\frac{\sqrt{14}}{7} & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| 118 | symmetry | $-\sqrt{3}xy$ |

continued ...

Table 8

| No. | multipole | matrix |
|-----|-------------------------------|---|
| | $\mathbb{Q}_{2,2}^{(a)}(E_2)$ | $\begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{14}}{7} \\ 0 & 0 & 0 & -\frac{\sqrt{42}}{14} & 0 \\ 0 & 0 & -\frac{\sqrt{42}}{14} & 0 & 0 \\ 0 & \frac{\sqrt{14}}{7} & 0 & 0 & 0 \end{bmatrix}$ |
| 119 | symmetry | $\frac{3x^4}{8} + \frac{3x^2y^2}{4} - 3x^2z^2 + \frac{3y^4}{8} - 3y^2z^2 + z^4$ |
| | $\mathbb{Q}_4^{(a)}(A)$ | $\begin{bmatrix} \frac{\sqrt{70}}{70} & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{70}}{70} & 0 & 0 & 0 \\ 0 & 0 & -\frac{2\sqrt{70}}{35} & 0 & 0 \\ 0 & 0 & 0 & -\frac{2\sqrt{70}}{35} & 0 \\ 0 & 0 & 0 & 0 & \frac{3\sqrt{70}}{35} \end{bmatrix}$ |
| 120 | symmetry | $\frac{\sqrt{70}xz(x^2-3y^2)}{4}$ |
| | $\mathbb{Q}_4^{(a)}(B, 1)$ | $\begin{bmatrix} 0 & 0 & \frac{1}{2} & 0 & 0 \\ 0 & 0 & 0 & -\frac{1}{2} & 0 \\ \frac{1}{2} & 0 & 0 & 0 & 0 \\ 0 & -\frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| 121 | symmetry | $\frac{\sqrt{70}yz(3x^2-y^2)}{4}$ |
| | $\mathbb{Q}_4^{(a)}(B, 2)$ | $\begin{bmatrix} 0 & 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & \frac{1}{2} & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 & 0 \\ \frac{1}{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| 122 | symmetry | $-\frac{\sqrt{10}yz(3x^2+3y^2-4z^2)}{4}$ |

continued ...

Table 8

| No. | multipole | matrix |
|-----|----------------------------------|---|
| | $\mathbb{Q}_{4,1}^{(a)}(E_1)$ | $\begin{bmatrix} 0 & 0 & 0 & \frac{\sqrt{7}}{14} & 0 \\ 0 & 0 & -\frac{\sqrt{7}}{14} & 0 & 0 \\ 0 & -\frac{\sqrt{7}}{14} & 0 & 0 & 0 \\ \frac{\sqrt{7}}{14} & 0 & 0 & 0 & \frac{\sqrt{21}}{7} \\ 0 & 0 & 0 & \frac{\sqrt{21}}{7} & 0 \end{bmatrix}$ |
| 123 | symmetry | $\frac{\sqrt{10}xz(3x^2+3y^2-4z^2)}{4}$ |
| | $\mathbb{Q}_{4,2}^{(a)}(E_1)$ | $\begin{bmatrix} 0 & 0 & \frac{\sqrt{7}}{14} & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{7}}{14} & 0 \\ \frac{\sqrt{7}}{14} & 0 & 0 & 0 & -\frac{\sqrt{21}}{7} \\ 0 & \frac{\sqrt{7}}{14} & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{21}}{7} & 0 & 0 \end{bmatrix}$ |
| 124 | symmetry | $\frac{\sqrt{35}(x^2-2xy-y^2)(x^2+2xy-y^2)}{8}$ |
| | $\mathbb{Q}_{4,1}^{(a)}(E_2, 1)$ | $\begin{bmatrix} \frac{\sqrt{2}}{2} & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{2}}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| 125 | symmetry | $\frac{\sqrt{35}xy(x-y)(x+y)}{2}$ |
| | $\mathbb{Q}_{4,2}^{(a)}(E_2, 1)$ | $\begin{bmatrix} 0 & \frac{\sqrt{2}}{2} & 0 & 0 & 0 \\ \frac{\sqrt{2}}{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| 126 | symmetry | $-\frac{\sqrt{5}(x-y)(x+y)(x^2+y^2-6z^2)}{4}$ |

continued ...

Table 8

| No. | multipole | matrix |
|-----|----------------------------------|--|
| | $\mathbb{Q}_{4,1}^{(a)}(E_2, 2)$ | $\begin{bmatrix} 0 & 0 & 0 & 0 & \frac{\sqrt{42}}{14} \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{14}}{7} & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{14}}{7} & 0 \\ \frac{\sqrt{42}}{14} & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| 127 | symmetry | $\frac{\sqrt{5}xy(x^2+y^2-6z^2)}{2}$ |
| | $\mathbb{Q}_{4,2}^{(a)}(E_2, 2)$ | $\begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{42}}{14} \\ 0 & 0 & 0 & -\frac{\sqrt{14}}{7} & 0 \\ 0 & 0 & -\frac{\sqrt{14}}{7} & 0 & 0 \\ 0 & -\frac{\sqrt{42}}{14} & 0 & 0 & 0 \end{bmatrix}$ |
| 128 | symmetry | z |
| | $\mathbb{M}_1^{(a)}(A)$ | $\begin{bmatrix} 0 & -\frac{\sqrt{10}i}{5} & 0 & 0 & 0 \\ \frac{\sqrt{10}i}{5} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{10}i}{10} & 0 \\ 0 & 0 & \frac{\sqrt{10}i}{10} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| 129 | symmetry | x |
| | $\mathbb{M}_{1,1}^{(a)}(E_1)$ | $\begin{bmatrix} 0 & 0 & 0 & \frac{\sqrt{10}i}{10} & 0 \\ 0 & 0 & -\frac{\sqrt{10}i}{10} & 0 & 0 \\ 0 & \frac{\sqrt{10}i}{10} & 0 & 0 & 0 \\ -\frac{\sqrt{10}i}{10} & 0 & 0 & 0 & -\frac{\sqrt{30}i}{10} \\ 0 & 0 & 0 & \frac{\sqrt{30}i}{10} & 0 \end{bmatrix}$ |
| 130 | symmetry | y |

continued ...

Table 8

| No. | multipole | matrix |
|-----|----------------------|--|
| | $M_{1,2}^{(a)}(E_1)$ | $\begin{bmatrix} 0 & 0 & \frac{\sqrt{10}i}{10} & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{10}i}{10} & 0 \\ -\frac{\sqrt{10}i}{10} & 0 & 0 & 0 & \frac{\sqrt{30}i}{10} \\ 0 & -\frac{\sqrt{10}i}{10} & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{30}i}{10} & 0 & 0 \end{bmatrix}$ |
| 131 | symmetry | $\frac{z(3x^2+3y^2-2z^2)}{2}$ |
| | $M_3^{(a)}(A)$ | $\begin{bmatrix} 0 & \frac{\sqrt{10}i}{10} & 0 & 0 & 0 \\ -\frac{\sqrt{10}i}{10} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{10}i}{5} & 0 \\ 0 & 0 & \frac{\sqrt{10}i}{5} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| 132 | symmetry | $\frac{\sqrt{10}y(3x^2-y^2)}{4}$ |
| | $M_3^{(a)}(B, 1)$ | $\begin{bmatrix} 0 & 0 & \frac{i}{2} & 0 & 0 \\ 0 & 0 & 0 & -\frac{i}{2} & 0 \\ -\frac{i}{2} & 0 & 0 & 0 & 0 \\ 0 & \frac{i}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| 133 | symmetry | $\frac{\sqrt{10}x(x^2-3y^2)}{4}$ |
| | $M_3^{(a)}(B, 2)$ | $\begin{bmatrix} 0 & 0 & 0 & -\frac{i}{2} & 0 \\ 0 & 0 & -\frac{i}{2} & 0 & 0 \\ 0 & \frac{i}{2} & 0 & 0 & 0 \\ \frac{i}{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| 134 | symmetry | $-\frac{\sqrt{6}x(x^2+y^2-4z^2)}{4}$ |

continued ...

