

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

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

Table 1: (s,s) block.

| No. | multipole                    | matrix                            |
|-----|------------------------------|-----------------------------------|
| 1   | symmetry                     | 1                                 |
|     | $\mathbb{Q}_0^{(a)}(A_{1g})$ | $\begin{bmatrix} 1 \end{bmatrix}$ |

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

Table 2: (s,p) block.

| No. | multipole                        | matrix  |
|-----|----------------------------------|---|
| 2   | symmetry                         | $z$   |
|     | $\mathbb{Q}_1^{(a)}(A_{2u})$     | $\begin{bmatrix} 0 & 0 & \frac{\sqrt{2}}{2} \end{bmatrix}$  |
| 3   | symmetry                         | $x$   |
|     | $\mathbb{Q}_{1,0}^{(a)}(E_{1u})$ | $\begin{bmatrix} \frac{\sqrt{2}}{2} & 0 & 0 \end{bmatrix}$  |
| 4   | symmetry                         | $y$   |
|     | $\mathbb{Q}_{1,1}^{(a)}(E_{1u})$ | $\begin{bmatrix} 0 & \frac{\sqrt{2}}{2} & 0 \end{bmatrix}$  |
| 5   | symmetry                         | $z$   |
|     | $\mathbb{T}_1^{(a)}(A_{2u})$     | $\begin{bmatrix} 0 & 0 & \frac{\sqrt{2}i}{2} \end{bmatrix}$ |
| 6   | symmetry                         | $x$   |
|     | $\mathbb{T}_{1,0}^{(a)}(E_{1u})$ | $\begin{bmatrix} \frac{\sqrt{2}i}{2} & 0 & 0 \end{bmatrix}$ |
| 7   | symmetry                         | $y$   |
|     | $\mathbb{T}_{1,1}^{(a)}(E_{1u})$ | $\begin{bmatrix} 0 & \frac{\sqrt{2}i}{2} & 0 \end{bmatrix}$ |

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

Table 3: (s,d) block.

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

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

Table 4: (s,f) block.

| No. | multipole                        | matrix  |
|-----|----------------------------------|---|
| 18  | symmetry                         | $-\frac{z(3x^2+3y^2-2z^2)}{2}$  |
|     | $\mathbb{Q}_3^{(a)}(A_{2u})$     | $\begin{bmatrix} 0 & 0 & 0 & \frac{\sqrt{2}}{2} & 0 & 0 & 0 \end{bmatrix}$                      |
| 19  | symmetry                         | $\frac{\sqrt{10}y(3x^2-y^2)}{4}$  |
|     | $\mathbb{Q}_3^{(a)}(B_{1u})$     | $\begin{bmatrix} 0 & 0 & -\frac{\sqrt{5}}{4} & 0 & 0 & -\frac{\sqrt{3}}{4} & 0 \end{bmatrix}$   |
| 20  | symmetry                         | $\frac{\sqrt{10}x(x^2-3y^2)}{4}$  |
|     | $\mathbb{Q}_3^{(a)}(B_{2u})$     | $\begin{bmatrix} 0 & \frac{\sqrt{5}}{4} & 0 & 0 & -\frac{\sqrt{3}}{4} & 0 & 0 \end{bmatrix}$    |
| 21  | symmetry                         | $-\frac{\sqrt{6}x(x^2+y^2-4z^2)}{4}$  |
|     | $\mathbb{Q}_{3,0}^{(a)}(E_{1u})$ | $\begin{bmatrix} 0 & -\frac{\sqrt{3}}{4} & 0 & 0 & -\frac{\sqrt{5}}{4} & 0 & 0 \end{bmatrix}$   |
| 22  | symmetry                         | $-\frac{\sqrt{6}y(x^2+y^2-4z^2)}{4}$  |
|     | $\mathbb{Q}_{3,1}^{(a)}(E_{1u})$ | $\begin{bmatrix} 0 & 0 & -\frac{\sqrt{3}}{4} & 0 & 0 & \frac{\sqrt{5}}{4} & 0 \end{bmatrix}$    |
| 23  | symmetry                         | $\sqrt{15}xyz$  |
|     | $\mathbb{Q}_{3,0}^{(a)}(E_{2u})$ | $\begin{bmatrix} \frac{\sqrt{2}}{2} & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$                      |
| 24  | symmetry                         | $\frac{\sqrt{15}z(x-y)(x+y)}{2}$  |
|     | $\mathbb{Q}_{3,1}^{(a)}(E_{2u})$ | $\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{2}}{2} \end{bmatrix}$                      |
| 25  | symmetry                         | $-\frac{z(3x^2+3y^2-2z^2)}{2}$  |
|     | $\mathbb{T}_3^{(a)}(A_{2u})$     | $\begin{bmatrix} 0 & 0 & 0 & \frac{\sqrt{2}i}{2} & 0 & 0 & 0 \end{bmatrix}$                     |
| 26  | symmetry                         | $\frac{\sqrt{10}y(3x^2-y^2)}{4}$  |
|     | $\mathbb{T}_3^{(a)}(B_{1u})$     | $\begin{bmatrix} 0 & 0 & -\frac{\sqrt{5}i}{4} & 0 & 0 & -\frac{\sqrt{3}i}{4} & 0 \end{bmatrix}$ |
| 27  | symmetry                         | $\frac{\sqrt{10}x(x^2-3y^2)}{4}$  |
|     | $\mathbb{T}_3^{(a)}(B_{2u})$     | $\begin{bmatrix} 0 & \frac{\sqrt{5}i}{4} & 0 & 0 & -\frac{\sqrt{3}i}{4} & 0 & 0 \end{bmatrix}$  |
| 28  | symmetry                         | $-\frac{\sqrt{6}x(x^2+y^2-4z^2)}{4}$  |
|     | $\mathbb{T}_{3,0}^{(a)}(E_{1u})$ | $\begin{bmatrix} 0 & -\frac{\sqrt{3}i}{4} & 0 & 0 & -\frac{\sqrt{5}i}{4} & 0 & 0 \end{bmatrix}$ |
| 29  | symmetry                         | $-\frac{\sqrt{6}y(x^2+y^2-4z^2)}{4}$  |
|     | $\mathbb{T}_{3,1}^{(a)}(E_{1u})$ | $\begin{bmatrix} 0 & 0 & -\frac{\sqrt{3}i}{4} & 0 & 0 & \frac{\sqrt{5}i}{4} & 0 \end{bmatrix}$  |
| 30  | symmetry                         | $\sqrt{15}xyz$  |
|     | $\mathbb{T}_{3,0}^{(a)}(E_{2u})$ | $\begin{bmatrix} \frac{\sqrt{2}i}{2} & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$                     |
| 31  | symmetry                         | $\frac{\sqrt{15}z(x-y)(x+y)}{2}$  |

continued ...

Table 4

| No. | multipole                        | matrix  |
|-----|----------------------------------|---|
|     | $\mathbb{T}_{3,1}^{(a)}(E_{2u})$ | $\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{2}i}{2} \end{bmatrix}$ |

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                         | $1$  |
|     | $\mathbb{Q}_0^{(a)}(A_{1g})$     | $\begin{bmatrix} \frac{\sqrt{3}}{3} & 0 & 0 \\ 0 & \frac{\sqrt{3}}{3} & 0 \\ 0 & 0 & \frac{\sqrt{3}}{3} \end{bmatrix}$   |
| 33  | symmetry                         | $-\frac{x^2}{2} - \frac{y^2}{2} + z^2$   |
|     | $\mathbb{Q}_2^{(a)}(A_{1g})$     | $\begin{bmatrix} -\frac{\sqrt{6}}{6} & 0 & 0 \\ 0 & -\frac{\sqrt{6}}{6} & 0 \\ 0 & 0 & \frac{\sqrt{6}}{3} \end{bmatrix}$ |
| 34  | symmetry                         | $\sqrt{3}yz$   |
|     | $\mathbb{Q}_{2,0}^{(a)}(E_{1g})$ | $\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{2}}{2} \\ 0 & \frac{\sqrt{2}}{2} & 0 \end{bmatrix}$                    |
| 35  | symmetry                         | $-\sqrt{3}xz$  |
|     | $\mathbb{Q}_{2,1}^{(a)}(E_{1g})$ | $\begin{bmatrix} 0 & 0 & -\frac{\sqrt{2}}{2} \\ 0 & 0 & 0 \\ -\frac{\sqrt{2}}{2} & 0 & 0 \end{bmatrix}$                  |
| 36  | symmetry                         | $\frac{\sqrt{3}(x-y)(x+y)}{2}$   |
|     | $\mathbb{Q}_{2,0}^{(a)}(E_{2g})$ | $\begin{bmatrix} \frac{\sqrt{2}}{2} & 0 & 0 \\ 0 & -\frac{\sqrt{2}}{2} & 0 \\ 0 & 0 & 0 \end{bmatrix}$                   |

*continued ...*

Table 5

| No. | multipole                        | matrix   |
|-----|----------------------------------|--|
| 37  | symmetry                         | $-\sqrt{3}xy$  |
|     | $\mathbb{Q}_{2,1}^{(a)}(E_{2g})$ | $\begin{bmatrix} 0 & -\frac{\sqrt{2}}{2} & 0 \\ -\frac{\sqrt{2}}{2} & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$  |
| 38  | symmetry                         | $z$  |
|     | $\mathbb{M}_1^{(a)}(A_{2g})$     | $\begin{bmatrix} 0 & -\frac{\sqrt{2}i}{2} & 0 \\ \frac{\sqrt{2}i}{2} & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$ |
| 39  | symmetry                         | $x$  |
|     | $\mathbb{M}_{1,0}^{(a)}(E_{1g})$ | $\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{2}i}{2} \\ 0 & \frac{\sqrt{2}i}{2} & 0 \end{bmatrix}$ |
| 40  | symmetry                         | $y$  |
|     | $\mathbb{M}_{1,1}^{(a)}(E_{1g})$ | $\begin{bmatrix} 0 & 0 & \frac{\sqrt{2}i}{2} \\ 0 & 0 & 0 \\ -\frac{\sqrt{2}i}{2} & 0 & 0 \end{bmatrix}$ |

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

Table 6: (p,d) block.

| No. | multipole                    | matrix   |
|-----|------------------------------|--|
| 41  | symmetry                     | $z$  |
|     | $\mathbb{Q}_1^{(a)}(A_{2u})$ | $\begin{bmatrix} 0 & 0 & 0 & \frac{\sqrt{15}}{10} & 0 \\ 0 & 0 & \frac{\sqrt{15}}{10} & 0 & 0 \\ \frac{\sqrt{5}}{5} & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| 42  | symmetry                     | $x$  |

*continued ...*

Table 6

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

continued ...

Table 6

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

continued ...

Table 6

| No. | multipole | matrix   |
|-----|-----------|--|
|     |           | $\begin{bmatrix} 0 & 0 & 0 & \frac{\sqrt{15}i}{10} & 0 \\ 0 & 0 & \frac{\sqrt{15}i}{10} & 0 & 0 \\ \frac{\sqrt{5}i}{5} & 0 & 0 & 0 & 0 \end{bmatrix}$                        |
| 57  | symmetry  | $x$  |
|     |           | $\begin{bmatrix} -\frac{\sqrt{5}i}{10} & \frac{\sqrt{15}i}{10} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{15}i}{10} \\ 0 & 0 & 0 & \frac{\sqrt{15}i}{10} & 0 \end{bmatrix}$  |
| 58  | symmetry  | $y$  |
|     |           | $\begin{bmatrix} 0 & 0 & 0 & 0 & \frac{\sqrt{15}i}{10} \\ -\frac{\sqrt{5}i}{10} & -\frac{\sqrt{15}i}{10} & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{15}i}{10} & 0 & 0 \end{bmatrix}$ |
| 59  | symmetry  | $-\frac{z(3x^2+3y^2-2z^2)}{2}$   |
|     |           | $\begin{bmatrix} 0 & 0 & 0 & -\frac{\sqrt{10}i}{10} & 0 \\ 0 & 0 & -\frac{\sqrt{10}i}{10} & 0 & 0 \\ \frac{\sqrt{30}i}{10} & 0 & 0 & 0 & 0 \end{bmatrix}$                    |
| 60  | symmetry  | $\frac{\sqrt{10}y(3x^2-y^2)}{4}$   |
|     |           | $\begin{bmatrix} 0 & 0 & 0 & 0 & \frac{i}{2} \\ 0 & \frac{i}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}$  |
| 61  | symmetry  | $\frac{\sqrt{10}x(x^2-3y^2)}{4}$   |
|     |           | $\begin{bmatrix} 0 & \frac{i}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{i}{2} \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}$   |
| 62  | symmetry  | $-\frac{\sqrt{6}x(x^2+y^2-4z^2)}{4}$   |
|     |           | $\begin{bmatrix} \frac{\sqrt{5}i}{5} & -\frac{\sqrt{15}i}{30} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{15}i}{30} \\ 0 & 0 & 0 & \frac{2\sqrt{15}i}{15} & 0 \end{bmatrix}$ |
| 63  | symmetry  | $-\frac{\sqrt{6}y(x^2+y^2-4z^2)}{4}$   |

continued ...

Table 6

| No. | multipole | matrix  |
|-----|-----------|---|
|     |           | $\begin{bmatrix} 0 & 0 & 0 & 0 & -\frac{\sqrt{15}i}{30} \\ \frac{\sqrt{5}i}{5} & \frac{\sqrt{15}i}{30} & 0 & 0 & 0 \\ 0 & 0 & \frac{2\sqrt{15}i}{15} & 0 & 0 \end{bmatrix}$ |
| 64  | symmetry  | $\sqrt{15}xyz$  |
|     |           | $\begin{bmatrix} 0 & 0 & \frac{\sqrt{6}i}{6} & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{6}i}{6} & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{6}i}{6} \end{bmatrix}$                           |
| 65  | symmetry  | $\frac{\sqrt{15}z(x-y)(x+y)}{2}$  |
|     |           | $\begin{bmatrix} 0 & 0 & 0 & \frac{\sqrt{6}i}{6} & 0 \\ 0 & 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 \\ 0 & \frac{\sqrt{6}i}{6} & 0 & 0 & 0 \end{bmatrix}$                          |
| 66  | symmetry  | $-\frac{x^2}{2} - \frac{y^2}{2} + z^2$  |
|     |           | $\begin{bmatrix} 0 & 0 & -\frac{i}{2} & 0 & 0 \\ 0 & 0 & 0 & \frac{i}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}$  |
| 67  | symmetry  | $\sqrt{3}yz$  |
|     |           | $\begin{bmatrix} \frac{i}{2} & \frac{\sqrt{3}i}{6} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{3}i}{6} \\ 0 & 0 & 0 & -\frac{\sqrt{3}i}{6} & 0 \end{bmatrix}$                |
| 68  | symmetry  | $-\sqrt{3}xz$   |
|     |           | $\begin{bmatrix} 0 & 0 & 0 & 0 & \frac{\sqrt{3}i}{6} \\ \frac{i}{2} & -\frac{\sqrt{3}i}{6} & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{3}i}{6} & 0 & 0 \end{bmatrix}$               |
| 69  | symmetry  | $\frac{\sqrt{3}(x-y)(x+y)}{2}$  |
|     |           | $\begin{bmatrix} 0 & 0 & -\frac{\sqrt{3}i}{6} & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{3}i}{6} & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{3}i}{3} \end{bmatrix}$                         |
| 70  | symmetry  | $-\sqrt{3}xy$   |

continued ...

Table 6

| No. | multipole                        | matrix   |
|-----|----------------------------------|--|
|     | $\mathbb{M}_{2,1}^{(a)}(E_{2u})$ | $\begin{bmatrix} 0 & 0 & 0 & -\frac{\sqrt{3}i}{6} & 0 \\ 0 & 0 & \frac{\sqrt{3}i}{6} & 0 & 0 \\ 0 & \frac{\sqrt{3}i}{3} & 0 & 0 & 0 \end{bmatrix}$ |

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

Table 7: (p,f) block.

| No. | multipole | matrix   |
|-----|-----------|--|
| 71  | symmetry  | $-\frac{x^2}{2} - \frac{y^2}{2} + z^2$ $\begin{bmatrix} 0 & -\frac{\sqrt{42}}{28} & 0 & 0 & -\frac{\sqrt{70}}{28} & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{42}}{28} & 0 & 0 & \frac{\sqrt{70}}{28} & 0 \\ 0 & 0 & 0 & \frac{\sqrt{42}}{14} & 0 & 0 & 0 \end{bmatrix}$ |
| 72  | symmetry  | $\sqrt{3}yz$ $\begin{bmatrix} \frac{\sqrt{210}}{42} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{14}}{14} & 0 & 0 & -\frac{\sqrt{210}}{42} \\ 0 & 0 & -\frac{\sqrt{14}}{14} & 0 & 0 & \frac{\sqrt{210}}{42} & 0 \end{bmatrix}$                        |
| 73  | symmetry  | $-\sqrt{3}xz$ $\begin{bmatrix} 0 & 0 & 0 & \frac{\sqrt{14}}{14} & 0 & 0 & -\frac{\sqrt{210}}{42} \\ -\frac{\sqrt{210}}{42} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{14}}{14} & 0 & 0 & \frac{\sqrt{210}}{42} & 0 & 0 \end{bmatrix}$                        |
| 74  | symmetry  | $\frac{\sqrt{3}(x-y)(x+y)}{2}$ $\begin{bmatrix} 0 & \frac{3\sqrt{14}}{28} & 0 & 0 & -\frac{\sqrt{210}}{84} & 0 & 0 \\ 0 & 0 & -\frac{3\sqrt{14}}{28} & 0 & 0 & -\frac{\sqrt{210}}{84} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{210}}{42} \end{bmatrix}$    |
| 75  | symmetry  | $-\sqrt{3}xy$  |

continued ...

Table 7

| No. | multipole                        | matrix  |
|-----|----------------------------------|---|
|     | $\mathbb{Q}_{2,1}^{(a)}(E_{2g})$ | $\begin{bmatrix} 0 & 0 & \frac{\sqrt{14}}{14} & 0 & 0 & \frac{\sqrt{210}}{42} & 0 \\ 0 & \frac{\sqrt{14}}{14} & 0 & 0 & -\frac{\sqrt{210}}{42} & 0 & 0 \\ -\frac{\sqrt{210}}{42} & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$   |
| 76  | symmetry                         | $\frac{3x^4}{8} + \frac{3x^2y^2}{4} - 3x^2z^2 + \frac{3y^4}{8} - 3y^2z^2 + z^4$<br>$\begin{bmatrix} 0 & \frac{3\sqrt{14}}{56} & 0 & 0 & \frac{\sqrt{210}}{56} & 0 & 0 \\ 0 & 0 & \frac{3\sqrt{14}}{56} & 0 & 0 & -\frac{\sqrt{210}}{56} & 0 \\ 0 & 0 & 0 & \frac{\sqrt{14}}{7} & 0 & 0 & 0 \end{bmatrix}$ |
| 77  | symmetry                         | $\frac{\sqrt{70}xz(x^2-3y^2)}{4}$<br>$\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{3}}{4} \\ -\frac{\sqrt{3}}{4} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{5}}{8} & 0 & 0 & -\frac{\sqrt{3}}{8} & 0 & 0 \end{bmatrix}$  |
| 78  | symmetry                         | $\frac{\sqrt{70}yz(3x^2-y^2)}{4}$<br>$\begin{bmatrix} \frac{\sqrt{3}}{4} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{3}}{4} \\ 0 & 0 & -\frac{\sqrt{5}}{8} & 0 & 0 & -\frac{\sqrt{3}}{8} & 0 \end{bmatrix}$  |
| 79  | symmetry                         | $-\frac{\sqrt{10}yz(3x^2+3y^2-4z^2)}{4}$<br>$\begin{bmatrix} -\frac{\sqrt{21}}{28} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{35}}{14} & 0 & 0 & \frac{\sqrt{21}}{28} \\ 0 & 0 & -\frac{3\sqrt{35}}{56} & 0 & 0 & \frac{5\sqrt{21}}{56} & 0 \end{bmatrix}$  |
| 80  | symmetry                         | $\frac{\sqrt{10}xz(3x^2+3y^2-4z^2)}{4}$<br>$\begin{bmatrix} 0 & 0 & 0 & -\frac{\sqrt{35}}{14} & 0 & 0 & \frac{\sqrt{21}}{28} \\ \frac{\sqrt{21}}{28} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{3\sqrt{35}}{56} & 0 & 0 & \frac{5\sqrt{21}}{56} & 0 & 0 \end{bmatrix}$  |
| 81  | symmetry                         | $\frac{\sqrt{35}(x^2-2xy-y^2)(x^2+2xy-y^2)}{8}$<br>$\begin{bmatrix} 0 & \frac{\sqrt{10}}{8} & 0 & 0 & -\frac{\sqrt{6}}{8} & 0 & 0 \\ 0 & 0 & \frac{\sqrt{10}}{8} & 0 & 0 & \frac{\sqrt{6}}{8} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$   |
| 82  | symmetry                         | $\frac{\sqrt{35}xy(x-y)(x+y)}{2}$   |

continued ...

Table 7

| No. | multipole                           | matrix   |
|-----|-------------------------------------|--|
|     | $\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)$ | $\begin{bmatrix} 0 & 0 & -\frac{\sqrt{10}}{8} & 0 & 0 & -\frac{\sqrt{6}}{8} & 0 \\ 0 & \frac{\sqrt{10}}{8} & 0 & 0 & -\frac{\sqrt{6}}{8} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$                           |
| 83  | symmetry                            | $-\frac{\sqrt{5}(x-y)(x+y)(x^2+y^2-6z^2)}{4}$  |
|     | $\mathbb{Q}_{4,0}^{(a)}(E_{2g}, 2)$ | $\begin{bmatrix} 0 & -\frac{\sqrt{70}}{28} & 0 & 0 & -\frac{\sqrt{42}}{28} & 0 & 0 \\ 0 & 0 & \frac{\sqrt{70}}{28} & 0 & 0 & -\frac{\sqrt{42}}{28} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{42}}{14} \end{bmatrix}$  |
| 84  | symmetry                            | $\frac{\sqrt{5}xy(x^2+y^2-6z^2)}{2}$   |
|     | $\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)$ | $\begin{bmatrix} 0 & 0 & \frac{\sqrt{70}}{56} & 0 & 0 & -\frac{3\sqrt{42}}{56} & 0 \\ 0 & \frac{\sqrt{70}}{56} & 0 & 0 & \frac{3\sqrt{42}}{56} & 0 & 0 \\ -\frac{\sqrt{42}}{14} & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| 85  | symmetry                            | $-\frac{z(3x^2+3y^2-2z^2)}{2}$   |
|     | $\mathbb{G}_3^{(a)}(A_{2g})$        | $\begin{bmatrix} 0 & 0 & -\frac{\sqrt{6}}{8} & 0 & 0 & \frac{\sqrt{10}}{8} & 0 \\ 0 & \frac{\sqrt{6}}{8} & 0 & 0 & \frac{\sqrt{10}}{8} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$                             |
| 86  | symmetry                            | $\frac{\sqrt{10}y(3x^2-y^2)}{4}$   |
|     | $\mathbb{G}_3^{(a)}(B_{1g})$        | $\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & -\frac{1}{4} \\ \frac{1}{4} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{15}}{8} & 0 & 0 & -\frac{3}{8} & 0 & 0 \end{bmatrix}$  |
| 87  | symmetry                            | $\frac{\sqrt{10}x(x^2-3y^2)}{4}$   |
|     | $\mathbb{G}_3^{(a)}(B_{2g})$        | $\begin{bmatrix} \frac{1}{4} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{4} \\ 0 & 0 & \frac{\sqrt{15}}{8} & 0 & 0 & \frac{3}{8} & 0 \end{bmatrix}$  |
| 88  | symmetry                            | $-\frac{\sqrt{6}x(x^2+y^2-4z^2)}{4}$   |
|     | $\mathbb{G}_{3,0}^{(a)}(E_{1g})$    | $\begin{bmatrix} \frac{\sqrt{15}}{12} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2} & 0 & 0 & -\frac{\sqrt{15}}{12} \\ 0 & 0 & \frac{1}{8} & 0 & 0 & -\frac{\sqrt{15}}{24} & 0 \end{bmatrix}$                     |
| 89  | symmetry                            | $-\frac{\sqrt{6}y(x^2+y^2-4z^2)}{4}$   |

continued ...

Table 7

| No. | multipole | matrix  |
|-----|-----------|---|
|     |           | $\begin{bmatrix} 0 & 0 & 0 & -\frac{1}{2} & 0 & 0 & -\frac{\sqrt{15}}{12} \\ -\frac{\sqrt{15}}{12} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{1}{8} & 0 & 0 & -\frac{\sqrt{15}}{24} & 0 & 0 \end{bmatrix}$                           |
| 90  | symmetry  | $\sqrt{15}xyz$  |
|     |           | $\begin{bmatrix} 0 & 0 & 0 & 0 & \frac{\sqrt{6}}{6} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{6}}{6} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{6}}{6} \end{bmatrix}$  |
| 91  | symmetry  | $\frac{\sqrt{15}z(x-y)(x+y)}{2}$  |
|     |           | $\begin{bmatrix} 0 & 0 & -\frac{\sqrt{10}}{8} & 0 & 0 & \frac{\sqrt{6}}{24} & 0 \\ 0 & -\frac{\sqrt{10}}{8} & 0 & 0 & -\frac{\sqrt{6}}{24} & 0 & 0 \\ -\frac{\sqrt{6}}{6} & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$                |
| 92  | symmetry  | $-\frac{x^2}{2} - \frac{y^2}{2} + z^2$  |
|     |           | $\begin{bmatrix} 0 & -\frac{\sqrt{42}i}{28} & 0 & 0 & -\frac{\sqrt{70}i}{28} & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{42}i}{28} & 0 & 0 & \frac{\sqrt{70}i}{28} & 0 \\ 0 & 0 & 0 & \frac{\sqrt{42}i}{14} & 0 & 0 & 0 \end{bmatrix}$      |
| 93  | symmetry  | $\sqrt{3}yz$  |
|     |           | $\begin{bmatrix} \frac{\sqrt{210}i}{42} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{14}i}{14} & 0 & 0 & -\frac{\sqrt{210}i}{42} \\ 0 & 0 & -\frac{\sqrt{14}i}{14} & 0 & 0 & \frac{\sqrt{210}i}{42} & 0 \end{bmatrix}$   |
| 94  | symmetry  | $-\sqrt{3}xz$   |
|     |           | $\begin{bmatrix} 0 & 0 & 0 & \frac{\sqrt{14}i}{14} & 0 & 0 & -\frac{\sqrt{210}i}{42} \\ -\frac{\sqrt{210}i}{42} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{14}i}{14} & 0 & 0 & \frac{\sqrt{210}i}{42} & 0 & 0 \end{bmatrix}$    |
| 95  | symmetry  | $\frac{\sqrt{3}(x-y)(x+y)}{2}$  |
|     |           | $\begin{bmatrix} 0 & \frac{3\sqrt{14}i}{28} & 0 & 0 & -\frac{\sqrt{210}i}{84} & 0 & 0 \\ 0 & 0 & -\frac{3\sqrt{14}i}{28} & 0 & 0 & -\frac{\sqrt{210}i}{84} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{210}i}{42} \end{bmatrix}$ |
| 96  | symmetry  | $-\sqrt{3}xy$   |

continued ...