Table 8

| No. | multipole | matrix |
|-----|-------------------------------|--|
| | $\mathbb{M}_{3,1}^{(a)}(E_1)$ | $\begin{bmatrix} 0 & 0 & 0 & -\frac{\sqrt{15}i}{10} & 0 \\ 0 & 0 & \frac{\sqrt{15}i}{10} & 0 & 0 \\ 0 & -\frac{\sqrt{15}i}{10} & 0 & 0 & 0 \\ \frac{\sqrt{15}i}{10} & 0 & 0 & 0 & -\frac{\sqrt{5}i}{5} \\ 0 & 0 & 0 & \frac{\sqrt{5}i}{5} & 0 \end{bmatrix}$ |
| 135 | symmetry | $-\frac{\sqrt{6}y(x^2+y^2-4z^2)}{4}$ |
| | $\mathbb{M}_{3,2}^{(a)}(E_1)$ | $\begin{bmatrix} 0 & 0 & -\frac{\sqrt{15}i}{10} & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{15}i}{10} & 0 \\ \frac{\sqrt{15}i}{10} & 0 & 0 & 0 & \frac{\sqrt{5}i}{5} \\ 0 & \frac{\sqrt{15}i}{10} & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{5}i}{5} & 0 & 0 \end{bmatrix}$ |
| 136 | symmetry | $\sqrt{15}xyz$ |
| | $\mathbb{M}_{3,1}^{(a)}(E_2)$ | $\begin{bmatrix} 0 & 0 & 0 & 0 & \frac{\sqrt{2}i}{2} \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ -\frac{\sqrt{2}i}{2} & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| 137 | symmetry | $\frac{\sqrt{15}z(x-y)(x+y)}{2}$ |
| | $\mathbb{M}_{3,2}^{(a)}(E_2)$ | $\begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{2}i}{2} \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{2}i}{2} & 0 & 0 & 0 \end{bmatrix}$ |

bra: = $\langle d_v |, \langle d_{xy} |, \langle d_{xz} |, \langle d_{yz} |, \langle d_u |$

ket: = $|f_2\rangle, |f_1\rangle, |f_{bz}\rangle, |f_3\rangle, |f_{3x}\rangle, |f_{3y}\rangle, |f_{az}\rangle$

Table 9: (d,f) block.

| No. | multipole | matrix |
|-----|----------------------|---|
| 138 | symmetry | z |
| | $Q_1^{(a)}(A)$ | $\begin{bmatrix} 0 & 0 & \frac{\sqrt{14}}{14} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{14}}{14} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{2\sqrt{35}}{35} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{2\sqrt{35}}{35} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{3\sqrt{70}}{70} \end{bmatrix}$ |
| 139 | symmetry | x |
| | $Q_{1,1}^{(a)}(E_1)$ | $\begin{bmatrix} \frac{\sqrt{21}}{14} & 0 & 0 & 0 & -\frac{\sqrt{35}}{70} & 0 & 0 \\ 0 & \frac{\sqrt{21}}{14} & 0 & 0 & 0 & -\frac{\sqrt{35}}{70} & 0 \\ 0 & 0 & \frac{\sqrt{14}}{14} & 0 & 0 & 0 & -\frac{\sqrt{210}}{70} \\ 0 & 0 & 0 & \frac{\sqrt{14}}{14} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{105}}{35} & 0 & 0 \end{bmatrix}$ |
| 140 | symmetry | y |
| | $Q_{1,2}^{(a)}(E_1)$ | $\begin{bmatrix} 0 & \frac{\sqrt{21}}{14} & 0 & 0 & 0 & \frac{\sqrt{35}}{70} & 0 \\ -\frac{\sqrt{21}}{14} & 0 & 0 & 0 & -\frac{\sqrt{35}}{70} & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{14}}{14} & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{14}}{14} & 0 & 0 & 0 & -\frac{\sqrt{210}}{70} \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{105}}{35} & 0 \end{bmatrix}$ |
| 141 | symmetry | $-\frac{z(3x^2+3y^2-2z^2)}{2}$ |
| | $Q_3^{(a)}(A)$ | $\begin{bmatrix} 0 & 0 & -\frac{\sqrt{6}}{6} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{6}}{6} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{15}}{30} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{15}}{30} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{30}}{15} \end{bmatrix}$ |
| 142 | symmetry | $\frac{\sqrt{10}y(3x^2-y^2)}{4}$ |

continued ...

Table 9

| No. | multipole | matrix |
|-----|----------------------|--|
| | $Q_3^{(a)}(B, 1)$ | $\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{6}}{12} & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{6}}{12} & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{15}}{12} & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{15}}{12} & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{30}}{12} & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| 143 | symmetry | $\frac{\sqrt{10}x(x^2-3y^2)}{4}$ |
| | $Q_3^{(a)}(B, 2)$ | $\begin{bmatrix} 0 & 0 & 0 & 0 & -\frac{\sqrt{6}}{12} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{6}}{12} & 0 \\ 0 & 0 & \frac{\sqrt{15}}{12} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{15}}{12} & 0 & 0 & 0 \\ -\frac{\sqrt{30}}{12} & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| 144 | symmetry | $-\frac{\sqrt{6}x(x^2+y^2-4z^2)}{4}$ |
| | $Q_{3,1}^{(a)}(E_1)$ | $\begin{bmatrix} -\frac{\sqrt{6}}{12} & 0 & 0 & 0 & \frac{\sqrt{10}}{10} & 0 & 0 \\ 0 & -\frac{\sqrt{6}}{12} & 0 & 0 & 0 & \frac{\sqrt{10}}{10} & 0 \\ 0 & 0 & \frac{1}{4} & 0 & 0 & 0 & \frac{\sqrt{15}}{30} \\ 0 & 0 & 0 & \frac{1}{4} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{30}}{20} & 0 & 0 \end{bmatrix}$ |
| 145 | symmetry | $-\frac{\sqrt{6}y(x^2+y^2-4z^2)}{4}$ |
| | $Q_{3,2}^{(a)}(E_1)$ | $\begin{bmatrix} 0 & -\frac{\sqrt{6}}{12} & 0 & 0 & 0 & -\frac{\sqrt{10}}{10} & 0 \\ \frac{\sqrt{6}}{12} & 0 & 0 & 0 & \frac{\sqrt{10}}{10} & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{4} & 0 & 0 & 0 \\ 0 & 0 & -\frac{1}{4} & 0 & 0 & 0 & \frac{\sqrt{15}}{30} \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{30}}{20} & 0 \end{bmatrix}$ |
| 146 | symmetry | $\sqrt{15}xyz$ |

continued ...

Table 9

| No. | multipole | matrix |
|-----|-------------------------------|---|
| | $\mathbb{Q}_{3,1}^{(a)}(E_2)$ | $\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{6}}{6} \\ 0 & \frac{\sqrt{15}}{12} & 0 & 0 & 0 & \frac{1}{4} & 0 \\ -\frac{\sqrt{15}}{12} & 0 & 0 & 0 & \frac{1}{4} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| 147 | symmetry | $\frac{\sqrt{15}z(x-y)(x+y)}{2}$ |
| | $\mathbb{Q}_{3,2}^{(a)}(E_2)$ | $\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{6}}{6} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{\sqrt{15}}{12} & 0 & 0 & 0 & \frac{1}{4} & 0 & 0 \\ 0 & \frac{\sqrt{15}}{12} & 0 & 0 & 0 & -\frac{1}{4} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| 148 | symmetry | $\frac{z(15x^4+30x^2y^2-40x^2z^2+15y^4-40y^2z^2+8z^4)}{8}$ |
| | $\mathbb{Q}_5^{(a)}(A)$ | $\begin{bmatrix} 0 & 0 & \frac{\sqrt{21}}{42} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{21}}{42} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{210}}{42} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{210}}{42} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{105}}{21} \end{bmatrix}$ |
| 149 | symmetry | $-\frac{\sqrt{70}y(3x^2-y^2)(x^2+y^2-8z^2)}{16}$ |
| | $\mathbb{Q}_5^{(a)}(B, 1)$ | $\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{3}}{6} & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{3}}{6} & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{30}}{15} & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{30}}{15} & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{15}}{15} & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| 150 | symmetry | $-\frac{\sqrt{70}x(x^2-3y^2)(x^2+y^2-8z^2)}{16}$ |

continued ...

Table 9

| No. | multipole | matrix |
|-----|-------------------------|--|
| | $Q_5^{(a)}(B, 2)$ | $\begin{bmatrix} 0 & 0 & 0 & 0 & \frac{\sqrt{3}}{6} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{3}}{6} & 0 \\ 0 & 0 & \frac{\sqrt{30}}{15} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{30}}{15} & 0 & 0 & 0 \\ \frac{\sqrt{15}}{15} & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| 151 | symmetry | $\frac{3\sqrt{14}x(x^4-10x^2y^2+5y^4)}{16}$ |
| | $Q_{5,1}^{(a)}(E_1, 1)$ | $\begin{bmatrix} \frac{1}{2} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{1}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| 152 | symmetry | $-\frac{3\sqrt{14}y(5x^4-10x^2y^2+y^4)}{16}$ |
| | $Q_{5,2}^{(a)}(E_1, 1)$ | $\begin{bmatrix} 0 & -\frac{1}{2} & 0 & 0 & 0 & 0 & 0 \\ -\frac{1}{2} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| 153 | symmetry | $\frac{\sqrt{15}x(x^4+2x^2y^2-12x^2z^2+y^4-12y^2z^2+8z^4)}{8}$ |
| | $Q_{5,1}^{(a)}(E_1, 2)$ | $\begin{bmatrix} \frac{\sqrt{210}}{420} & 0 & 0 & 0 & -\frac{\sqrt{14}}{28} & 0 & 0 \\ 0 & \frac{\sqrt{210}}{420} & 0 & 0 & 0 & -\frac{\sqrt{14}}{28} & 0 \\ 0 & 0 & -\frac{\sqrt{35}}{35} & 0 & 0 & 0 & \frac{2\sqrt{21}}{21} \\ 0 & 0 & 0 & -\frac{\sqrt{35}}{35} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{42}}{14} & 0 & 0 \end{bmatrix}$ |
| 154 | symmetry | $\frac{\sqrt{15}y(x^4+2x^2y^2-12x^2z^2+y^4-12y^2z^2+8z^4)}{8}$ |

continued ...