Table 7

| No. | multipole                        | matrix   |
|-----|----------------------------------|--|
|     | $\mathbb{T}_{2,1}^{(a)}(E_{2g})$ | $\begin{bmatrix} 0 & 0 & \frac{\sqrt{14}i}{14} & 0 & 0 & \frac{\sqrt{210}i}{42} & 0 \\ 0 & \frac{\sqrt{14}i}{14} & 0 & 0 & -\frac{\sqrt{210}i}{42} & 0 & 0 \\ -\frac{\sqrt{210}i}{42} & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$   |
| 97  | symmetry                         | $\frac{3x^4}{8} + \frac{3x^2y^2}{4} - 3x^2z^2 + \frac{3y^4}{8} - 3y^2z^2 + z^4$<br>$\begin{bmatrix} 0 & \frac{3\sqrt{14}i}{56} & 0 & 0 & \frac{\sqrt{210}i}{56} & 0 & 0 \\ 0 & 0 & \frac{3\sqrt{14}i}{56} & 0 & 0 & -\frac{\sqrt{210}i}{56} & 0 \\ 0 & 0 & 0 & \frac{\sqrt{14}i}{7} & 0 & 0 & 0 \end{bmatrix}$ |
| 98  | symmetry                         | $\frac{\sqrt{70}xz(x^2-3y^2)}{4}$<br>$\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{3}i}{4} \\ -\frac{\sqrt{3}i}{4} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{5}i}{8} & 0 & 0 & -\frac{\sqrt{3}i}{8} & 0 & 0 \end{bmatrix}$   |
| 99  | symmetry                         | $\frac{\sqrt{70}yz(3x^2-y^2)}{4}$<br>$\begin{bmatrix} \frac{\sqrt{3}i}{4} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{3}i}{4} \\ 0 & 0 & -\frac{\sqrt{5}i}{8} & 0 & 0 & -\frac{\sqrt{3}i}{8} & 0 \end{bmatrix}$   |
| 100 | symmetry                         | $-\frac{\sqrt{10}yz(3x^2+3y^2-4z^2)}{4}$<br>$\begin{bmatrix} -\frac{\sqrt{21}i}{28} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{35}i}{14} & 0 & 0 & \frac{\sqrt{21}i}{28} \\ 0 & 0 & -\frac{3\sqrt{35}i}{56} & 0 & 0 & \frac{5\sqrt{21}i}{56} & 0 \end{bmatrix}$  |
| 101 | symmetry                         | $\frac{\sqrt{10}xz(3x^2+3y^2-4z^2)}{4}$<br>$\begin{bmatrix} 0 & 0 & 0 & -\frac{\sqrt{35}i}{14} & 0 & 0 & \frac{\sqrt{21}i}{28} \\ \frac{\sqrt{21}i}{28} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{3\sqrt{35}i}{56} & 0 & 0 & \frac{5\sqrt{21}i}{56} & 0 & 0 \end{bmatrix}$  |
| 102 | symmetry                         | $\frac{\sqrt{35}(x^2-2xy-y^2)(x^2+2xy-y^2)}{8}$<br>$\begin{bmatrix} 0 & \frac{\sqrt{10}i}{8} & 0 & 0 & -\frac{\sqrt{6}i}{8} & 0 & 0 \\ 0 & 0 & \frac{\sqrt{10}i}{8} & 0 & 0 & \frac{\sqrt{6}i}{8} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$  |
| 103 | symmetry                         | $\frac{\sqrt{35}xy(x-y)(x+y)}{2}$  |

continued ...

Table 7

| No. | multipole                           | matrix  |
|-----|-------------------------------------|---|
|     | $\mathbb{T}_{4,1}^{(a)}(E_{2g}, 1)$ | $\begin{bmatrix} 0 & 0 & -\frac{\sqrt{10}i}{8} & 0 & 0 & -\frac{\sqrt{6}i}{8} & 0 \\ 0 & \frac{\sqrt{10}i}{8} & 0 & 0 & -\frac{\sqrt{6}i}{8} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$                            |
| 104 | symmetry                            | $-\frac{\sqrt{5}(x-y)(x+y)(x^2+y^2-6z^2)}{4}$   |
|     | $\mathbb{T}_{4,0}^{(a)}(E_{2g}, 2)$ | $\begin{bmatrix} 0 & -\frac{\sqrt{70}i}{28} & 0 & 0 & -\frac{\sqrt{42}i}{28} & 0 & 0 \\ 0 & 0 & \frac{\sqrt{70}i}{28} & 0 & 0 & -\frac{\sqrt{42}i}{28} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{42}i}{14} \end{bmatrix}$  |
| 105 | symmetry                            | $\frac{\sqrt{5}xy(x^2+y^2-6z^2)}{2}$  |
|     | $\mathbb{T}_{4,1}^{(a)}(E_{2g}, 2)$ | $\begin{bmatrix} 0 & 0 & \frac{\sqrt{70}i}{56} & 0 & 0 & -\frac{3\sqrt{42}i}{56} & 0 \\ 0 & \frac{\sqrt{70}i}{56} & 0 & 0 & \frac{3\sqrt{42}i}{56} & 0 & 0 \\ -\frac{\sqrt{42}i}{14} & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| 106 | symmetry                            | $-\frac{z(3x^2+3y^2-2z^2)}{2}$  |
|     | $\mathbb{M}_3^{(a)}(A_{2g})$        | $\begin{bmatrix} 0 & 0 & \frac{\sqrt{6}i}{8} & 0 & 0 & -\frac{\sqrt{10}i}{8} & 0 \\ 0 & -\frac{\sqrt{6}i}{8} & 0 & 0 & -\frac{\sqrt{10}i}{8} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$                            |
| 107 | symmetry                            | $\frac{\sqrt{10}y(3x^2-y^2)}{4}$  |
|     | $\mathbb{M}_3^{(a)}(B_{1g})$        | $\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & \frac{i}{4} \\ -\frac{i}{4} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{15}i}{8} & 0 & 0 & \frac{3i}{8} & 0 & 0 \end{bmatrix}$   |
| 108 | symmetry                            | $\frac{\sqrt{10}x(x^2-3y^2)}{4}$  |
|     | $\mathbb{M}_3^{(a)}(B_{2g})$        | $\begin{bmatrix} -\frac{i}{4} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\frac{i}{4} \\ 0 & 0 & -\frac{\sqrt{15}i}{8} & 0 & 0 & -\frac{3i}{8} & 0 \end{bmatrix}$   |
| 109 | symmetry                            | $-\frac{\sqrt{6}x(x^2+y^2-4z^2)}{4}$  |
|     | $\mathbb{M}_{3,0}^{(a)}(E_{1g})$    | $\begin{bmatrix} -\frac{\sqrt{15}i}{12} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{i}{2} & 0 & 0 & \frac{\sqrt{15}i}{12} \\ 0 & 0 & -\frac{i}{8} & 0 & 0 & \frac{\sqrt{15}i}{24} & 0 \end{bmatrix}$                      |
| 110 | symmetry                            | $-\frac{\sqrt{6}y(x^2+y^2-4z^2)}{4}$  |

continued ...

Table 7

| No. | multipole                        | matrix   |
|-----|----------------------------------|--|
|     | $\mathbb{M}_{3,1}^{(a)}(E_{1g})$ | $\begin{bmatrix} 0 & 0 & 0 & \frac{i}{2} & 0 & 0 & \frac{\sqrt{15}i}{12} \\ \frac{\sqrt{15}i}{12} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{i}{8} & 0 & 0 & \frac{\sqrt{15}i}{24} & 0 & 0 \end{bmatrix}$                |
| 111 | symmetry                         | $\sqrt{15}xyz$   |
|     | $\mathbb{M}_{3,0}^{(a)}(E_{2g})$ | $\begin{bmatrix} 0 & 0 & 0 & 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{6}i}{6} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{6}i}{6} \end{bmatrix}$                                       |
| 112 | symmetry                         | $\frac{\sqrt{15}z(x-y)(x+y)}{2}$   |
|     | $\mathbb{M}_{3,1}^{(a)}(E_{2g})$ | $\begin{bmatrix} 0 & 0 & \frac{\sqrt{10}i}{8} & 0 & 0 & -\frac{\sqrt{6}i}{24} & 0 \\ 0 & \frac{\sqrt{10}i}{8} & 0 & 0 & \frac{\sqrt{6}i}{24} & 0 & 0 \\ \frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$ |

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

Table 8: (d,d) block.

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

continued ...

Table 8

| No. | multipole | matrix  |
|-----|-----------|---|
|     |           | $\begin{bmatrix} \frac{\sqrt{14}}{7} & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{14}}{7} & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{14}}{14} & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{14}}{14} & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{14}}{7} \end{bmatrix}$                           |
| 115 | symmetry  | $\sqrt{3}yz$  |
|     |           | $\begin{bmatrix} 0 & 0 & \frac{\sqrt{14}}{14} & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{42}}{14} & 0 & 0 \\ \frac{\sqrt{14}}{14} & -\frac{\sqrt{42}}{14} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{42}}{14} \\ 0 & 0 & 0 & \frac{\sqrt{42}}{14} & 0 \end{bmatrix}$     |
| 116 | symmetry  | $-\sqrt{3}xz$   |
|     |           | $\begin{bmatrix} 0 & 0 & 0 & -\frac{\sqrt{14}}{14} & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{42}}{14} & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{42}}{14} \\ -\frac{\sqrt{14}}{14} & -\frac{\sqrt{42}}{14} & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{42}}{14} & 0 & 0 \end{bmatrix}$ |
| 117 | symmetry  | $\frac{\sqrt{3}(x-y)(x+y)}{2}$  |
|     |           | $\begin{bmatrix} 0 & -\frac{\sqrt{14}}{7} & 0 & 0 & 0 \\ -\frac{\sqrt{14}}{7} & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{42}}{14} & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{42}}{14} & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}$  |
| 118 | symmetry  | $-\sqrt{3}xy$   |

continued ...

Table 8

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

continued ...

Table 8

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

continued ...

Table 8

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

*continued ...*

Table 8

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

continued ...

Table 8

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

bra: =  $\langle d_u |, \langle d_{xz} |, \langle d_{yz} |, \langle d_{xy} |, \langle d_v |$ ket: =  $|f_{az}\rangle, |f_1\rangle, |f_2\rangle, |f_{3x}\rangle, |f_{3y}\rangle, |f_3\rangle, |f_{bz}\rangle$

Table 9: (d,f) block.

| No. | multipole | matrix   |
|-----|-----------|--|
| 138 | symmetry  | $z$  |
|     |           | $\begin{bmatrix} 0 & 0 & 0 & \frac{3\sqrt{70}}{70} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{14}}{14} \\ \mathbb{Q}_1^{(a)}(A_{2u}) & 0 & 0 & -\frac{\sqrt{210}}{70} & 0 & 0 & \frac{\sqrt{14}}{14} \\ 0 & 0 & -\frac{\sqrt{210}}{70} & 0 & 0 & -\frac{\sqrt{14}}{14} & 0 \\ \frac{\sqrt{14}}{14} & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$  |
| 139 | symmetry  | $x$  |
|     |           | $\begin{bmatrix} 0 & -\frac{3\sqrt{70}}{140} & 0 & 0 & -\frac{\sqrt{42}}{28} & 0 & 0 \\ 0 & \frac{3\sqrt{210}}{140} & 0 & 0 & -\frac{\sqrt{14}}{28} & 0 & 0 \\ \mathbb{Q}_{1,0}^{(a)}(E_{1u}) & \frac{\sqrt{14}}{14} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{210}}{70} & 0 & 0 & \frac{\sqrt{14}}{14} \\ 0 & 0 & -\frac{\sqrt{210}}{70} & 0 & 0 & -\frac{\sqrt{14}}{14} & 0 \end{bmatrix}$ |
| 140 | symmetry  | $y$  |
|     |           | $\begin{bmatrix} 0 & 0 & -\frac{3\sqrt{70}}{140} & 0 & 0 & \frac{\sqrt{42}}{28} & 0 \\ 0 & 0 & -\frac{3\sqrt{210}}{140} & 0 & 0 & -\frac{\sqrt{14}}{28} & 0 \\ \mathbb{Q}_{1,1}^{(a)}(E_{1u}) & 0 & 0 & 0 & -\frac{\sqrt{210}}{70} & 0 & -\frac{\sqrt{14}}{14} \\ \frac{\sqrt{14}}{14} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{210}}{70} & 0 & 0 & \frac{\sqrt{14}}{14} & 0 & 0 \end{bmatrix}$ |
| 141 | symmetry  | $-\frac{z(3x^2+3y^2-2z^2)}{2}$   |
|     |           | $\begin{bmatrix} 0 & 0 & 0 & \frac{\sqrt{30}}{15} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{6}}{6} \\ \mathbb{Q}_3^{(a)}(A_{2u}) & 0 & 0 & -\frac{\sqrt{10}}{40} & 0 & 0 & \frac{\sqrt{6}}{24} \\ 0 & -\frac{\sqrt{10}}{40} & 0 & 0 & 0 & -\frac{\sqrt{6}}{24} & 0 \\ -\frac{\sqrt{6}}{6} & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$   |
| 142 | symmetry  | $\frac{\sqrt{10}y(3x^2-y^2)}{4}$   |

*continued ...*

Table 9

| No. | multipole | matrix  |
|-----|-----------|---|
|     |           | $\begin{bmatrix} 0 & 0 & \frac{5\sqrt{3}}{24} & 0 & 0 & \frac{\sqrt{5}}{8} & 0 \\ 0 & 0 & \frac{1}{8} & 0 & 0 & -\frac{\sqrt{15}}{24} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{15}}{12} \\ \frac{\sqrt{15}}{12} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{8} & 0 & 0 & \frac{\sqrt{15}}{24} & 0 & 0 \end{bmatrix}$          |
| 143 | symmetry  | $\frac{\sqrt{10}x(x^2-3y^2)}{4}$  |
|     |           | $\begin{bmatrix} 0 & -\frac{5\sqrt{3}}{24} & 0 & 0 & \frac{\sqrt{5}}{8} & 0 & 0 \\ 0 & \frac{1}{8} & 0 & 0 & \frac{\sqrt{15}}{24} & 0 & 0 \\ -\frac{\sqrt{15}}{12} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{15}}{12} \\ 0 & 0 & -\frac{1}{8} & 0 & 0 & \frac{\sqrt{15}}{24} & 0 \end{bmatrix}$        |
| 144 | symmetry  | $-\frac{\sqrt{6}x(x^2+y^2-4z^2)}{4}$  |
|     |           | $\begin{bmatrix} 0 & -\frac{3\sqrt{5}}{40} & 0 & 0 & -\frac{\sqrt{3}}{8} & 0 & 0 \\ 0 & -\frac{11\sqrt{15}}{120} & 0 & 0 & -\frac{1}{8} & 0 & 0 \\ \frac{1}{4} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{15}}{30} & 0 & 0 & \frac{1}{4} \\ 0 & 0 & -\frac{\sqrt{15}}{120} & 0 & 0 & \frac{3}{8} & 0 \end{bmatrix}$ |
| 145 | symmetry  | $-\frac{\sqrt{6}y(x^2+y^2-4z^2)}{4}$  |
|     |           | $\begin{bmatrix} 0 & 0 & -\frac{3\sqrt{5}}{40} & 0 & 0 & \frac{\sqrt{3}}{8} & 0 \\ 0 & 0 & \frac{11\sqrt{15}}{120} & 0 & 0 & -\frac{1}{8} & 0 \\ 0 & 0 & 0 & \frac{\sqrt{15}}{30} & 0 & 0 & -\frac{1}{4} \\ \frac{1}{4} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{15}}{120} & 0 & 0 & -\frac{3}{8} & 0 & 0 \end{bmatrix}$ |
| 146 | symmetry  | $\sqrt{15}xyz$  |

continued ...