Table 9

| No. | multipole | matrix |
|-----|-------------------------|---|
| | $Q_{5,2}^{(a)}(E_1, 2)$ | $\begin{bmatrix} 0 & \frac{\sqrt{210}}{420} & 0 & 0 & 0 & \frac{\sqrt{14}}{28} & 0 \\ -\frac{\sqrt{210}}{420} & 0 & 0 & 0 & -\frac{\sqrt{14}}{28} & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{35}}{35} & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{35}}{35} & 0 & 0 & 0 & \frac{2\sqrt{21}}{21} \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{42}}{14} & 0 \end{bmatrix}$ |
| 155 | symmetry | $-\frac{3\sqrt{35}xyz(x-y)(x+y)}{2}$ |
| | $Q_{5,1}^{(a)}(E_2, 1)$ | $\begin{bmatrix} 0 & 0 & 0 & -\frac{\sqrt{15}}{10} & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{15}}{10} & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{10}}{10} & 0 & 0 & 0 & 0 & 0 \\ -\frac{\sqrt{10}}{10} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| 156 | symmetry | $\frac{3\sqrt{35}z(x^2-2xy-y^2)(x^2+2xy-y^2)}{8}$ |
| | $Q_{5,2}^{(a)}(E_2, 1)$ | $\begin{bmatrix} 0 & 0 & \frac{\sqrt{15}}{10} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{15}}{10} & 0 & 0 & 0 \\ \frac{\sqrt{10}}{10} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{10}}{10} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| 157 | symmetry | $-\frac{\sqrt{105}xyz(x^2+y^2-2z^2)}{2}$ |
| | $Q_{5,1}^{(a)}(E_2, 2)$ | $\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{3}}{6} \\ 0 & -\frac{\sqrt{30}}{60} & 0 & 0 & 0 & \frac{\sqrt{2}}{4} & 0 \\ \frac{\sqrt{30}}{60} & 0 & 0 & 0 & \frac{\sqrt{2}}{4} & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{15}}{10} & 0 & 0 & 0 \end{bmatrix}$ |
| 158 | symmetry | $-\frac{\sqrt{105}z(x-y)(x+y)(x^2+y^2-2z^2)}{4}$ |

continued ...

Table 9

| No. | multipole | matrix |
|-----|----------------------------------|--|
| | $\mathbb{Q}_{5,2}^{(a)}(E_2, 2)$ | $\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{3}}{6} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -\frac{\sqrt{30}}{60} & 0 & 0 & 0 & \frac{\sqrt{2}}{4} & 0 & 0 \\ 0 & -\frac{\sqrt{30}}{60} & 0 & 0 & 0 & -\frac{\sqrt{2}}{4} & 0 \\ 0 & 0 & \frac{\sqrt{15}}{10} & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| 159 | symmetry | $-\frac{x^2}{2} - \frac{y^2}{2} + z^2$ |
| | $\mathbb{G}_2^{(a)}(A)$ | $\begin{bmatrix} 0 & 0 & 0 & \frac{\sqrt{35}}{14} & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{35}}{14} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{14}}{14} & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{14}}{14} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| 160 | symmetry | $\sqrt{3}yz$ |
| | $\mathbb{G}_{2,1}^{(a)}(E_1)$ | $\begin{bmatrix} -\frac{\sqrt{70}}{28} & 0 & 0 & 0 & -\frac{\sqrt{42}}{28} & 0 & 0 \\ 0 & -\frac{\sqrt{70}}{28} & 0 & 0 & 0 & -\frac{\sqrt{42}}{28} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{7}}{7} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{14}}{14} & 0 & 0 \end{bmatrix}$ |
| 161 | symmetry | $-\sqrt{3}xz$ |
| | $\mathbb{G}_{2,2}^{(a)}(E_1)$ | $\begin{bmatrix} 0 & -\frac{\sqrt{70}}{28} & 0 & 0 & 0 & \frac{\sqrt{42}}{28} & 0 \\ \frac{\sqrt{70}}{28} & 0 & 0 & 0 & -\frac{\sqrt{42}}{28} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{7}}{7} \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{14}}{14} & 0 \end{bmatrix}$ |
| 162 | symmetry | $\frac{\sqrt{3}(x-y)(x+y)}{2}$ |

continued ...

Table 9

| No. | multipole | matrix |
|-----|-------------------------------|---|
| | $\mathbb{G}_{2,1}^{(a)}(E_2)$ | $\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{7}}{14} \\ 0 & -\frac{\sqrt{70}}{28} & 0 & 0 & 0 & \frac{\sqrt{42}}{28} & 0 \\ \frac{\sqrt{70}}{28} & 0 & 0 & 0 & \frac{\sqrt{42}}{28} & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{35}}{14} & 0 & 0 & 0 \end{bmatrix}$ |
| 163 | symmetry | $-\sqrt{3}xy$ |
| | $\mathbb{G}_{2,2}^{(a)}(E_2)$ | $\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{7}}{14} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -\frac{\sqrt{70}}{28} & 0 & 0 & 0 & \frac{\sqrt{42}}{28} & 0 & 0 \\ 0 & -\frac{\sqrt{70}}{28} & 0 & 0 & 0 & -\frac{\sqrt{42}}{28} & 0 \\ 0 & 0 & -\frac{\sqrt{35}}{14} & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| 164 | symmetry | $\frac{3x^4}{8} + \frac{3x^2y^2}{4} - 3x^2z^2 + \frac{3y^4}{8} - 3y^2z^2 + z^4$ |
| | $\mathbb{G}_4^{(a)}(A)$ | $\begin{bmatrix} 0 & 0 & 0 & -\frac{\sqrt{14}}{14} & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{14}}{14} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{35}}{14} & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{35}}{14} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| 165 | symmetry | $\frac{\sqrt{70}xz(x^2-3y^2)}{4}$ |
| | $\mathbb{G}_4^{(a)}(B,1)$ | $\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{2}}{4} & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{2}}{4} & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{5}}{20} & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{5}}{20} & 0 & 0 & 0 & 0 \\ 0 & -\frac{3\sqrt{10}}{20} & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| 166 | symmetry | $\frac{\sqrt{70}yz(3x^2-y^2)}{4}$ |

continued ...

Table 9

| No. | multipole | matrix |
|-----|----------------------------------|---|
| | $\mathbb{G}_4^{(a)}(B, 2)$ | $\begin{bmatrix} 0 & 0 & 0 & 0 & -\frac{\sqrt{2}}{4} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{2}}{4} & 0 \\ 0 & 0 & \frac{\sqrt{5}}{20} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{5}}{20} & 0 & 0 & 0 \\ \frac{3\sqrt{10}}{20} & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| 167 | symmetry | $-\frac{\sqrt{10}yz(3x^2+3y^2-4z^2)}{4}$ |
| | $\mathbb{G}_{4,1}^{(a)}(E_1)$ | $\begin{bmatrix} \frac{\sqrt{210}}{140} & 0 & 0 & 0 & \frac{\sqrt{14}}{14} & 0 & 0 \\ 0 & \frac{\sqrt{210}}{140} & 0 & 0 & 0 & \frac{\sqrt{14}}{14} & 0 \\ 0 & 0 & -\frac{\sqrt{35}}{20} & 0 & 0 & 0 & -\frac{\sqrt{21}}{14} \\ 0 & 0 & 0 & -\frac{\sqrt{35}}{20} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{42}}{28} & 0 & 0 \end{bmatrix}$ |
| 168 | symmetry | $\frac{\sqrt{10}xz(3x^2+3y^2-4z^2)}{4}$ |
| | $\mathbb{G}_{4,2}^{(a)}(E_1)$ | $\begin{bmatrix} 0 & \frac{\sqrt{210}}{140} & 0 & 0 & 0 & -\frac{\sqrt{14}}{14} & 0 \\ -\frac{\sqrt{210}}{140} & 0 & 0 & 0 & \frac{\sqrt{14}}{14} & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{35}}{20} & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{35}}{20} & 0 & 0 & 0 & -\frac{\sqrt{21}}{14} \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{42}}{28} & 0 \end{bmatrix}$ |
| 169 | symmetry | $\frac{\sqrt{35}(x^2-2xy-y^2)(x^2+2xy-y^2)}{8}$ |
| | $\mathbb{G}_{4,1}^{(a)}(E_2, 1)$ | $\begin{bmatrix} 0 & 0 & 0 & \frac{\sqrt{10}}{10} & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{10}}{10} & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{15}}{10} & 0 & 0 & 0 & 0 & 0 \\ -\frac{\sqrt{15}}{10} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| 170 | symmetry | $\frac{\sqrt{35}xy(x-y)(x+y)}{2}$ |

continued ...

Table 9

| No. | multipole | matrix |
|-----|----------------------------------|--|
| | $\mathbb{G}_{4,2}^{(a)}(E_2, 1)$ | $\begin{bmatrix} 0 & 0 & -\frac{\sqrt{10}}{10} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{10}}{10} & 0 & 0 & 0 \\ \frac{\sqrt{15}}{10} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{15}}{10} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| 171 | symmetry | $-\frac{\sqrt{5}(x-y)(x+y)(x^2+y^2-6z^2)}{4}$ |
| | $\mathbb{G}_{4,1}^{(a)}(E_2, 2)$ | $\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{42}}{14} \\ 0 & \frac{3\sqrt{105}}{140} & 0 & 0 & 0 & \frac{\sqrt{7}}{28} & 0 \\ -\frac{3\sqrt{105}}{140} & 0 & 0 & 0 & \frac{\sqrt{7}}{28} & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{210}}{35} & 0 & 0 & 0 \end{bmatrix}$ |
| 172 | symmetry | $\frac{\sqrt{5}xy(x^2+y^2-6z^2)}{2}$ |
| | $\mathbb{G}_{4,2}^{(a)}(E_2, 2)$ | $\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{42}}{14} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{3\sqrt{105}}{140} & 0 & 0 & 0 & \frac{\sqrt{7}}{28} & 0 & 0 \\ 0 & \frac{3\sqrt{105}}{140} & 0 & 0 & 0 & -\frac{\sqrt{7}}{28} & 0 \\ 0 & 0 & -\frac{\sqrt{210}}{35} & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| 173 | symmetry | z |
| | $\mathbb{T}_1^{(a)}(A)$ | $\begin{bmatrix} 0 & 0 & \frac{\sqrt{14}i}{14} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{14}i}{14} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{2\sqrt{35}i}{35} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{2\sqrt{35}i}{35} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{3\sqrt{70}i}{70} \end{bmatrix}$ |
| 174 | symmetry | x |

continued ...

Table 9

| No. | multipole | matrix |
|-----|-------------------------------|---|
| | $\mathbb{T}_{1,1}^{(a)}(E_1)$ | $\begin{bmatrix} \frac{\sqrt{21}i}{14} & 0 & 0 & 0 & -\frac{\sqrt{35}i}{70} & 0 & 0 \\ 0 & \frac{\sqrt{21}i}{14} & 0 & 0 & 0 & -\frac{\sqrt{35}i}{70} & 0 \\ 0 & 0 & \frac{\sqrt{14}i}{14} & 0 & 0 & 0 & -\frac{\sqrt{210}i}{70} \\ 0 & 0 & 0 & \frac{\sqrt{14}i}{14} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{105}i}{35} & 0 & 0 \end{bmatrix}$ |
| 175 | symmetry | y $\mathbb{T}_{1,2}^{(a)}(E_1) \begin{bmatrix} 0 & \frac{\sqrt{21}i}{14} & 0 & 0 & 0 & \frac{\sqrt{35}i}{70} & 0 \\ -\frac{\sqrt{21}i}{14} & 0 & 0 & 0 & -\frac{\sqrt{35}i}{70} & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{14}i}{14} & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{14}i}{14} & 0 & 0 & 0 & -\frac{\sqrt{210}i}{70} \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{105}i}{35} & 0 \end{bmatrix}$ |
| 176 | symmetry | $-\frac{z(3x^2+3y^2-2z^2)}{2}$ $\mathbb{T}_3^{(a)}(A) \begin{bmatrix} 0 & 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{15}i}{30} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{15}i}{30} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{30}i}{15} \end{bmatrix}$ |
| 177 | symmetry | $\frac{\sqrt{10}y(3x^2-y^2)}{4}$ $\mathbb{T}_3^{(a)}(B, 1) \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{6}i}{12} & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{6}i}{12} & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{15}i}{12} & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{15}i}{12} & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{30}i}{12} & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| 178 | symmetry | $\frac{\sqrt{10}x(x^2-3y^2)}{4}$ |

continued ...

Table 9

| No. | multipole | matrix |
|-----|-------------------------------|--|
| | $\mathbb{T}_3^{(a)}(B, 2)$ | $\begin{bmatrix} 0 & 0 & 0 & 0 & -\frac{\sqrt{6}i}{12} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{6}i}{12} & 0 \\ 0 & 0 & \frac{\sqrt{15}i}{12} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{15}i}{12} & 0 & 0 & 0 \\ -\frac{\sqrt{30}i}{12} & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| 179 | symmetry | $-\frac{\sqrt{6}x(x^2+y^2-4z^2)}{4}$ |
| | $\mathbb{T}_{3,1}^{(a)}(E_1)$ | $\begin{bmatrix} -\frac{\sqrt{6}i}{12} & 0 & 0 & 0 & \frac{\sqrt{10}i}{10} & 0 & 0 \\ 0 & -\frac{\sqrt{6}i}{12} & 0 & 0 & 0 & \frac{\sqrt{10}i}{10} & 0 \\ 0 & 0 & \frac{i}{4} & 0 & 0 & 0 & \frac{\sqrt{15}i}{30} \\ 0 & 0 & 0 & \frac{i}{4} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{30}i}{20} & 0 & 0 \end{bmatrix}$ |
| 180 | symmetry | $-\frac{\sqrt{6}y(x^2+y^2-4z^2)}{4}$ |
| | $\mathbb{T}_{3,2}^{(a)}(E_1)$ | $\begin{bmatrix} 0 & -\frac{\sqrt{6}i}{12} & 0 & 0 & 0 & -\frac{\sqrt{10}i}{10} & 0 \\ \frac{\sqrt{6}i}{12} & 0 & 0 & 0 & \frac{\sqrt{10}i}{10} & 0 & 0 \\ 0 & 0 & 0 & \frac{i}{4} & 0 & 0 & 0 \\ 0 & 0 & -\frac{i}{4} & 0 & 0 & 0 & \frac{\sqrt{15}i}{30} \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{30}i}{20} & 0 \end{bmatrix}$ |
| 181 | symmetry | $\sqrt{15}xyz$ |
| | $\mathbb{T}_{3,1}^{(a)}(E_2)$ | $\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{6}i}{6} \\ 0 & \frac{\sqrt{15}i}{12} & 0 & 0 & 0 & \frac{i}{4} & 0 \\ -\frac{\sqrt{15}i}{12} & 0 & 0 & 0 & \frac{i}{4} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| 182 | symmetry | $\frac{\sqrt{15}z(x-y)(x+y)}{2}$ |

continued ...

Table 9

| No. | multipole | matrix |
|-----|-------------------------------|--|
| | $\mathbb{T}_{3,2}^{(a)}(E_2)$ | $\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{6}i}{6} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{\sqrt{15}i}{12} & 0 & 0 & 0 & \frac{i}{4} & 0 & 0 \\ 0 & \frac{\sqrt{15}i}{12} & 0 & 0 & 0 & -\frac{i}{4} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| 183 | symmetry | $\frac{z(15x^4+30x^2y^2-40x^2z^2+15y^4-40y^2z^2+8z^4)}{8}$ |
| | $\mathbb{T}_5^{(a)}(A)$ | $\begin{bmatrix} 0 & 0 & \frac{\sqrt{21}i}{42} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{21}i}{42} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{210}i}{42} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{210}i}{42} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{105}i}{21} \end{bmatrix}$ |
| 184 | symmetry | $-\frac{\sqrt{70}y(3x^2-y^2)(x^2+y^2-8z^2)}{16}$ |
| | $\mathbb{T}_5^{(a)}(B,1)$ | $\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{3}i}{6} & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{3}i}{6} & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{30}i}{15} & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{30}i}{15} & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{15}i}{15} & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| 185 | symmetry | $-\frac{\sqrt{70}x(x^2-3y^2)(x^2+y^2-8z^2)}{16}$ |
| | $\mathbb{T}_5^{(a)}(B,2)$ | $\begin{bmatrix} 0 & 0 & 0 & 0 & \frac{\sqrt{3}i}{6} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{3}i}{6} & 0 \\ 0 & 0 & \frac{\sqrt{30}i}{15} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{30}i}{15} & 0 & 0 & 0 \\ \frac{\sqrt{15}i}{15} & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| 186 | symmetry | $\frac{3\sqrt{14}x(x^4-10x^2y^2+5y^4)}{16}$ |

continued ...