Table 9

| No. | multipole | matrix  |
|-----|-----------|---|
|     |           | $\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{6}}{6} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{6}}{6} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{6}}{6} & 0 & 0 & 0 \end{bmatrix}$   |
| 147 | symmetry  | $\frac{\sqrt{15}z(x-y)(x+y)}{2}$  |
|     |           | $\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{6}}{6} & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{6}}{24} & 0 & 0 & -\frac{\sqrt{10}}{8} & 0 \\ 0 & \frac{\sqrt{6}}{24} & 0 & 0 & -\frac{\sqrt{10}}{8} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$  |
| 148 | symmetry  | $\frac{z(15x^4+30x^2y^2-40x^2z^2+15y^4-40y^2z^2+8z^4)}{8}$  |
|     |           | $\begin{bmatrix} 0 & 0 & 0 & \frac{\sqrt{105}}{21} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{21}}{42} \\ 0 & 0 & \frac{\sqrt{35}}{28} & 0 & 0 & -\frac{5\sqrt{21}}{84} & 0 \\ 0 & \frac{\sqrt{35}}{28} & 0 & 0 & \frac{5\sqrt{21}}{84} & 0 & 0 \\ \frac{\sqrt{21}}{42} & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$                |
| 149 | symmetry  | $-\frac{\sqrt{70}y(3x^2-y^2)(x^2+y^2-8z^2)}{16}$  |
|     |           | $\begin{bmatrix} 0 & 0 & -\frac{\sqrt{6}}{12} & 0 & 0 & -\frac{\sqrt{10}}{20} & 0 \\ 0 & 0 & -\frac{\sqrt{2}}{8} & 0 & 0 & \frac{\sqrt{30}}{24} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{30}}{15} \\ \frac{\sqrt{30}}{15} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{2}}{8} & 0 & 0 & -\frac{\sqrt{30}}{24} & 0 & 0 \end{bmatrix}$ |
| 150 | symmetry  | $-\frac{\sqrt{70}x(x^2-3y^2)(x^2+y^2-8z^2)}{16}$  |

continued ...

Table 9

| No. | multipole | matrix  |
|-----|-----------|---|
|     |           | $\begin{bmatrix} 0 & \frac{\sqrt{6}}{12} & 0 & 0 & -\frac{\sqrt{10}}{20} & 0 & 0 \\ 0 & -\frac{\sqrt{2}}{8} & 0 & 0 & -\frac{\sqrt{30}}{24} & 0 & 0 \\ -\frac{\sqrt{30}}{15} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{30}}{15} \\ 0 & 0 & \frac{\sqrt{2}}{8} & 0 & 0 & -\frac{\sqrt{30}}{24} & 0 \end{bmatrix}$                             |
| 151 | symmetry  | $\frac{3\sqrt{14}x(x^4 - 10x^2y^2 + 5y^4)}{16}$   |
|     |           | $\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{10}}{8} & 0 & 0 & -\frac{\sqrt{6}}{8} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{10}}{8} & 0 & 0 & \frac{\sqrt{6}}{8} & 0 \end{bmatrix}$  |
| 152 | symmetry  | $\frac{-3\sqrt{14}y(5x^4 - 10x^2y^2 + y^4)}{16}$  |
|     |           | $\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{10}}{8} & 0 & 0 & \frac{\sqrt{6}}{8} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{10}}{8} & 0 & 0 & \frac{\sqrt{6}}{8} & 0 & 0 \end{bmatrix}$  |
| 153 | symmetry  | $\frac{\sqrt{15}x(x^4 + 2x^2y^2 - 12x^2z^2 + y^4 - 12y^2z^2 + 8z^4)}{8}$  |
|     |           | $\begin{bmatrix} 0 & -\frac{3\sqrt{7}}{28} & 0 & 0 & -\frac{\sqrt{105}}{28} & 0 & 0 \\ 0 & \frac{\sqrt{21}}{42} & 0 & 0 & \frac{\sqrt{35}}{70} & 0 & 0 \\ -\frac{\sqrt{35}}{35} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{2\sqrt{21}}{21} & 0 & 0 & -\frac{\sqrt{35}}{35} \\ 0 & 0 & \frac{\sqrt{21}}{84} & 0 & 0 & -\frac{3\sqrt{35}}{140} & 0 \end{bmatrix}$ |
| 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  |
|-----|-------------------------------------|---|
|     | $\mathbb{Q}_{5,1}^{(a)}(E_{1u}, 2)$ | $\begin{bmatrix} 0 & 0 & -\frac{3\sqrt{7}}{28} & 0 & 0 & \frac{\sqrt{105}}{28} & 0 \\ 0 & 0 & -\frac{\sqrt{21}}{42} & 0 & 0 & \frac{\sqrt{35}}{70} & 0 \\ 0 & 0 & 0 & \frac{2\sqrt{21}}{21} & 0 & 0 & \frac{\sqrt{35}}{35} \\ -\frac{\sqrt{35}}{35} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{21}}{84} & 0 & 0 & \frac{3\sqrt{35}}{140} & 0 & 0 \end{bmatrix}$ |
| 155 | symmetry                            | $-\frac{3\sqrt{35}xyz(x-y)(x+y)}{2}$  |
|     | $\mathbb{Q}_{5,0}^{(a)}(E_{2u}, 1)$ | $\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -\frac{\sqrt{15}}{10} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{1}{4} & 0 & 0 & \frac{\sqrt{15}}{20} & 0 & 0 \\ 0 & 0 & \frac{1}{4} & 0 & 0 & \frac{\sqrt{15}}{20} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{15}}{10} \end{bmatrix}$  |
| 156 | symmetry                            | $\frac{3\sqrt{35}z(x^2-2xy-y^2)(x^2+2xy-y^2)}{8}$   |
|     | $\mathbb{Q}_{5,1}^{(a)}(E_{2u}, 1)$ | $\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{15}}{10} \\ 0 & 0 & \frac{1}{4} & 0 & 0 & \frac{\sqrt{15}}{20} & 0 \\ 0 & \frac{1}{4} & 0 & 0 & -\frac{\sqrt{15}}{20} & 0 & 0 \\ -\frac{\sqrt{15}}{10} & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$   |
| 157 | symmetry                            | $-\frac{\sqrt{105}xyz(x^2+y^2-2z^2)}{2}$  |
|     | $\mathbb{Q}_{5,0}^{(a)}(E_{2u}, 2)$ | $\begin{bmatrix} \frac{\sqrt{15}}{10} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{3}}{12} & 0 & 0 & -\frac{3\sqrt{5}}{20} & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{3}}{12} & 0 & 0 & \frac{3\sqrt{5}}{20} & 0 \\ 0 & 0 & 0 & \frac{\sqrt{3}}{6} & 0 & 0 & 0 \end{bmatrix}$  |
| 158 | symmetry                            | $-\frac{\sqrt{105}z(x-y)(x+y)(x^2+y^2-2z^2)}{4}$  |

continued ...

Table 9

| No. | multipole | matrix  |
|-----|-----------|---|
|     |           | $\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{15}}{10} \\ 0 & 0 & 0 & \frac{\sqrt{3}}{6} & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{3}}{6} & 0 & 0 & -\frac{\sqrt{5}}{10} & 0 \\ 0 & -\frac{\sqrt{3}}{6} & 0 & 0 & -\frac{\sqrt{5}}{10} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$  |
| 159 | symmetry  | $-\frac{x^2}{2} - \frac{y^2}{2} + z^2$<br>$\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{\sqrt{35}}{14} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{21}}{28} & 0 & 0 & \frac{\sqrt{35}}{28} & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{21}}{28} & 0 & 0 & \frac{\sqrt{35}}{28} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{35}}{14} \end{bmatrix}$ |
| 160 | symmetry  | $\sqrt{3}yz$<br>$\begin{bmatrix} 0 & -\frac{\sqrt{21}}{28} & 0 & 0 & -\frac{\sqrt{35}}{28} & 0 & 0 \\ 0 & -\frac{\sqrt{7}}{28} & 0 & 0 & \frac{\sqrt{105}}{28} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{7}}{7} & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{7}}{7} & 0 & 0 & 0 & 0 \end{bmatrix}$                             |
| 161 | symmetry  | $-\sqrt{3}xz$<br>$\begin{bmatrix} 0 & 0 & -\frac{\sqrt{21}}{28} & 0 & 0 & \frac{\sqrt{35}}{28} & 0 \\ 0 & 0 & \frac{\sqrt{7}}{28} & 0 & 0 & \frac{\sqrt{105}}{28} & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{7}}{7} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{7}}{7} & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$                              |
| 162 | symmetry  | $\frac{\sqrt{3}(x-y)(x+y)}{2}$  |

*continued ...*

Table 9

| No. | multipole | matrix   |
|-----|-----------|--|
|     |           | $\begin{bmatrix} -\frac{\sqrt{35}}{14} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{7}}{28} & 0 & 0 & -\frac{\sqrt{105}}{28} & 0 & 0 \\ 0 & 0 & \frac{\sqrt{7}}{28} & 0 & 0 & \frac{\sqrt{105}}{28} & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{7}}{14} & 0 & 0 & 0 \end{bmatrix}$                        |
| 163 | symmetry  | $-\sqrt{3}xy$  |
|     |           | $\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{35}}{14} \\ 0 & 0 & 0 & -\frac{\sqrt{7}}{14} & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{7}}{7} & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{7}}{7} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$  |
| 164 | symmetry  | $\frac{3x^4}{8} + \frac{3x^2y^2}{4} - 3x^2z^2 + \frac{3y^4}{8} - 3y^2z^2 + z^4$  |
|     |           | $\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -\frac{\sqrt{14}}{14} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{210}}{56} & 0 & 0 & \frac{5\sqrt{14}}{56} & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{210}}{56} & 0 & 0 & \frac{5\sqrt{14}}{56} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{14}}{14} \end{bmatrix}$                    |
| 165 | symmetry  | $\frac{\sqrt{70}xz(x^2-3y^2)}{4}$  |
|     |           | $\begin{bmatrix} 0 & 0 & \frac{3}{8} & 0 & 0 & \frac{3\sqrt{15}}{40} & 0 \\ 0 & 0 & -\frac{\sqrt{3}}{8} & 0 & 0 & \frac{\sqrt{5}}{8} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{5}}{20} \\ -\frac{\sqrt{5}}{20} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{3}}{8} & 0 & 0 & -\frac{\sqrt{5}}{8} & 0 & 0 \end{bmatrix}$ |
| 166 | symmetry  | $\frac{\sqrt{70}yz(3x^2-y^2)}{4}$  |

continued ...

Table 9

| No. | multipole | matrix  |
|-----|-----------|---|
|     |           | $\begin{bmatrix} 0 & \frac{3}{8} & 0 & 0 & -\frac{3\sqrt{15}}{40} & 0 & 0 \\ 0 & \frac{\sqrt{3}}{8} & 0 & 0 & \frac{\sqrt{5}}{8} & 0 & 0 \\ -\frac{\sqrt{5}}{20} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{5}}{20} \\ 0 & 0 & -\frac{\sqrt{3}}{8} & 0 & 0 & \frac{\sqrt{5}}{8} & 0 \end{bmatrix}$  |
| 167 | symmetry  | $-\frac{\sqrt{10}yz(3x^2+3y^2-4z^2)}{4}$  |
|     |           | $\begin{bmatrix} 0 & -\frac{3\sqrt{7}}{56} & 0 & 0 & -\frac{\sqrt{105}}{56} & 0 & 0 \\ 0 & -\frac{\sqrt{21}}{56} & 0 & 0 & -\frac{13\sqrt{35}}{280} & 0 & 0 \\ -\frac{\sqrt{35}}{20} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{21}}{14} & 0 & 0 & -\frac{\sqrt{35}}{20} \\ 0 & 0 & -\frac{3\sqrt{21}}{56} & 0 & 0 & \frac{\sqrt{35}}{40} & 0 \end{bmatrix}$ |
| 168 | symmetry  | $\frac{\sqrt{10}xz(3x^2+3y^2-4z^2)}{4}$   |
|     |           | $\begin{bmatrix} 0 & 0 & -\frac{3\sqrt{7}}{56} & 0 & 0 & \frac{\sqrt{105}}{56} & 0 \\ 0 & 0 & \frac{\sqrt{21}}{56} & 0 & 0 & -\frac{13\sqrt{35}}{280} & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{21}}{14} & 0 & 0 & \frac{\sqrt{35}}{20} \\ -\frac{\sqrt{35}}{20} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{3\sqrt{21}}{56} & 0 & 0 & -\frac{\sqrt{35}}{40} & 0 & 0 \end{bmatrix}$   |
| 169 | symmetry  | $\frac{\sqrt{35}(x^2-2xy-y^2)(x^2+2xy-y^2)}{8}$   |
|     |           | $\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{\sqrt{10}}{10} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{6}}{8} & 0 & 0 & \frac{3\sqrt{10}}{40} & 0 & 0 \\ 0 & 0 & \frac{\sqrt{6}}{8} & 0 & 0 & \frac{3\sqrt{10}}{40} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{10}}{10} \end{bmatrix}$  |
| 170 | symmetry  | $\frac{\sqrt{35}xy(x-y)(x+y)}{2}$   |

continued ...