Table 9

| No. | multipole | matrix |
|-----|----------------------------------|--|
| | $\mathbb{T}_{5,1}^{(a)}(E_1, 1)$ | $\begin{bmatrix} \frac{i}{2} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{i}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| 187 | symmetry | $-\frac{3\sqrt{14}y(5x^4-10x^2y^2+y^4)}{16}$ |
| | $\mathbb{T}_{5,2}^{(a)}(E_1, 1)$ | $\begin{bmatrix} 0 & -\frac{i}{2} & 0 & 0 & 0 & 0 & 0 \\ -\frac{i}{2} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| 188 | symmetry | $\frac{\sqrt{15}x(x^4+2x^2y^2-12x^2z^2+y^4-12y^2z^2+8z^4)}{8}$ |
| | $\mathbb{T}_{5,1}^{(a)}(E_1, 2)$ | $\begin{bmatrix} \frac{\sqrt{210}i}{420} & 0 & 0 & 0 & -\frac{\sqrt{14}i}{28} & 0 & 0 \\ 0 & \frac{\sqrt{210}i}{420} & 0 & 0 & 0 & -\frac{\sqrt{14}i}{28} & 0 \\ 0 & 0 & -\frac{\sqrt{35}i}{35} & 0 & 0 & 0 & \frac{2\sqrt{21}i}{21} \\ 0 & 0 & 0 & -\frac{\sqrt{35}i}{35} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{42}i}{14} & 0 & 0 \end{bmatrix}$ |
| 189 | symmetry | $\frac{\sqrt{15}y(x^4+2x^2y^2-12x^2z^2+y^4-12y^2z^2+8z^4)}{8}$ |
| | $\mathbb{T}_{5,2}^{(a)}(E_1, 2)$ | $\begin{bmatrix} 0 & \frac{\sqrt{210}i}{420} & 0 & 0 & 0 & \frac{\sqrt{14}i}{28} & 0 \\ -\frac{\sqrt{210}i}{420} & 0 & 0 & 0 & -\frac{\sqrt{14}i}{28} & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{35}i}{35} & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{35}i}{35} & 0 & 0 & 0 & \frac{2\sqrt{21}i}{21} \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{42}i}{14} & 0 \end{bmatrix}$ |
| 190 | symmetry | $-\frac{3\sqrt{35}xyz(x-y)(x+y)}{2}$ |

continued ...

Table 9

| No. | multipole | matrix |
|-----|----------------------------------|--|
| | $\mathbb{T}_{5,1}^{(a)}(E_2, 1)$ | $\begin{bmatrix} 0 & 0 & 0 & -\frac{\sqrt{15}i}{10} & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{15}i}{10} & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{10}i}{10} & 0 & 0 & 0 & 0 & 0 \\ -\frac{\sqrt{10}i}{10} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| 191 | symmetry | $\frac{3\sqrt{35}z(x^2-2xy-y^2)(x^2+2xy-y^2)}{8}$ |
| | $\mathbb{T}_{5,2}^{(a)}(E_2, 1)$ | $\begin{bmatrix} 0 & 0 & \frac{\sqrt{15}i}{10} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{15}i}{10} & 0 & 0 & 0 \\ \frac{\sqrt{10}i}{10} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{10}i}{10} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| 192 | symmetry | $-\frac{\sqrt{105}xyz(x^2+y^2-2z^2)}{2}$ |
| | $\mathbb{T}_{5,1}^{(a)}(E_2, 2)$ | $\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{3}i}{6} \\ 0 & -\frac{\sqrt{30}i}{60} & 0 & 0 & 0 & \frac{\sqrt{2}i}{4} & 0 \\ \frac{\sqrt{30}i}{60} & 0 & 0 & 0 & \frac{\sqrt{2}i}{4} & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{15}i}{10} & 0 & 0 & 0 \end{bmatrix}$ |
| 193 | symmetry | $\frac{\sqrt{105}z(x-y)(x+y)(x^2+y^2-2z^2)}{4}$ |
| | $\mathbb{T}_{5,2}^{(a)}(E_2, 2)$ | $\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{3}i}{6} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -\frac{\sqrt{30}i}{60} & 0 & 0 & 0 & \frac{\sqrt{2}i}{4} & 0 & 0 \\ 0 & -\frac{\sqrt{30}i}{60} & 0 & 0 & 0 & -\frac{\sqrt{2}i}{4} & 0 \\ 0 & 0 & \frac{\sqrt{15}i}{10} & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| 194 | symmetry | $-\frac{x^2}{2} - \frac{y^2}{2} + z^2$ |

continued ...

Table 9

| No. | multipole | matrix |
|-----|----------------------|---|
| | $M_2^{(a)}(A)$ | $\begin{bmatrix} 0 & 0 & 0 & -\frac{\sqrt{35}i}{14} & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{35}i}{14} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{14}i}{14} & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{14}i}{14} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| 195 | symmetry | $\sqrt{3}yz$ |
| | $M_{2,1}^{(a)}(E_1)$ | $\begin{bmatrix} \frac{\sqrt{70}i}{28} & 0 & 0 & 0 & \frac{\sqrt{42}i}{28} & 0 & 0 \\ 0 & \frac{\sqrt{70}i}{28} & 0 & 0 & 0 & \frac{\sqrt{42}i}{28} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{7}i}{7} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{14}i}{14} & 0 & 0 \end{bmatrix}$ |
| 196 | symmetry | $-\sqrt{3}xz$ |
| | $M_{2,2}^{(a)}(E_1)$ | $\begin{bmatrix} 0 & \frac{\sqrt{70}i}{28} & 0 & 0 & 0 & -\frac{\sqrt{42}i}{28} & 0 \\ -\frac{\sqrt{70}i}{28} & 0 & 0 & 0 & \frac{\sqrt{42}i}{28} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{7}i}{7} \\ 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{14}i}{14} & 0 \end{bmatrix}$ |
| 197 | symmetry | $\frac{\sqrt{3}(x-y)(x+y)}{2}$ |
| | $M_{2,1}^{(a)}(E_2)$ | $\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{7}i}{14} \\ 0 & \frac{\sqrt{70}i}{28} & 0 & 0 & 0 & -\frac{\sqrt{42}i}{28} & 0 \\ -\frac{\sqrt{70}i}{28} & 0 & 0 & 0 & -\frac{\sqrt{42}i}{28} & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{35}i}{14} & 0 & 0 & 0 \end{bmatrix}$ |
| 198 | symmetry | $-\sqrt{3}xy$ |

continued ...

Table 9

| No. | multipole | matrix |
|-----|----------------------|---|
| | $M_{2,2}^{(a)}(E_2)$ | $\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{7}i}{14} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{\sqrt{70}i}{28} & 0 & 0 & 0 & -\frac{\sqrt{42}i}{28} & 0 & 0 \\ 0 & \frac{\sqrt{70}i}{28} & 0 & 0 & 0 & \frac{\sqrt{42}i}{28} & 0 \\ 0 & 0 & \frac{\sqrt{35}i}{14} & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| 199 | symmetry | $\frac{3x^4}{8} + \frac{3x^2y^2}{4} - 3x^2z^2 + \frac{3y^4}{8} - 3y^2z^2 + z^4$ |
| | $M_4^{(a)}(A)$ | $\begin{bmatrix} 0 & 0 & 0 & \frac{\sqrt{14}i}{14} & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{14}i}{14} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{35}i}{14} & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{35}i}{14} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| 200 | symmetry | $\frac{\sqrt{70}xz(x^2-3y^2)}{4}$ |
| | $M_4^{(a)}(B, 1)$ | $\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{2}i}{4} & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{2}i}{4} & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{5}i}{20} & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{5}i}{20} & 0 & 0 & 0 & 0 \\ 0 & \frac{3\sqrt{10}i}{20} & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| 201 | symmetry | $\frac{\sqrt{70}yz(3x^2-y^2)}{4}$ |
| | $M_4^{(a)}(B, 2)$ | $\begin{bmatrix} 0 & 0 & 0 & 0 & \frac{\sqrt{2}i}{4} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{2}i}{4} & 0 \\ 0 & 0 & -\frac{\sqrt{5}i}{20} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{5}i}{20} & 0 & 0 & 0 \\ -\frac{3\sqrt{10}i}{20} & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| 202 | symmetry | $-\frac{\sqrt{10}yz(3x^2+3y^2-4z^2)}{4}$ |

continued ...

Table 9

| No. | multipole | matrix |
|-----|-------------------------|--|
| | $M_{4,1}^{(a)}(E_1)$ | $\begin{bmatrix} -\frac{\sqrt{210}i}{140} & 0 & 0 & 0 & -\frac{\sqrt{14}i}{14} & 0 & 0 \\ 0 & -\frac{\sqrt{210}i}{140} & 0 & 0 & 0 & -\frac{\sqrt{14}i}{14} & 0 \\ 0 & 0 & \frac{\sqrt{35}i}{20} & 0 & 0 & 0 & \frac{\sqrt{21}i}{14} \\ 0 & 0 & 0 & \frac{\sqrt{35}i}{20} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{42}i}{28} & 0 & 0 \end{bmatrix}$ |
| 203 | symmetry | $\frac{\sqrt{10}xz(3x^2+3y^2-4z^2)}{4}$ |
| | $M_{4,2}^{(a)}(E_1)$ | $\begin{bmatrix} 0 & -\frac{\sqrt{210}i}{140} & 0 & 0 & 0 & \frac{\sqrt{14}i}{14} & 0 \\ \frac{\sqrt{210}i}{140} & 0 & 0 & 0 & -\frac{\sqrt{14}i}{14} & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{35}i}{20} & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{35}i}{20} & 0 & 0 & 0 & \frac{\sqrt{21}i}{14} \\ 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{42}i}{28} & 0 \end{bmatrix}$ |
| 204 | symmetry | $\frac{\sqrt{35}(x^2-2xy-y^2)(x^2+2xy-y^2)}{8}$ |
| | $M_{4,1}^{(a)}(E_2, 1)$ | $\begin{bmatrix} 0 & 0 & 0 & -\frac{\sqrt{10}i}{10} & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{10}i}{10} & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{15}i}{10} & 0 & 0 & 0 & 0 & 0 \\ \frac{\sqrt{15}i}{10} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| 205 | symmetry | $\frac{\sqrt{35}xy(x-y)(x+y)}{2}$ |
| | $M_{4,2}^{(a)}(E_2, 1)$ | $\begin{bmatrix} 0 & 0 & \frac{\sqrt{10}i}{10} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{10}i}{10} & 0 & 0 & 0 \\ -\frac{\sqrt{15}i}{10} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{15}i}{10} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| 206 | symmetry | $-\frac{\sqrt{5}(x-y)(x+y)(x^2+y^2-6z^2)}{4}$ |

continued ...

Table 9

| No. | multipole | matrix |
|-----|-----------|--|
| | | $\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{42}i}{14} \\ 0 & -\frac{3\sqrt{105}i}{140} & 0 & 0 & 0 & -\frac{\sqrt{7}i}{28} & 0 \\ \frac{3\sqrt{105}i}{140} & 0 & 0 & 0 & -\frac{\sqrt{7}i}{28} & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{210}i}{35} & 0 & 0 & 0 \end{bmatrix}$ |
| 207 | symmetry | $\frac{\sqrt{5}xy(x^2+y^2-6z^2)}{2}$ |
| | | $\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{42}i}{14} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -\frac{3\sqrt{105}i}{140} & 0 & 0 & 0 & -\frac{\sqrt{7}i}{28} & 0 & 0 \\ 0 & -\frac{3\sqrt{105}i}{140} & 0 & 0 & 0 & \frac{\sqrt{7}i}{28} & 0 \\ 0 & 0 & \frac{\sqrt{210}i}{35} & 0 & 0 & 0 & 0 \end{bmatrix}$ |

bra: = $\langle f_2 |, \langle f_1 |, \langle f_{bz} |, \langle f_3 |, \langle f_{3x} |, \langle f_{3y} |, \langle f_{az} |$
ket: = $|f_2\rangle, |f_1\rangle, |f_{bz}\rangle, |f_3\rangle, |f_{3x}\rangle, |f_{3y}\rangle, |f_{az}\rangle$

Table 10: (f,f) block.

| No. | multipole | matrix |
|-----|-----------|--|
| 208 | symmetry | 1 |
| | | $\begin{bmatrix} \frac{\sqrt{7}}{7} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{7}}{7} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{7}}{7} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{7}}{7} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{7}}{7} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{7}}{7} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{7}}{7} \end{bmatrix}$ |
| 209 | symmetry | $-\frac{x^2}{2} - \frac{y^2}{2} + z^2$ |

continued ...

Table 10

| No. | multipole | matrix |
|-----|----------------------|--|
| | $Q_{2,1}^{(a)}(E_2)$ | $\begin{bmatrix} 0 & 0 & 0 & 0 & -\frac{\sqrt{105}}{42} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{105}}{42} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{105}}{21} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -\frac{\sqrt{105}}{42} & 0 & 0 & 0 & \frac{\sqrt{7}}{7} & 0 & 0 \\ 0 & -\frac{\sqrt{105}}{42} & 0 & 0 & 0 & -\frac{\sqrt{7}}{7} & 0 \\ 0 & 0 & -\frac{\sqrt{105}}{21} & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| 213 | symmetry | $-\sqrt{3}xy$ |
| | $Q_{2,2}^{(a)}(E_2)$ | $\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{105}}{42} & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{105}}{42} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{105}}{21} \\ 0 & \frac{\sqrt{105}}{42} & 0 & 0 & 0 & -\frac{\sqrt{7}}{7} & 0 \\ -\frac{\sqrt{105}}{42} & 0 & 0 & 0 & -\frac{\sqrt{7}}{7} & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{105}}{21} & 0 & 0 & 0 \end{bmatrix}$ |
| 214 | symmetry | $\frac{3x^4}{8} + \frac{3x^2y^2}{4} - 3x^2z^2 + \frac{3y^4}{8} - 3y^2z^2 + z^4$ |
| | $Q_4^{(a)}(A)$ | $\begin{bmatrix} \frac{3\sqrt{154}}{154} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{3\sqrt{154}}{154} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{154}}{22} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{154}}{22} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{154}}{154} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{154}}{154} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{3\sqrt{154}}{77} \end{bmatrix}$ |
| 215 | symmetry | $\frac{\sqrt{70}xz(x^2-3y^2)}{4}$ |

continued ...

Table 10

| No. | multipole | matrix |
|-----|-------------------------------|--|
| | $\mathbb{Q}_4^{(a)}(B, 1)$ | $\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & -\frac{3\sqrt{22}}{22} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{22}}{22} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{22}}{22} & 0 \\ 0 & 0 & \frac{\sqrt{22}}{22} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{22}}{22} & 0 & 0 & 0 \\ -\frac{3\sqrt{22}}{22} & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| 216 | symmetry | $\frac{\sqrt{70}yz(3x^2-y^2)}{4}$ $\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\frac{3\sqrt{22}}{22} \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{22}}{22} & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{22}}{22} & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{22}}{22} & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{22}}{22} & 0 & 0 & 0 & 0 \\ 0 & -\frac{3\sqrt{22}}{22} & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| | $\mathbb{Q}_4^{(a)}(B, 2)$ | |
| 217 | symmetry | $-\frac{\sqrt{10}yz(3x^2+3y^2-4z^2)}{4}$ $\begin{bmatrix} 0 & 0 & 0 & \frac{\sqrt{2310}}{154} & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{2310}}{154} & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{2310}}{154} & 0 & 0 & 0 & -\frac{2\sqrt{154}}{77} & 0 \\ \frac{\sqrt{2310}}{154} & 0 & 0 & 0 & \frac{2\sqrt{154}}{77} & 0 & 0 \\ 0 & 0 & 0 & \frac{2\sqrt{154}}{77} & 0 & 0 & 0 \\ 0 & 0 & -\frac{2\sqrt{154}}{77} & 0 & 0 & 0 & \frac{\sqrt{2310}}{154} \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{2310}}{154} & 0 \end{bmatrix}$ |
| | $\mathbb{Q}_{4,1}^{(a)}(E_1)$ | |
| 218 | symmetry | $\frac{\sqrt{10}xz(3x^2+3y^2-4z^2)}{4}$ |

continued ...

Table 10

| No. | multipole | matrix | | | | | | |
|-----|----------------------------------|---|---------------------------|---------------------------|---------------------------|----------------------------|---------------------------|----------------------------|
| | $\mathbb{Q}_{4,2}^{(a)}(E_1)$ | 0 | 0 | $\frac{\sqrt{2310}}{154}$ | 0 | 0 | 0 | 0 |
| | | 0 | 0 | 0 | $\frac{\sqrt{2310}}{154}$ | 0 | 0 | 0 |
| | | $\frac{\sqrt{2310}}{154}$ | 0 | 0 | 0 | $-\frac{2\sqrt{154}}{77}$ | 0 | 0 |
| | | 0 | $\frac{\sqrt{2310}}{154}$ | 0 | 0 | 0 | $-\frac{2\sqrt{154}}{77}$ | 0 |
| | | 0 | 0 | $-\frac{2\sqrt{154}}{77}$ | 0 | 0 | 0 | $-\frac{\sqrt{2310}}{154}$ |
| | | 0 | 0 | 0 | $-\frac{2\sqrt{154}}{77}$ | 0 | 0 | 0 |
| | | 0 | 0 | 0 | 0 | $-\frac{\sqrt{2310}}{154}$ | 0 | 0 |
| 219 | symmetry | $\frac{\sqrt{35}(x^2-2xy-y^2)(x^2+2xy-y^2)}{8}$ | | | | | | |
| | $\mathbb{Q}_{4,1}^{(a)}(E_2, 1)$ | 0 | 0 | 0 | 0 | $-\frac{\sqrt{66}}{22}$ | 0 | 0 |
| | | 0 | 0 | 0 | 0 | 0 | $\frac{\sqrt{66}}{22}$ | 0 |
| | | 0 | 0 | $\frac{\sqrt{110}}{22}$ | 0 | 0 | 0 | 0 |
| | | 0 | 0 | 0 | $-\frac{\sqrt{110}}{22}$ | 0 | 0 | 0 |
| | | $-\frac{\sqrt{66}}{22}$ | 0 | 0 | 0 | 0 | 0 | 0 |
| | | 0 | $\frac{\sqrt{66}}{22}$ | 0 | 0 | 0 | 0 | 0 |
| | | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 220 | symmetry | $\frac{\sqrt{35}xy(x-y)(x+y)}{2}$ | | | | | | |
| | $\mathbb{Q}_{4,2}^{(a)}(E_2, 1)$ | 0 | 0 | 0 | 0 | 0 | $-\frac{\sqrt{66}}{22}$ | 0 |
| | | 0 | 0 | 0 | 0 | $-\frac{\sqrt{66}}{22}$ | 0 | 0 |
| | | 0 | 0 | 0 | $\frac{\sqrt{110}}{22}$ | 0 | 0 | 0 |
| | | 0 | 0 | $\frac{\sqrt{110}}{22}$ | 0 | 0 | 0 | 0 |
| | | 0 | $-\frac{\sqrt{66}}{22}$ | 0 | 0 | 0 | 0 | 0 |
| | | $-\frac{\sqrt{66}}{22}$ | 0 | 0 | 0 | 0 | 0 | 0 |
| | | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 221 | symmetry | $-\frac{\sqrt{5}(x-y)(x+y)(x^2+y^2-6z^2)}{4}$ | | | | | | |

continued ...