Table 9

| No. | multipole | matrix  |
|-----|-----------|---|
|     |           | $\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{10}}{10} \\ 0 & 0 & \frac{\sqrt{6}}{8} & 0 & 0 & \frac{3\sqrt{10}}{40} & 0 \\ 0 & \frac{\sqrt{6}}{8} & 0 & 0 & -\frac{3\sqrt{10}}{40} & 0 & 0 \\ \frac{\sqrt{10}}{10} & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$                                 |
| 171 | symmetry  | $-\frac{\sqrt{5}(x-y)(x+y)(x^2+y^2-6z^2)}{4}$   |
|     |           | $\begin{bmatrix} -\frac{\sqrt{210}}{35} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{42}}{28} & 0 & 0 & \frac{\sqrt{70}}{140} & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{42}}{28} & 0 & 0 & -\frac{\sqrt{70}}{140} & 0 \\ 0 & 0 & 0 & \frac{\sqrt{42}}{14} & 0 & 0 & 0 \end{bmatrix}$                          |
| 172 | symmetry  | $\frac{\sqrt{5}xy(x^2+y^2-6z^2)}{2}$  |
|     |           | $\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{210}}{35} \\ 0 & 0 & 0 & \frac{\sqrt{42}}{14} & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{42}}{56} & 0 & 0 & -\frac{\sqrt{70}}{40} & 0 \\ 0 & \frac{\sqrt{42}}{56} & 0 & 0 & -\frac{\sqrt{70}}{40} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$                            |
| 173 | symmetry  | $z$   |
|     |           | $\begin{bmatrix} 0 & 0 & 0 & \frac{3\sqrt{70}i}{70} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{14}i}{14} \\ 0 & 0 & -\frac{\sqrt{210}i}{70} & 0 & 0 & \frac{\sqrt{14}i}{14} & 0 \\ 0 & -\frac{\sqrt{210}i}{70} & 0 & 0 & -\frac{\sqrt{14}i}{14} & 0 & 0 \\ \frac{\sqrt{14}i}{14} & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| 174 | symmetry  | $x$   |

continued ...

Table 9

| No. | multipole | matrix  |
|-----|-----------|---|
|     |           | $\begin{bmatrix} 0 & -\frac{3\sqrt{70}i}{140} & 0 & 0 & -\frac{\sqrt{42}i}{28} & 0 & 0 \\ 0 & \frac{3\sqrt{210}i}{140} & 0 & 0 & -\frac{\sqrt{14}i}{28} & 0 & 0 \\ \frac{\sqrt{14}i}{14} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{210}i}{70} & 0 & 0 & \frac{\sqrt{14}i}{14} \\ 0 & 0 & -\frac{\sqrt{210}i}{70} & 0 & 0 & -\frac{\sqrt{14}i}{14} & 0 \end{bmatrix}$        |
| 175 | symmetry  | $y$<br>$\begin{bmatrix} 0 & 0 & -\frac{3\sqrt{70}i}{140} & 0 & 0 & \frac{\sqrt{42}i}{28} & 0 \\ 0 & 0 & -\frac{3\sqrt{210}i}{140} & 0 & 0 & -\frac{\sqrt{14}i}{28} & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{210}i}{70} & 0 & 0 & -\frac{\sqrt{14}i}{14} \\ \frac{\sqrt{14}i}{14} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{210}i}{70} & 0 & 0 & \frac{\sqrt{14}i}{14} & 0 & 0 \end{bmatrix}$ |
| 176 | symmetry  | $-\frac{z(3x^2+3y^2-2z^2)}{2}$<br>$\begin{bmatrix} 0 & 0 & 0 & \frac{\sqrt{30}i}{15} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{6}i}{6} \\ 0 & 0 & -\frac{\sqrt{10}i}{40} & 0 & 0 & \frac{\sqrt{6}i}{24} & 0 \\ 0 & -\frac{\sqrt{10}i}{40} & 0 & 0 & -\frac{\sqrt{6}i}{24} & 0 & 0 \\ -\frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$                            |
| 177 | symmetry  | $\frac{\sqrt{10}y(3x^2-y^2)}{4}$<br>$\begin{bmatrix} 0 & 0 & \frac{5\sqrt{3}i}{24} & 0 & 0 & \frac{\sqrt{5}i}{8} & 0 \\ 0 & 0 & \frac{i}{8} & 0 & 0 & -\frac{\sqrt{15}i}{24} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{15}i}{12} \\ \frac{\sqrt{15}i}{12} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{i}{8} & 0 & 0 & \frac{\sqrt{15}i}{24} & 0 & 0 \end{bmatrix}$                          |
| 178 | symmetry  | $\frac{\sqrt{10}x(x^2-3y^2)}{4}$  |

continued ...

Table 9

| No. | multipole | matrix  |
|-----|-----------|---|
|     |           | $\begin{bmatrix} 0 & -\frac{5\sqrt{3}i}{24} & 0 & 0 & \frac{\sqrt{5}i}{8} & 0 & 0 \\ 0 & \frac{i}{8} & 0 & 0 & \frac{\sqrt{15}i}{24} & 0 & 0 \\ -\frac{\sqrt{15}i}{12} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{15}i}{12} \\ 0 & 0 & -\frac{i}{8} & 0 & 0 & \frac{\sqrt{15}i}{24} & 0 \end{bmatrix}$        |
| 179 | symmetry  | $-\frac{\sqrt{6}x(x^2+y^2-4z^2)}{4}$  |
|     |           | $\begin{bmatrix} 0 & -\frac{3\sqrt{5}i}{40} & 0 & 0 & -\frac{\sqrt{3}i}{8} & 0 & 0 \\ 0 & -\frac{11\sqrt{15}i}{120} & 0 & 0 & -\frac{i}{8} & 0 & 0 \\ \frac{i}{4} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{15}i}{30} & 0 & 0 & \frac{i}{4} \\ 0 & 0 & -\frac{\sqrt{15}i}{120} & 0 & 0 & \frac{3i}{8} & 0 \end{bmatrix}$ |
| 180 | symmetry  | $-\frac{\sqrt{6}y(x^2+y^2-4z^2)}{4}$  |
|     |           | $\begin{bmatrix} 0 & 0 & -\frac{3\sqrt{5}i}{40} & 0 & 0 & \frac{\sqrt{3}i}{8} & 0 \\ 0 & 0 & \frac{11\sqrt{15}i}{120} & 0 & 0 & -\frac{i}{8} & 0 \\ 0 & 0 & 0 & \frac{\sqrt{15}i}{30} & 0 & 0 & -\frac{i}{4} \\ \frac{i}{4} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{15}i}{120} & 0 & 0 & -\frac{3i}{8} & 0 & 0 \end{bmatrix}$ |
| 181 | symmetry  | $\sqrt{15}xyz$  |
|     |           | $\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 & 0 \end{bmatrix}$  |
| 182 | symmetry  | $\frac{\sqrt{15}z(x-y)(x+y)}{2}$  |

continued ...

Table 9

| No. | multipole                        | matrix   |
|-----|----------------------------------|--|
|     | $\mathbb{T}_{3,1}^{(a)}(E_{2u})$ | $\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{6}i}{24} & 0 & 0 & -\frac{\sqrt{10}i}{8} & 0 \\ 0 & \frac{\sqrt{6}i}{24} & 0 & 0 & -\frac{\sqrt{10}i}{8} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$  |
| 183 | symmetry                         | $\frac{z(15x^4 + 30x^2y^2 - 40x^2z^2 + 15y^4 - 40y^2z^2 + 8z^4)}{8}$ $\begin{bmatrix} 0 & 0 & 0 & \frac{\sqrt{105}i}{21} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{21}i}{42} \\ 0 & 0 & \frac{\sqrt{35}i}{28} & 0 & 0 & -\frac{5\sqrt{21}i}{84} & 0 \\ 0 & \frac{\sqrt{35}i}{28} & 0 & 0 & \frac{5\sqrt{21}i}{84} & 0 & 0 \\ \frac{\sqrt{21}i}{42} & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$   |
| 184 | symmetry                         | $-\frac{\sqrt{70}y(3x^2 - y^2)(x^2 + y^2 - 8z^2)}{16}$ $\begin{bmatrix} 0 & 0 & -\frac{\sqrt{6}i}{12} & 0 & 0 & -\frac{\sqrt{10}i}{20} & 0 \\ 0 & 0 & -\frac{\sqrt{2}i}{8} & 0 & 0 & \frac{\sqrt{30}i}{24} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{30}i}{15} \\ \frac{\sqrt{30}i}{15} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{2}i}{8} & 0 & 0 & -\frac{\sqrt{30}i}{24} & 0 & 0 \end{bmatrix}$ |
| 185 | symmetry                         | $-\frac{\sqrt{70}x(x^2 - 3y^2)(x^2 + y^2 - 8z^2)}{16}$ $\begin{bmatrix} 0 & \frac{\sqrt{6}i}{12} & 0 & 0 & -\frac{\sqrt{10}i}{20} & 0 & 0 \\ 0 & -\frac{\sqrt{2}i}{8} & 0 & 0 & -\frac{\sqrt{30}i}{24} & 0 & 0 \\ -\frac{\sqrt{30}i}{15} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{30}i}{15} \\ 0 & 0 & \frac{\sqrt{2}i}{8} & 0 & 0 & -\frac{\sqrt{30}i}{24} & 0 \end{bmatrix}$ |
| 186 | symmetry                         | $\frac{3\sqrt{14}x(x^4 - 10x^2y^2 + 5y^4)}{16}$  |

continued ...

Table 9

| No. | multipole | matrix   |
|-----|-----------|--|
|     |           | $\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{10}i}{8} & 0 & 0 & -\frac{\sqrt{6}i}{8} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{10}i}{8} & 0 & 0 & \frac{\sqrt{6}i}{8} & 0 \end{bmatrix}$   |
| 187 | symmetry  | $-\frac{3\sqrt{14}y(5x^4 - 10x^2y^2 + y^4)}{16}$   |
|     |           | $\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{10}i}{8} & 0 & 0 & \frac{\sqrt{6}i}{8} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{10}i}{8} & 0 & 0 & \frac{\sqrt{6}i}{8} & 0 & 0 \end{bmatrix}$   |
| 188 | symmetry  | $\frac{\sqrt{15}x(x^4 + 2x^2y^2 - 12x^2z^2 + y^4 - 12y^2z^2 + 8z^4)}{8}$   |
|     |           | $\begin{bmatrix} 0 & -\frac{3\sqrt{7}i}{28} & 0 & 0 & -\frac{\sqrt{105}i}{28} & 0 & 0 \\ 0 & \frac{\sqrt{21}i}{42} & 0 & 0 & \frac{\sqrt{35}i}{70} & 0 & 0 \\ -\frac{\sqrt{35}i}{35} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{2\sqrt{21}i}{21} & 0 & 0 & -\frac{\sqrt{35}i}{35} \\ 0 & 0 & \frac{\sqrt{21}i}{84} & 0 & 0 & -\frac{3\sqrt{35}i}{140} & 0 \end{bmatrix}$ |
| 189 | symmetry  | $\frac{\sqrt{15}y(x^4 + 2x^2y^2 - 12x^2z^2 + y^4 - 12y^2z^2 + 8z^4)}{8}$   |
|     |           | $\begin{bmatrix} 0 & 0 & -\frac{3\sqrt{7}i}{28} & 0 & 0 & \frac{\sqrt{105}i}{28} & 0 \\ 0 & 0 & -\frac{\sqrt{21}i}{42} & 0 & 0 & \frac{\sqrt{35}i}{70} & 0 \\ 0 & 0 & 0 & \frac{2\sqrt{21}i}{21} & 0 & 0 & \frac{\sqrt{35}i}{35} \\ -\frac{\sqrt{35}i}{35} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{21}i}{84} & 0 & 0 & \frac{3\sqrt{35}i}{140} & 0 & 0 \end{bmatrix}$   |
| 190 | symmetry  | $-\frac{3\sqrt{35}xyz(x-y)(x+y)}{2}$   |

continued ...

Table 9

| No. | multipole | matrix   |
|-----|-----------|--|
|     |           | $\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -\frac{\sqrt{15}i}{10} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{i}{4} & 0 & 0 & \frac{\sqrt{15}i}{20} & 0 & 0 \\ 0 & 0 & \frac{i}{4} & 0 & 0 & \frac{\sqrt{15}i}{20} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{15}i}{10} \end{bmatrix}$                 |
| 191 | symmetry  | $\frac{3\sqrt{35}z(x^2-2xy-y^2)(x^2+2xy-y^2)}{8}$  |
|     |           | $\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{15}i}{10} \\ 0 & 0 & \frac{i}{4} & 0 & 0 & \frac{\sqrt{15}i}{20} & 0 \\ 0 & \frac{i}{4} & 0 & 0 & -\frac{\sqrt{15}i}{20} & 0 & 0 \\ -\frac{\sqrt{15}i}{10} & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$                  |
| 192 | symmetry  | $-\frac{\sqrt{105}xyz(x^2+y^2-2z^2)}{2}$   |
|     |           | $\begin{bmatrix} \frac{\sqrt{15}i}{10} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{3}i}{12} & 0 & 0 & -\frac{3\sqrt{5}i}{20} & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{3}i}{12} & 0 & 0 & \frac{3\sqrt{5}i}{20} & 0 \\ 0 & 0 & 0 & \frac{\sqrt{3}i}{6} & 0 & 0 & 0 \end{bmatrix}$ |
| 193 | symmetry  | $-\frac{\sqrt{105}z(x-y)(x+y)(x^2+y^2-2z^2)}{4}$   |
|     |           | $\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{15}i}{10} \\ 0 & 0 & 0 & \frac{\sqrt{3}i}{6} & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{3}i}{6} & 0 & 0 & -\frac{\sqrt{5}i}{10} & 0 \\ 0 & -\frac{\sqrt{3}i}{6} & 0 & 0 & -\frac{\sqrt{5}i}{10} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$     |
| 194 | symmetry  | $-\frac{x^2}{2} - \frac{y^2}{2} + z^2$   |

*continued ...*

Table 9

| No. | multipole | matrix  |
|-----|-----------|---|
|     |           | $\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -\frac{\sqrt{35}i}{14} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{21}i}{28} & 0 & 0 & -\frac{\sqrt{35}i}{28} & 0 & 0 \\ 0 & 0 & \frac{\sqrt{21}i}{28} & 0 & 0 & -\frac{\sqrt{35}i}{28} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{35}i}{14} \end{bmatrix}$ |
| 195 | symmetry  | $\sqrt{3}yz$  |
|     |           | $\begin{bmatrix} 0 & \frac{\sqrt{21}i}{28} & 0 & 0 & \frac{\sqrt{35}i}{28} & 0 & 0 \\ 0 & \frac{\sqrt{7}i}{28} & 0 & 0 & -\frac{\sqrt{105}i}{28} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{7}i}{7} & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{7}i}{7} & 0 & 0 & 0 & 0 \end{bmatrix}$       |
| 196 | symmetry  | $-\sqrt{3}xz$   |
|     |           | $\begin{bmatrix} 0 & 0 & \frac{\sqrt{21}i}{28} & 0 & 0 & -\frac{\sqrt{35}i}{28} & 0 \\ 0 & 0 & -\frac{\sqrt{7}i}{28} & 0 & 0 & -\frac{\sqrt{105}i}{28} & 0 \\ 0 & 0 & 0 & \frac{\sqrt{7}i}{7} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{7}i}{7} & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$     |
| 197 | symmetry  | $\frac{\sqrt{3}(x-y)(x+y)}{2}$  |
|     |           | $\begin{bmatrix} \frac{\sqrt{35}i}{14} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{7}i}{28} & 0 & 0 & \frac{\sqrt{105}i}{28} & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{7}i}{28} & 0 & 0 & -\frac{\sqrt{105}i}{28} & 0 \\ 0 & 0 & 0 & \frac{\sqrt{7}i}{14} & 0 & 0 & 0 \end{bmatrix}$   |
| 198 | symmetry  | $-\sqrt{3}xy$   |

continued ...

Table 9

| No. | multipole | matrix   |
|-----|-----------|--|
|     |           | $\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{35}i}{14} \\ 0 & 0 & 0 & \frac{\sqrt{7}i}{14} & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{7}i}{7} & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{7}i}{7} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$  |
| 199 | symmetry  | $\frac{3x^4}{8} + \frac{3x^2y^2}{4} - 3x^2z^2 + \frac{3y^4}{8} - 3y^2z^2 + z^4$<br>$\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{\sqrt{14}i}{14} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{210}i}{56} & 0 & 0 & -\frac{5\sqrt{14}i}{56} & 0 & 0 \\ 0 & 0 & \frac{\sqrt{210}i}{56} & 0 & 0 & -\frac{5\sqrt{14}i}{56} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{14}i}{14} \end{bmatrix}$ |
| 200 | symmetry  | $\frac{\sqrt{70}xz(x^2-3y^2)}{4}$<br>$\begin{bmatrix} 0 & 0 & -\frac{3i}{8} & 0 & 0 & -\frac{3\sqrt{15}i}{40} & 0 \\ 0 & 0 & \frac{\sqrt{3}i}{8} & 0 & 0 & -\frac{\sqrt{5}i}{8} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{5}i}{20} \\ \frac{\sqrt{5}i}{20} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{3}i}{8} & 0 & 0 & \frac{\sqrt{5}i}{8} & 0 & 0 \end{bmatrix}$                              |
| 201 | symmetry  | $\frac{\sqrt{70}yz(3x^2-y^2)}{4}$<br>$\begin{bmatrix} 0 & -\frac{3i}{8} & 0 & 0 & \frac{3\sqrt{15}i}{40} & 0 & 0 \\ 0 & -\frac{\sqrt{3}i}{8} & 0 & 0 & -\frac{\sqrt{5}i}{8} & 0 & 0 \\ \frac{\sqrt{5}i}{20} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{5}i}{20} \\ 0 & 0 & \frac{\sqrt{3}i}{8} & 0 & 0 & -\frac{\sqrt{5}i}{8} & 0 \end{bmatrix}$                            |
| 202 | symmetry  | $-\frac{\sqrt{10}yz(3x^2+3y^2-4z^2)}{4}$   |

continued ...

Table 9

| No. | multipole | matrix  |
|-----|-----------|---|
|     |           | $\begin{bmatrix} 0 & \frac{3\sqrt{7}i}{56} & 0 & 0 & \frac{\sqrt{105}i}{56} & 0 & 0 \\ 0 & \frac{\sqrt{21}i}{56} & 0 & 0 & \frac{13\sqrt{35}i}{280} & 0 & 0 \\ \frac{\sqrt{35}i}{20} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{21}i}{14} & 0 & 0 & \frac{\sqrt{35}i}{20} \\ 0 & 0 & \frac{3\sqrt{21}i}{56} & 0 & 0 & -\frac{\sqrt{35}i}{40} & 0 \end{bmatrix}$   |
| 203 | symmetry  | $\frac{\sqrt{10}xz(3x^2+3y^2-4z^2)}{4}$   |
|     |           | $\begin{bmatrix} 0 & 0 & \frac{3\sqrt{7}i}{56} & 0 & 0 & -\frac{\sqrt{105}i}{56} & 0 \\ 0 & 0 & -\frac{\sqrt{21}i}{56} & 0 & 0 & \frac{13\sqrt{35}i}{280} & 0 \\ 0 & 0 & 0 & \frac{\sqrt{21}i}{14} & 0 & 0 & -\frac{\sqrt{35}i}{20} \\ \frac{\sqrt{35}i}{20} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{3\sqrt{21}i}{56} & 0 & 0 & \frac{\sqrt{35}i}{40} & 0 & 0 \end{bmatrix}$ |
| 204 | symmetry  | $\frac{\sqrt{35}(x^2-2xy-y^2)(x^2+2xy-y^2)}{8}$   |
|     |           | $\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -\frac{\sqrt{10}i}{10} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{6}i}{8} & 0 & 0 & -\frac{3\sqrt{10}i}{40} & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{6}i}{8} & 0 & 0 & -\frac{3\sqrt{10}i}{40} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{10}i}{10} \end{bmatrix}$  |
| 205 | symmetry  | $\frac{\sqrt{35}xy(x-y)(x+y)}{2}$   |
|     |           | $\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{10}i}{10} \\ 0 & 0 & -\frac{\sqrt{6}i}{8} & 0 & 0 & -\frac{3\sqrt{10}i}{40} & 0 \\ 0 & -\frac{\sqrt{6}i}{8} & 0 & 0 & \frac{3\sqrt{10}i}{40} & 0 & 0 \\ -\frac{\sqrt{10}i}{10} & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$   |
| 206 | symmetry  | $-\frac{\sqrt{5}(x-y)(x+y)(x^2+y^2-6z^2)}{4}$   |

continued ...

Table 9

| No. | multipole                           | matrix   |
|-----|-------------------------------------|--|
|     | $\mathbb{M}_{4,0}^{(a)}(E_{2u}, 2)$ | $\begin{bmatrix} \frac{\sqrt{210}i}{35} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{42}i}{28} & 0 & 0 & -\frac{\sqrt{70}i}{140} & 0 & 0 \\ 0 & 0 & \frac{\sqrt{42}i}{28} & 0 & 0 & \frac{\sqrt{70}i}{140} & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{42}i}{14} & 0 & 0 & 0 \end{bmatrix}$                                     |
| 207 | symmetry                            | $\frac{\sqrt{5}xy(x^2+y^2-6z^2)}{2}$ $\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{210}i}{35} \\ 0 & 0 & 0 & -\frac{\sqrt{42}i}{14} & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{42}i}{56} & 0 & 0 & \frac{\sqrt{70}i}{40} & 0 \\ 0 & -\frac{\sqrt{42}i}{56} & 0 & 0 & \frac{\sqrt{70}i}{40} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$ |

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

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  |
|-----|-----------|---|
|     |           | $\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{21}}{21} & 0 & 0 & \frac{\sqrt{35}}{14} & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{21}}{21} & 0 & 0 & -\frac{\sqrt{35}}{14} & 0 \\ 0 & 0 & 0 & \frac{2\sqrt{21}}{21} & 0 & 0 & 0 \\ 0 & \frac{\sqrt{35}}{14} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{35}}{14} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$   |
| 210 | symmetry  | $\sqrt{3}yz$  |
|     |           | $\begin{bmatrix} 0 & -\frac{\sqrt{105}}{21} & 0 & 0 & 0 & 0 & 0 \\ -\frac{\sqrt{105}}{21} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{7}}{28} & 0 & 0 & -\frac{\sqrt{105}}{84} \\ 0 & 0 & -\frac{\sqrt{7}}{28} & 0 & 0 & \frac{\sqrt{105}}{84} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{105}}{84} & 0 & 0 & -\frac{5\sqrt{7}}{28} \\ 0 & 0 & -\frac{\sqrt{105}}{84} & 0 & 0 & -\frac{5\sqrt{7}}{28} & 0 \end{bmatrix}$ |
| 211 | symmetry  | $-\sqrt{3}xz$   |
|     |           | $\begin{bmatrix} 0 & 0 & \frac{\sqrt{105}}{21} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{7}}{28} & 0 & 0 & -\frac{\sqrt{105}}{84} \\ \frac{\sqrt{105}}{21} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{7}}{28} & 0 & 0 & \frac{\sqrt{105}}{84} & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{105}}{84} & 0 & 0 & \frac{5\sqrt{7}}{28} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{105}}{84} & 0 & 0 & 0 & \frac{5\sqrt{7}}{28} & 0 \end{bmatrix}$       |
| 212 | symmetry  | $\frac{\sqrt{3}(x-y)(x+y)}{2}$  |

continued ...

Table 10

| No. | multipole | matrix  |
|-----|-----------|---|
|     |           | $\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{7}}{7} & 0 & 0 & \frac{\sqrt{105}}{42} & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{7}}{7} & 0 & 0 & \frac{\sqrt{105}}{42} & 0 \\ \mathbb{Q}_{2,0}^{(a)}(E_{2g}) & 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{105}}{21} \\ 0 & \frac{\sqrt{105}}{42} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{105}}{42} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{105}}{21} & 0 & 0 & 0 \end{bmatrix}$   |
| 213 | symmetry  | $-\sqrt{3}xy$   |
|     |           | $\begin{bmatrix} 0 & 0 & 0 & \frac{\sqrt{105}}{21} & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{7}}{28} & 0 & 0 & \frac{\sqrt{105}}{84} & 0 \\ 0 & \frac{\sqrt{7}}{28} & 0 & 0 & -\frac{\sqrt{105}}{84} & 0 & 0 \\ \frac{\sqrt{105}}{21} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{105}}{84} & 0 & 0 & \frac{5\sqrt{7}}{28} & 0 \\ 0 & \frac{\sqrt{105}}{84} & 0 & 0 & \frac{5\sqrt{7}}{28} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$   |
| 214 | symmetry  | $\frac{3x^4}{8} + \frac{3x^2y^2}{4} - 3x^2z^2 + \frac{3y^4}{8} - 3y^2z^2 + z^4$   |
|     |           | $\begin{bmatrix} -\frac{\sqrt{154}}{22} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{9\sqrt{154}}{616} & 0 & 0 & -\frac{\sqrt{2310}}{616} & 0 & 0 \\ 0 & 0 & \frac{9\sqrt{154}}{616} & 0 & 0 & \frac{\sqrt{2310}}{616} & 0 \\ \mathbb{Q}_4^{(a)}(A_{1g}) & 0 & 0 & 0 & \frac{3\sqrt{154}}{77} & 0 & 0 \\ 0 & -\frac{\sqrt{2310}}{616} & 0 & 0 & \frac{\sqrt{154}}{88} & 0 & 0 \\ 0 & 0 & \frac{\sqrt{2310}}{616} & 0 & 0 & \frac{\sqrt{154}}{88} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{154}}{22} \end{bmatrix}$ |
| 215 | symmetry  | $\frac{\sqrt{70}xz(x^2-3y^2)}{4}$   |

continued ...