Table 10

| No. | multipole | matrix |
|-----|----------------------------------|---|
| | $\mathbb{Q}_{4,1}^{(a)}(E_2, 2)$ | $\begin{bmatrix} 0 & 0 & 0 & 0 & \frac{3\sqrt{462}}{154} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{3\sqrt{462}}{154} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{462}}{154} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{3\sqrt{462}}{154} & 0 & 0 & 0 & \frac{\sqrt{770}}{77} & 0 & 0 \\ 0 & \frac{3\sqrt{462}}{154} & 0 & 0 & 0 & -\frac{\sqrt{770}}{77} & 0 \\ 0 & 0 & -\frac{\sqrt{462}}{154} & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| 222 | symmetry | $\frac{\sqrt{5xy}(x^2+y^2-6z^2)}{2}$ |
| | $\mathbb{Q}_{4,2}^{(a)}(E_2, 2)$ | $\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & \frac{3\sqrt{462}}{154} & 0 \\ 0 & 0 & 0 & 0 & -\frac{3\sqrt{462}}{154} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{462}}{154} \\ 0 & -\frac{3\sqrt{462}}{154} & 0 & 0 & 0 & -\frac{\sqrt{770}}{77} & 0 \\ \frac{3\sqrt{462}}{154} & 0 & 0 & 0 & -\frac{\sqrt{770}}{77} & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{462}}{154} & 0 & 0 & 0 \end{bmatrix}$ |
| 223 | symmetry | $-\frac{5x^6}{16} - \frac{15x^4y^2}{16} + \frac{45x^4z^2}{8} - \frac{15x^2y^4}{16} + \frac{45x^2y^2z^2}{4} - \frac{15x^2z^4}{2} - \frac{5y^6}{16} + \frac{45y^4z^2}{8} - \frac{15y^2z^4}{2} + z^6$ |
| | $\mathbb{Q}_6^{(a)}(A, 1)$ | $\begin{bmatrix} -\frac{\sqrt{231}}{462} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{231}}{462} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{231}}{77} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{231}}{77} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{5\sqrt{231}}{154} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{5\sqrt{231}}{154} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{10\sqrt{231}}{231} \end{bmatrix}$ |
| 224 | symmetry | $\frac{\sqrt{462}(x-y)(x+y)(x^2-4xy+y^2)(x^2+4xy+y^2)}{32}$ |

continued ...

Table 10

| No. | multipole | matrix |
|-----|----------------------------|--|
| | $\mathbb{Q}_6^{(a)}(A, 2)$ | $\begin{bmatrix} \frac{\sqrt{2}}{2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{2}}{2} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| 225 | symmetry | $\frac{\sqrt{462xy(x^2-3y^2)(3x^2-y^2)}}{16}$ $\begin{bmatrix} 0 & \frac{\sqrt{2}}{2} & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{\sqrt{2}}{2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| | $\mathbb{Q}_6^{(a)}(A, 3)$ | |
| 226 | symmetry | $-\frac{\sqrt{210xz(x^2-3y^2)(3x^2+3y^2-8z^2)}}{16}$ $\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{11}}{11} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{3\sqrt{11}}{22} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{3\sqrt{11}}{22} & 0 \\ 0 & 0 & \frac{3\sqrt{11}}{22} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{3\sqrt{11}}{22} & 0 & 0 & 0 \\ \frac{\sqrt{11}}{11} & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| | $\mathbb{Q}_6^{(a)}(B, 1)$ | |
| 227 | symmetry | $-\frac{\sqrt{210yz(3x^2-y^2)(3x^2+3y^2-8z^2)}}{16}$ |

continued ...

Table 10

| No. | multipole | matrix |
|-----|----------------------------------|---|
| | $\mathbb{Q}_6^{(a)}(B, 2)$ | $\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{11}}{11} \\ 0 & 0 & 0 & 0 & 0 & \frac{3\sqrt{11}}{22} & 0 \\ 0 & 0 & 0 & 0 & \frac{3\sqrt{11}}{22} & 0 & 0 \\ 0 & 0 & 0 & \frac{3\sqrt{11}}{22} & 0 & 0 & 0 \\ 0 & 0 & \frac{3\sqrt{11}}{22} & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{11}}{11} & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| 228 | symmetry | $\frac{3\sqrt{154}yz(5x^4-10x^2y^2+y^4)}{16}$ $\begin{bmatrix} 0 & 0 & 0 & \frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{2} & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 & 0 & 0 & 0 \\ \frac{1}{2} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| | $\mathbb{Q}_{6,1}^{(a)}(E_1, 1)$ | |
| 229 | symmetry | $\frac{3\sqrt{154}xz(x^4-10x^2y^2+5y^4)}{16}$ $\begin{bmatrix} 0 & 0 & \frac{1}{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{1}{2} & 0 & 0 & 0 \\ \frac{1}{2} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{1}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| | $\mathbb{Q}_{6,2}^{(a)}(E_1, 1)$ | |
| 230 | symmetry | $\frac{\sqrt{21}yz(5x^4+10x^2y^2-20x^2z^2+5y^4-20y^2z^2+8z^4)}{8}$ |

continued ...

Table 10

| No. | multipole | matrix |
|-----|----------------------------------|---|
| | $\mathbb{Q}_{6,1}^{(a)}(E_1, 2)$ | $\begin{bmatrix} 0 & 0 & 0 & -\frac{\sqrt{66}}{132} & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{66}}{132} & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{66}}{132} & 0 & 0 & 0 & \frac{\sqrt{110}}{44} & 0 \\ -\frac{\sqrt{66}}{132} & 0 & 0 & 0 & -\frac{\sqrt{110}}{44} & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{110}}{44} & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{110}}{44} & 0 & 0 & 0 & \frac{5\sqrt{66}}{66} \\ 0 & 0 & 0 & 0 & 0 & \frac{5\sqrt{66}}{66} & 0 \end{bmatrix}$ |
| 231 | symmetry | $-\frac{\sqrt{21}xz(5x^4+10x^2y^2-20x^2z^2+5y^4-20y^2z^2+8z^4)}{8}$ |
| | $\mathbb{Q}_{6,2}^{(a)}(E_1, 2)$ | $\begin{bmatrix} 0 & 0 & -\frac{\sqrt{66}}{132} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{66}}{132} & 0 & 0 & 0 \\ -\frac{\sqrt{66}}{132} & 0 & 0 & 0 & \frac{\sqrt{110}}{44} & 0 & 0 \\ 0 & -\frac{\sqrt{66}}{132} & 0 & 0 & 0 & \frac{\sqrt{110}}{44} & 0 \\ 0 & 0 & \frac{\sqrt{110}}{44} & 0 & 0 & 0 & -\frac{5\sqrt{66}}{66} \\ 0 & 0 & 0 & \frac{\sqrt{110}}{44} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{5\sqrt{66}}{66} & 0 & 0 \end{bmatrix}$ |
| 232 | symmetry | $-\frac{3\sqrt{7}(x^2+y^2-10z^2)(x^2-2xy-y^2)(x^2+2xy-y^2)}{16}$ |
| | $\mathbb{Q}_{6,1}^{(a)}(E_2, 1)$ | $\begin{bmatrix} 0 & 0 & 0 & 0 & \frac{\sqrt{55}}{22} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{55}}{22} & 0 \\ 0 & 0 & \frac{\sqrt{33}}{11} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{33}}{11} & 0 & 0 & 0 \\ \frac{\sqrt{55}}{22} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{55}}{22} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| 233 | symmetry | $-\frac{3\sqrt{7}xy(x-y)(x+y)(x^2+y^2-10z^2)}{4}$ |

continued ...

Table 10

| No. | multipole | matrix |
|-----|----------------------------------|---|
| | $\mathbb{Q}_{6,2}^{(a)}(E_2, 1)$ | $\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{55}}{22} & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{55}}{22} & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{33}}{11} & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{33}}{11} & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{55}}{22} & 0 & 0 & 0 & 0 & 0 \\ \frac{\sqrt{55}}{22} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| 234 | symmetry | $\frac{\sqrt{210}(x-y)(x+y)(x^4+2x^2y^2-16x^2z^2+y^4-16y^2z^2+16z^4)}{32}$ $\begin{bmatrix} 0 & 0 & 0 & 0 & -\frac{\sqrt{66}}{66} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{66}}{66} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{2\sqrt{66}}{33} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -\frac{\sqrt{66}}{66} & 0 & 0 & 0 & \frac{\sqrt{110}}{22} & 0 & 0 \\ 0 & -\frac{\sqrt{66}}{66} & 0 & 0 & 0 & -\frac{\sqrt{110}}{22} & 0 \\ 0 & 0 & \frac{2\sqrt{66}}{33} & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| 235 | symmetry | $-\frac{\sqrt{210}xy(x^4+2x^2y^2-16x^2z^2+y^4-16y^2z^2+16z^4)}{16}$ $\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{66}}{66} & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{66}}{66} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\frac{2\sqrt{66}}{33} \\ 0 & \frac{\sqrt{66}}{66} & 0 & 0 & 0 & -\frac{\sqrt{110}}{22} & 0 \\ -\frac{\sqrt{66}}{66} & 0 & 0 & 0 & -\frac{\sqrt{110}}{22} & 0 & 0 \\ 0 & 0 & 0 & -\frac{2\sqrt{66}}{33} & 0 & 0 & 0 \end{bmatrix}$ |
| 236 | symmetry | z |

continued ...