Table 10

| No. | multipole | matrix  |
|-----|-----------|---|
|     |           | $\begin{bmatrix} 0 & 0 & \frac{\sqrt{33}}{44} & 0 & 0 & -\frac{\sqrt{55}}{44} & 0 \\ 0 & 0 & 0 & -\frac{3\sqrt{55}}{44} & 0 & 0 & -\frac{\sqrt{33}}{44} \\ \frac{\sqrt{33}}{44} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{3\sqrt{55}}{44} & 0 & 0 & \frac{3\sqrt{33}}{44} & 0 & 0 \\ 0 & 0 & 0 & \frac{3\sqrt{33}}{44} & 0 & 0 & -\frac{\sqrt{55}}{44} \\ -\frac{\sqrt{55}}{44} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{33}}{44} & 0 & 0 & -\frac{\sqrt{55}}{44} & 0 & 0 \end{bmatrix}$                       |
| 216 | symmetry  | $\frac{\sqrt{70}yz(3x^2-y^2)}{4}$   |
|     |           | $\begin{bmatrix} 0 & -\frac{\sqrt{33}}{44} & 0 & 0 & -\frac{\sqrt{55}}{44} & 0 & 0 \\ -\frac{\sqrt{33}}{44} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{3\sqrt{55}}{44} & 0 & 0 & -\frac{\sqrt{33}}{44} \\ 0 & 0 & \frac{3\sqrt{55}}{44} & 0 & 0 & \frac{3\sqrt{33}}{44} & 0 \\ -\frac{\sqrt{55}}{44} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{3\sqrt{33}}{44} & 0 & 0 & \frac{\sqrt{55}}{44} \\ 0 & 0 & -\frac{\sqrt{33}}{44} & 0 & 0 & \frac{\sqrt{55}}{44} & 0 \end{bmatrix}$                         |
| 217 | symmetry  | $-\frac{\sqrt{10}yz(3x^2+3y^2-4z^2)}{4}$  |
|     |           | $\begin{bmatrix} 0 & \frac{\sqrt{231}}{308} & 0 & 0 & -\frac{\sqrt{385}}{44} & 0 & 0 \\ \frac{\sqrt{231}}{308} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{3\sqrt{385}}{308} & 0 & 0 & \frac{9\sqrt{231}}{308} \\ 0 & 0 & -\frac{3\sqrt{385}}{308} & 0 & 0 & \frac{5\sqrt{231}}{308} & 0 \\ -\frac{\sqrt{385}}{44} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{5\sqrt{231}}{308} & 0 & 0 & -\frac{\sqrt{385}}{308} \\ 0 & 0 & \frac{9\sqrt{231}}{308} & 0 & 0 & -\frac{\sqrt{385}}{308} & 0 \end{bmatrix}$ |
| 218 | symmetry  | $\frac{\sqrt{10}xz(3x^2+3y^2-4z^2)}{4}$   |

continued ...

Table 10

| No. | multipole | matrix  |
|-----|-----------|---|
|     |           | $\begin{bmatrix} 0 & 0 & -\frac{\sqrt{231}}{308} & 0 & 0 & -\frac{\sqrt{385}}{44} & 0 \\ 0 & 0 & 0 & \frac{3\sqrt{385}}{308} & 0 & 0 & \frac{9\sqrt{231}}{308} \\ -\frac{\sqrt{231}}{308} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{3\sqrt{385}}{308} & 0 & 0 & \frac{5\sqrt{231}}{308} & 0 & 0 \\ 0 & 0 & 0 & \frac{5\sqrt{231}}{308} & 0 & 0 & \frac{\sqrt{385}}{308} \\ -\frac{\sqrt{385}}{44} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{9\sqrt{231}}{308} & 0 & 0 & \frac{\sqrt{385}}{308} & 0 & 0 \end{bmatrix}$ |
| 219 | symmetry  | $\frac{\sqrt{35}(x^2-2xy-y^2)(x^2+2xy-y^2)}{8}$   |
|     |           | $\begin{bmatrix} -\frac{\sqrt{110}}{22} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{3\sqrt{110}}{88} & 0 & 0 & \frac{\sqrt{66}}{88} & 0 & 0 \\ 0 & 0 & \frac{3\sqrt{110}}{88} & 0 & 0 & -\frac{\sqrt{66}}{88} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{66}}{88} & 0 & 0 & -\frac{3\sqrt{110}}{88} & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{66}}{88} & 0 & 0 & -\frac{3\sqrt{110}}{88} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{110}}{22} \end{bmatrix}$  |
| 220 | symmetry  | $\frac{\sqrt{35}xy(x-y)(x+y)}{2}$   |
|     |           | $\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{110}}{22} \\ 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{66}}{22} & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{66}}{22} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{66}}{22} & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{66}}{22} & 0 & 0 & 0 & 0 & 0 \\ \frac{\sqrt{110}}{22} & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$   |
| 221 | symmetry  | $-\frac{\sqrt{5}(x-y)(x+y)(x^2+y^2-6z^2)}{4}$   |

continued ...

Table 10

| No. | multipole | matrix  |
|-----|-----------|---|
|     |           | $\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{3\sqrt{770}}{308} & 0 & 0 & \frac{\sqrt{462}}{308} & 0 & 0 \\ 0 & 0 & \frac{3\sqrt{770}}{308} & 0 & 0 & \frac{\sqrt{462}}{308} & 0 \\ \mathbb{Q}_{4,0}^{(a)}(E_{2g}, 2) & 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{462}}{154} \\ 0 & \frac{\sqrt{462}}{308} & 0 & 0 & \frac{\sqrt{770}}{44} & 0 & 0 \\ 0 & 0 & \frac{\sqrt{462}}{308} & 0 & 0 & -\frac{\sqrt{770}}{44} & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{462}}{154} & 0 & 0 & 0 \end{bmatrix}$   |
| 222 | symmetry  | $\frac{\sqrt{5}xy(x^2+y^2-6z^2)}{2}$ $\begin{bmatrix} 0 & 0 & 0 & \frac{\sqrt{462}}{154} & 0 & 0 & 0 \\ 0 & 0 & -\frac{3\sqrt{770}}{154} & 0 & 0 & \frac{\sqrt{462}}{77} & 0 \\ 0 & -\frac{3\sqrt{770}}{154} & 0 & 0 & -\frac{\sqrt{462}}{77} & 0 & 0 \\ \mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2) & \frac{\sqrt{462}}{154} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{462}}{77} & 0 & 0 & -\frac{\sqrt{770}}{154} & 0 \\ 0 & \frac{\sqrt{462}}{77} & 0 & 0 & -\frac{\sqrt{770}}{154} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$  |
| 223 | symmetry  | $-\frac{5x^6}{16} - \frac{15x^4y^2}{16} + \frac{45x^4z^2}{8} - \frac{15x^2y^4}{16} + \frac{45x^2y^2z^2}{4} - \frac{15x^2z^4}{2} - \frac{5y^6}{16} + \frac{45y^4z^2}{8} - \frac{15y^2z^4}{2} + z^6$ $\begin{bmatrix} \frac{\sqrt{231}}{77} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{25\sqrt{231}}{1848} & 0 & 0 & -\frac{\sqrt{385}}{88} & 0 & 0 \\ 0 & 0 & -\frac{25\sqrt{231}}{1848} & 0 & 0 & \frac{\sqrt{385}}{88} & 0 \\ \mathbb{Q}_6^{(a)}(A_{1g}, 1) & 0 & 0 & 0 & \frac{10\sqrt{231}}{231} & 0 & 0 \\ 0 & -\frac{\sqrt{385}}{88} & 0 & 0 & -\frac{13\sqrt{231}}{616} & 0 & 0 \\ 0 & 0 & \frac{\sqrt{385}}{88} & 0 & 0 & -\frac{13\sqrt{231}}{616} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{231}}{77} \end{bmatrix}$ |
| 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  |
|-----|---------------------------------|---|
|     |                                 | $\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{5\sqrt{2}}{16} & 0 & 0 & -\frac{\sqrt{30}}{16} & 0 & 0 \\ 0 & 0 & -\frac{5\sqrt{2}}{16} & 0 & 0 & -\frac{\sqrt{30}}{16} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{30}}{16} & 0 & 0 & \frac{3\sqrt{2}}{16} & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{30}}{16} & 0 & 0 & -\frac{3\sqrt{2}}{16} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$   |
| 225 | $\mathbb{Q}_6^{(a)}(A_{1g}, 2)$ | $\frac{\sqrt{462}xy(x^2-3y^2)(3x^2-y^2)}{16}$   |
|     |                                 | $\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{5\sqrt{2}}{16} & 0 & 0 & -\frac{\sqrt{30}}{16} & 0 \\ 0 & -\frac{5\sqrt{2}}{16} & 0 & 0 & \frac{\sqrt{30}}{16} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{30}}{16} & 0 & 0 & \frac{3\sqrt{2}}{16} & 0 \\ 0 & -\frac{\sqrt{30}}{16} & 0 & 0 & \frac{3\sqrt{2}}{16} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$   |
| 226 | $\mathbb{Q}_6^{(a)}(A_{2g})$    | $\frac{-\sqrt{210}xz(x^2-3y^2)(3x^2+3y^2-8z^2)}{16}$  |
|     |                                 | $\begin{bmatrix} 0 & 0 & \frac{3\sqrt{66}}{88} & 0 & 0 & -\frac{3\sqrt{110}}{88} & 0 \\ 0 & 0 & 0 & \frac{\sqrt{110}}{44} & 0 & 0 & -\frac{3\sqrt{66}}{88} \\ \frac{3\sqrt{66}}{88} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{110}}{44} & 0 & 0 & -\frac{\sqrt{66}}{44} & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{66}}{44} & 0 & 0 & -\frac{3\sqrt{110}}{88} \\ -\frac{3\sqrt{110}}{88} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{3\sqrt{66}}{88} & 0 & 0 & -\frac{3\sqrt{110}}{88} & 0 & 0 \end{bmatrix}$ |
| 227 | $\mathbb{Q}_6^{(a)}(B_{1g})$    | $\frac{-\sqrt{210}yz(3x^2-y^2)(3x^2+3y^2-8z^2)}{16}$  |

continued ...

Table 10

| No. | multipole | matrix   |
|-----|-----------|--|
|     |           | $\begin{bmatrix} 0 & -\frac{3\sqrt{66}}{88} & 0 & 0 & -\frac{3\sqrt{110}}{88} & 0 & 0 \\ -\frac{3\sqrt{66}}{88} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{110}}{44} & 0 & 0 & -\frac{3\sqrt{66}}{88} \\ \mathbb{Q}_6^{(a)}(B_{2g}) & 0 & 0 & -\frac{\sqrt{110}}{44} & 0 & 0 & -\frac{\sqrt{66}}{44} \\ -\frac{3\sqrt{110}}{88} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{66}}{44} & 0 & 0 & \frac{3\sqrt{110}}{88} \\ 0 & 0 & -\frac{3\sqrt{66}}{88} & 0 & 0 & \frac{3\sqrt{110}}{88} & 0 \end{bmatrix}$ |
| 228 | symmetry  | $\frac{3\sqrt{154}yz(5x^4-10x^2y^2+y^4)}{16}$  |
|     |           | $\begin{bmatrix} 0 & \frac{\sqrt{10}}{8} & 0 & 0 & -\frac{\sqrt{6}}{8} & 0 & 0 \\ \frac{\sqrt{10}}{8} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{10}}{8} \\ \mathbb{Q}_{6,0}^{(a)}(E_{1g}, 1) & 0 & 0 & 0 & 0 & 0 & 0 \\ -\frac{\sqrt{6}}{8} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{6}}{8} \\ 0 & 0 & -\frac{\sqrt{10}}{8} & 0 & 0 & -\frac{\sqrt{6}}{8} & 0 \end{bmatrix}$  |
| 229 | symmetry  | $\frac{3\sqrt{154}xz(x^4-10x^2y^2+5y^4)}{16}$  |
|     |           | $\begin{bmatrix} 0 & 0 & \frac{\sqrt{10}}{8} & 0 & 0 & \frac{\sqrt{6}}{8} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{10}}{8} \\ \frac{\sqrt{10}}{8} & 0 & 0 & 0 & 0 & 0 & 0 \\ \mathbb{Q}_{6,1}^{(a)}(E_{1g}, 1) & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{6}}{8} \\ \frac{\sqrt{6}}{8} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{10}}{8} & 0 & 0 & -\frac{\sqrt{6}}{8} & 0 & 0 \end{bmatrix}$  |
| 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  |
|-----|-------------------------------------|---|
|     |                                     | $\begin{bmatrix} 0 & \frac{\sqrt{165}}{132} & 0 & 0 & \frac{3\sqrt{11}}{44} & 0 & 0 \\ \frac{\sqrt{165}}{132} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{5\sqrt{11}}{44} & 0 & 0 & -\frac{\sqrt{165}}{66} \\ 0 & 0 & -\frac{5\sqrt{11}}{44} & 0 & 0 & \frac{5\sqrt{165}}{132} & 0 \\ \frac{3\sqrt{11}}{44} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{5\sqrt{165}}{132} & 0 & 0 & \frac{\sqrt{11}}{22} \\ 0 & 0 & -\frac{\sqrt{165}}{66} & 0 & 0 & \frac{\sqrt{11}}{22} & 0 \end{bmatrix}$   |
| 231 | $\mathbb{Q}_{6,0}^{(a)}(E_{1g}, 2)$ | $-\frac{\sqrt{21}xz(5x^4+10x^2y^2-20x^2z^2+5y^4-20y^2z^2+8z^4)}{8}$   |
|     |                                     | $\begin{bmatrix} 0 & 0 & -\frac{\sqrt{165}}{132} & 0 & 0 & \frac{3\sqrt{11}}{44} & 0 \\ 0 & 0 & 0 & \frac{5\sqrt{11}}{44} & 0 & 0 & -\frac{\sqrt{165}}{66} \\ -\frac{\sqrt{165}}{132} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{5\sqrt{11}}{44} & 0 & 0 & \frac{5\sqrt{165}}{132} & 0 & 0 \\ 0 & 0 & 0 & \frac{5\sqrt{165}}{132} & 0 & 0 & -\frac{\sqrt{11}}{22} \\ \frac{3\sqrt{11}}{44} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{165}}{66} & 0 & 0 & -\frac{\sqrt{11}}{22} & 0 & 0 \end{bmatrix}$ |
| 232 | $\mathbb{Q}_{6,1}^{(a)}(E_{1g}, 2)$ | $-\frac{3\sqrt{7}(x^2+y^2-10z^2)(x^2-2xy-y^2)(x^2+2xy-y^2)}{16}$  |
|     |                                     | $\begin{bmatrix} -\frac{\sqrt{33}}{11} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{5\sqrt{33}}{88} & 0 & 0 & -\frac{\sqrt{55}}{88} & 0 & 0 \\ 0 & 0 & -\frac{5\sqrt{33}}{88} & 0 & 0 & \frac{\sqrt{55}}{88} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{55}}{88} & 0 & 0 & \frac{5\sqrt{33}}{88} & 0 & 0 \\ 0 & 0 & \frac{\sqrt{55}}{88} & 0 & 0 & \frac{5\sqrt{33}}{88} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{33}}{11} \end{bmatrix}$  |
| 233 | $\mathbb{Q}_{6,0}^{(a)}(E_{2g}, 1)$ | $-\frac{3\sqrt{7}xy(x-y)(x+y)(x^2+y^2-10z^2)}{4}$   |

continued ...