Table 10

| No. | multipole | matrix |
|-----|-------------------------|---|
| | $\mathbb{M}_3^{(a)}(A)$ | $\begin{bmatrix} 0 & \frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 & 0 \\ -\frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{6}i}{6} & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{6}i}{6} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| 240 | symmetry | $\frac{\sqrt{10}y(3x^2-y^2)}{4}$ $\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{6}i}{6} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{6}i}{6} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{6}i}{6} & 0 \\ 0 & 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{6}i}{6} & 0 & 0 & 0 \\ \frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| 241 | symmetry | $\frac{\sqrt{10}x(x^2-3y^2)}{4}$ $\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{6}i}{6} \\ 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{6}i}{6} & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{6}i}{6} & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| 242 | symmetry | $-\frac{\sqrt{6}x(x^2+y^2-4z^2)}{4}$ |

continued ...

Table 10

| No. | multipole | matrix |
|-----|----------------------|--|
| | $M_{3,1}^{(a)}(E_1)$ | $\begin{bmatrix} 0 & 0 & 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 & 0 \\ \frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{6}i}{6} \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{6}i}{6} & 0 \end{bmatrix}$ |
| 243 | symmetry | $-\frac{\sqrt{6}y(x^2+y^2-4z^2)}{4}$ |
| | $M_{3,2}^{(a)}(E_1)$ | $\begin{bmatrix} 0 & 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 & 0 \\ \frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{6}i}{6} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 \end{bmatrix}$ |
| 244 | symmetry | $\sqrt{15}xyz$ |
| | $M_{3,1}^{(a)}(E_2)$ | $\begin{bmatrix} 0 & 0 & 0 & 0 & \frac{\sqrt{6}i}{6} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{6}i}{6} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{6}i}{6} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -\frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| 245 | symmetry | $\frac{\sqrt{15}z(x-y)(x+y)}{2}$ |

continued ...

Table 10

| No. | multipole | matrix |
|-----|----------------------|--|
| | $M_{3,2}^{(a)}(E_2)$ | $\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{6}i}{6} & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{6}i}{6} \\ 0 & \frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 & 0 \\ -\frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{6}i}{6} & 0 & 0 & 0 \end{bmatrix}$ |
| 246 | symmetry | $\frac{z(15x^4+30x^2y^2-40x^2z^2+15y^4-40y^2z^2+8z^4)}{8}$ |
| | $M_5^{(a)}(A)$ | $\begin{bmatrix} 0 & -\frac{\sqrt{21}i}{42} & 0 & 0 & 0 & 0 & 0 \\ \frac{\sqrt{21}i}{42} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{2\sqrt{21}i}{21} & 0 & 0 & 0 \\ 0 & 0 & -\frac{2\sqrt{21}i}{21} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{5\sqrt{21}i}{42} & 0 \\ 0 & 0 & 0 & 0 & \frac{5\sqrt{21}i}{42} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| 247 | symmetry | $-\frac{\sqrt{70}y(3x^2-y^2)(x^2+y^2-8z^2)}{16}$ |
| | $M_5^{(a)}(B, 1)$ | $\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{3}i}{3} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{3}i}{6} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{3}i}{6} & 0 \\ 0 & 0 & -\frac{\sqrt{3}i}{6} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{3}i}{6} & 0 & 0 & 0 \\ -\frac{\sqrt{3}i}{3} & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| 248 | symmetry | $-\frac{\sqrt{70}x(x^2-3y^2)(x^2+y^2-8z^2)}{16}$ |

continued ...

Table 10

| No. | multipole | matrix |
|-----|-------------------|--|
| | $M_5^{(a)}(B, 2)$ | $\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{3}i}{3} \\ 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{3}i}{6} & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{3}i}{6} & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{3}i}{6} & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{3}i}{6} & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{3}i}{3} & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| 249 | symmetry | $\frac{3\sqrt{14}x(x^4-10x^2y^2+5y^4)}{16}$ $\begin{bmatrix} 0 & 0 & 0 & -\frac{i}{2} & 0 & 0 & 0 \\ 0 & 0 & -\frac{i}{2} & 0 & 0 & 0 & 0 \\ 0 & \frac{i}{2} & 0 & 0 & 0 & 0 & 0 \\ \frac{i}{2} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| 250 | symmetry | $-\frac{3\sqrt{14}y(5x^4-10x^2y^2+y^4)}{16}$ $\begin{bmatrix} 0 & 0 & -\frac{i}{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{i}{2} & 0 & 0 & 0 \\ \frac{i}{2} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{i}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| 251 | symmetry | $\frac{\sqrt{15}x(x^4+2x^2y^2-12x^2z^2+y^4-12y^2z^2+8z^4)}{8}$ |

continued ...

Table 10

| No. | multipole | matrix |
|-----|-------------------------|--|
| | $M_{5,1}^{(a)}(E_1, 2)$ | $\begin{bmatrix} 0 & 0 & 0 & \frac{\sqrt{210i}}{84} & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{210i}}{84} & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{210i}}{84} & 0 & 0 & 0 & -\frac{3\sqrt{14i}}{28} & 0 \\ -\frac{\sqrt{210i}}{84} & 0 & 0 & 0 & \frac{3\sqrt{14i}}{28} & 0 & 0 \\ 0 & 0 & 0 & -\frac{3\sqrt{14i}}{28} & 0 & 0 & 0 \\ 0 & 0 & \frac{3\sqrt{14i}}{28} & 0 & 0 & 0 & -\frac{\sqrt{210i}}{42} \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{210i}}{42} & 0 \end{bmatrix}$ |
| 252 | symmetry | $\frac{\sqrt{15}y(x^4+2x^2y^2-12x^2z^2+y^4-12y^2z^2+8z^4)}{8}$ |
| | $M_{5,2}^{(a)}(E_1, 2)$ | $\begin{bmatrix} 0 & 0 & \frac{\sqrt{210i}}{84} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{210i}}{84} & 0 & 0 & 0 \\ -\frac{\sqrt{210i}}{84} & 0 & 0 & 0 & -\frac{3\sqrt{14i}}{28} & 0 & 0 \\ 0 & -\frac{\sqrt{210i}}{84} & 0 & 0 & 0 & -\frac{3\sqrt{14i}}{28} & 0 \\ 0 & 0 & \frac{3\sqrt{14i}}{28} & 0 & 0 & 0 & \frac{\sqrt{210i}}{42} \\ 0 & 0 & 0 & \frac{3\sqrt{14i}}{28} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{210i}}{42} & 0 & 0 \end{bmatrix}$ |
| 253 | symmetry | $-\frac{3\sqrt{35}xyz(x-y)(x+y)}{2}$ |
| | $M_{5,1}^{(a)}(E_2, 1)$ | $\begin{bmatrix} 0 & 0 & 0 & 0 & -\frac{i}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{i}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{i}{2} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{i}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| 254 | symmetry | $\frac{3\sqrt{35}z(x^2-2xy-y^2)(x^2+2xy-y^2)}{8}$ |

continued ...

Table 10

| No. | multipole | matrix |
|-----|-------------------------|--|
| | $M_{5,2}^{(a)}(E_2, 1)$ | $\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & -\frac{i}{2} & 0 \\ 0 & 0 & 0 & 0 & -\frac{i}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{i}{2} & 0 & 0 & 0 & 0 & 0 \\ \frac{i}{2} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| 255 | symmetry | $-\frac{\sqrt{105}xyz(x^2+y^2-2z^2)}{2}$ |
| | $M_{5,1}^{(a)}(E_2, 2)$ | $\begin{bmatrix} 0 & 0 & 0 & 0 & -\frac{\sqrt{3}i}{6} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{3}i}{6} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{3}i}{3} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{\sqrt{3}i}{6} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{3}i}{6} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{3}i}{3} & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| 256 | symmetry | $-\frac{\sqrt{105}z(x-y)(x+y)(x^2+y^2-2z^2)}{4}$ |
| | $M_{5,2}^{(a)}(E_2, 2)$ | $\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{3}i}{6} & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{3}i}{6} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{3}i}{3} \\ 0 & -\frac{\sqrt{3}i}{6} & 0 & 0 & 0 & 0 & 0 \\ \frac{\sqrt{3}i}{6} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{3}i}{3} & 0 & 0 & 0 \end{bmatrix}$ |