Table 10

| No. | multipole                           | matrix  |
|-----|-------------------------------------|---|
|     | $\mathbb{Q}_{6,1}^{(a)}(E_{2g}, 1)$ | $\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{33}}{11} \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{55}}{22} & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{55}}{22} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{55}}{22} & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{55}}{22} & 0 & 0 & 0 & 0 & 0 \\ \frac{\sqrt{33}}{11} & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$   |
| 234 | symmetry                            | $\frac{\sqrt{210}(x-y)(x+y)(x^4+2x^2y^2-16x^2z^2+y^4-16y^2z^2+16z^4)}{32}$  |
|     | $\mathbb{Q}_{6,0}^{(a)}(E_{2g}, 2)$ | $\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{5\sqrt{110}}{176} & 0 & 0 & \frac{17\sqrt{66}}{528} & 0 & 0 \\ 0 & 0 & -\frac{5\sqrt{110}}{176} & 0 & 0 & \frac{17\sqrt{66}}{528} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{2\sqrt{66}}{33} \\ 0 & \frac{17\sqrt{66}}{528} & 0 & 0 & \frac{3\sqrt{110}}{176} & 0 & 0 \\ 0 & 0 & \frac{17\sqrt{66}}{528} & 0 & 0 & -\frac{3\sqrt{110}}{176} & 0 \\ 0 & 0 & 0 & \frac{2\sqrt{66}}{33} & 0 & 0 & 0 \end{bmatrix}$   |
| 235 | symmetry                            | $-\frac{\sqrt{210}xy(x^4+2x^2y^2-16x^2z^2+y^4-16y^2z^2+16z^4)}{16}$   |
|     | $\mathbb{Q}_{6,1}^{(a)}(E_{2g}, 2)$ | $\begin{bmatrix} 0 & 0 & 0 & -\frac{2\sqrt{66}}{33} & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{110}}{176} & 0 & 0 & \frac{13\sqrt{66}}{528} & 0 \\ 0 & -\frac{\sqrt{110}}{176} & 0 & 0 & -\frac{13\sqrt{66}}{528} & 0 & 0 \\ -\frac{2\sqrt{66}}{33} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{13\sqrt{66}}{528} & 0 & 0 & \frac{7\sqrt{110}}{176} & 0 \\ 0 & \frac{13\sqrt{66}}{528} & 0 & 0 & \frac{7\sqrt{110}}{176} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| 236 | symmetry                            | $z$   |

continued ...

Table 10

| No. | multipole | matrix   |
|-----|-----------|--|
|     |           | $\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{7}i}{7} \\ 0 & 0 & \frac{3\sqrt{7}i}{28} & 0 & 0 & \frac{\sqrt{105}i}{28} & 0 \\ 0 & -\frac{3\sqrt{7}i}{28} & 0 & 0 & \frac{\sqrt{105}i}{28} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{105}i}{28} & 0 & 0 & -\frac{\sqrt{7}i}{28} & 0 \\ 0 & -\frac{\sqrt{105}i}{28} & 0 & 0 & \frac{\sqrt{7}i}{28} & 0 & 0 \\ -\frac{\sqrt{7}i}{7} & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| 237 | symmetry  | $\begin{bmatrix} 0 & 0 & 0 & 0 & \frac{\sqrt{7}i}{7} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{3\sqrt{7}i}{28} & 0 & 0 & \frac{\sqrt{105}i}{28} \\ 0 & 0 & -\frac{3\sqrt{7}i}{28} & 0 & 0 & \frac{\sqrt{105}i}{28} & 0 \\ -\frac{\sqrt{7}i}{7} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{105}i}{28} & 0 & 0 & -\frac{\sqrt{7}i}{28} \\ 0 & 0 & -\frac{\sqrt{105}i}{28} & 0 & 0 & \frac{\sqrt{7}i}{28} & 0 \end{bmatrix}$ |
| 238 | symmetry  | $\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{7}i}{7} & 0 \\ 0 & 0 & 0 & -\frac{3\sqrt{7}i}{28} & 0 & 0 & \frac{\sqrt{105}i}{28} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{3\sqrt{7}i}{28} & 0 & 0 & \frac{\sqrt{105}i}{28} & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{105}i}{28} & 0 & 0 & \frac{\sqrt{7}i}{28} \\ -\frac{\sqrt{7}i}{7} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{105}i}{28} & 0 & 0 & -\frac{\sqrt{7}i}{28} & 0 & 0 \end{bmatrix}$ |
| 239 | symmetry  | $-\frac{z(3x^2+3y^2-2z^2)}{2}$   |

continued ...

Table 10

| No. | multipole | matrix  |
|-----|-----------|---|
|     |           | $\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{6}i}{6} \\ 0 & 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{6}i}{6} & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 \\ -\frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$  |
| 240 | symmetry  | $\frac{\sqrt{10}y(3x^2-y^2)}{4}$  |
|     |           | $\begin{bmatrix} 0 & 0 & \frac{i}{4} & 0 & 0 & -\frac{\sqrt{15}i}{12} & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{15}i}{12} & 0 & 0 & \frac{i}{4} \\ -\frac{i}{4} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{15}i}{12} & 0 & 0 & -\frac{i}{4} & 0 & 0 \\ 0 & 0 & 0 & \frac{i}{4} & 0 & 0 & \frac{\sqrt{15}i}{12} \\ \frac{\sqrt{15}i}{12} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{i}{4} & 0 & 0 & -\frac{\sqrt{15}i}{12} & 0 & 0 \end{bmatrix}$ |
| 241 | symmetry  | $\frac{\sqrt{10}x(x^2-3y^2)}{4}$  |
|     |           | $\begin{bmatrix} 0 & \frac{i}{4} & 0 & 0 & \frac{\sqrt{15}i}{12} & 0 & 0 \\ -\frac{i}{4} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{15}i}{12} & 0 & 0 & -\frac{i}{4} \\ 0 & 0 & \frac{\sqrt{15}i}{12} & 0 & 0 & \frac{i}{4} & 0 \\ -\frac{\sqrt{15}i}{12} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{i}{4} & 0 & 0 & \frac{\sqrt{15}i}{12} \\ 0 & 0 & \frac{i}{4} & 0 & 0 & -\frac{\sqrt{15}i}{12} & 0 \end{bmatrix}$ |
| 242 | symmetry  | $-\frac{\sqrt{6}x(x^2+y^2-4z^2)}{4}$  |

continued ...

Table 10

| No. | multipole                        | matrix   |
|-----|----------------------------------|--|
|     | $\mathbb{M}_{3,0}^{(a)}(E_{1g})$ | $\begin{bmatrix} 0 & \frac{\sqrt{15}i}{12} & 0 & 0 & -\frac{i}{4} & 0 & 0 \\ -\frac{\sqrt{15}i}{12} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{i}{4} & 0 & 0 & -\frac{\sqrt{15}i}{12} \\ 0 & 0 & -\frac{i}{4} & 0 & 0 & \frac{\sqrt{15}i}{12} & 0 \\ \frac{i}{4} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{15}i}{12} & 0 & 0 & -\frac{i}{4} \\ 0 & 0 & \frac{\sqrt{15}i}{12} & 0 & 0 & \frac{i}{4} & 0 \end{bmatrix}$                                      |
| 243 | symmetry                         | $-\frac{\sqrt{6}y(x^2+y^2-4z^2)}{4}$ $\begin{bmatrix} 0 & 0 & -\frac{\sqrt{15}i}{12} & 0 & 0 & -\frac{i}{4} & 0 \\ 0 & 0 & 0 & -\frac{i}{4} & 0 & 0 & -\frac{\sqrt{15}i}{12} \\ \frac{\sqrt{15}i}{12} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{i}{4} & 0 & 0 & \frac{\sqrt{15}i}{12} & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{15}i}{12} & 0 & 0 & \frac{i}{4} \\ \frac{i}{4} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{15}i}{12} & 0 & 0 & -\frac{i}{4} & 0 & 0 \end{bmatrix}$ |
| 244 | symmetry                         | $\sqrt{15}xyz$ $\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{6}i}{6} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{6}i}{6} \\ 0 & \frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{6}i}{6} & 0 & 0 & 0 \end{bmatrix}$  |
| 245 | symmetry                         | $\frac{\sqrt{15}z(x-y)(x+y)}{2}$   |

continued ...

Table 10

| No. | multipole                        | matrix  |
|-----|----------------------------------|---|
|     | $\mathbb{M}_{3,1}^{(a)}(E_{2g})$ | $\begin{bmatrix} 0 & 0 & 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{6}i}{6} & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 \\ \frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$  |
| 246 | symmetry                         | $\frac{z(15x^4+30x^2y^2-40x^2z^2+15y^4-40y^2z^2+8z^4)}{8}$  |
|     | $\mathbb{M}_5^{(a)}(A_{2g})$     | $\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & -\frac{2\sqrt{21}i}{21} \\ 0 & 0 & -\frac{5\sqrt{21}i}{168} & 0 & 0 & \frac{3\sqrt{35}i}{56} & 0 \\ 0 & \frac{5\sqrt{21}i}{168} & 0 & 0 & \frac{3\sqrt{35}i}{56} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{3\sqrt{35}i}{56} & 0 & 0 & \frac{11\sqrt{21}i}{168} & 0 \\ 0 & -\frac{3\sqrt{35}i}{56} & 0 & 0 & -\frac{11\sqrt{21}i}{168} & 0 & 0 \\ \frac{2\sqrt{21}i}{21} & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$              |
| 247 | symmetry                         | $-\frac{\sqrt{70}y(3x^2-y^2)(x^2+y^2-8z^2)}{16}$  |
|     | $\mathbb{M}_5^{(a)}(B_{1g})$     | $\begin{bmatrix} 0 & 0 & \frac{\sqrt{2}i}{8} & 0 & 0 & -\frac{\sqrt{30}i}{24} & 0 \\ 0 & 0 & 0 & \frac{\sqrt{30}i}{12} & 0 & 0 & \frac{\sqrt{2}i}{8} \\ -\frac{\sqrt{2}i}{8} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{30}i}{12} & 0 & 0 & \frac{\sqrt{2}i}{4} & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{2}i}{4} & 0 & 0 & \frac{\sqrt{30}i}{24} \\ \frac{\sqrt{30}i}{24} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{2}i}{8} & 0 & 0 & -\frac{\sqrt{30}i}{24} & 0 & 0 \end{bmatrix}$ |
| 248 | symmetry                         | $-\frac{\sqrt{70}x(x^2-3y^2)(x^2+y^2-8z^2)}{16}$  |

continued ...

Table 10

| No. | multipole | matrix  |
|-----|-----------|---|
|     |           | $\begin{bmatrix} 0 & \frac{\sqrt{2}i}{8} & 0 & 0 & \frac{\sqrt{30}i}{24} & 0 & 0 \\ -\frac{\sqrt{2}i}{8} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{30}i}{12} & 0 & 0 & -\frac{\sqrt{2}i}{8} \\ 0 & 0 & -\frac{\sqrt{30}i}{12} & 0 & 0 & -\frac{\sqrt{2}i}{4} & 0 \\ -\frac{\sqrt{30}i}{24} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{2}i}{4} & 0 & 0 & \frac{\sqrt{30}i}{24} \\ 0 & 0 & \frac{\sqrt{2}i}{8} & 0 & 0 & -\frac{\sqrt{30}i}{24} & 0 \end{bmatrix}$ |
| 249 | symmetry  | $\frac{3\sqrt{14}x(x^4 - 10x^2y^2 + 5y^4)}{16}$   |
|     |           | $\begin{bmatrix} 0 & \frac{\sqrt{10}i}{8} & 0 & 0 & -\frac{\sqrt{6}i}{8} & 0 & 0 \\ -\frac{\sqrt{10}i}{8} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{10}i}{8} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{\sqrt{6}i}{8} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{6}i}{8} \\ 0 & 0 & -\frac{\sqrt{10}i}{8} & 0 & 0 & -\frac{\sqrt{6}i}{8} & 0 \end{bmatrix}$   |
| 250 | symmetry  | $-\frac{3\sqrt{14}y(5x^4 - 10x^2y^2 + y^4)}{16}$  |
|     |           | $\begin{bmatrix} 0 & 0 & \frac{\sqrt{10}i}{8} & 0 & 0 & \frac{\sqrt{6}i}{8} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{10}i}{8} \\ -\frac{\sqrt{10}i}{8} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{6}i}{8} \\ -\frac{\sqrt{6}i}{8} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{10}i}{8} & 0 & 0 & -\frac{\sqrt{6}i}{8} & 0 & 0 \end{bmatrix}$   |
| 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  |
|-----|-----------|---|
|     |           | $\begin{bmatrix} 0 & -\frac{\sqrt{21}i}{12} & 0 & 0 & -\frac{\sqrt{35}i}{28} & 0 & 0 \\ \frac{\sqrt{21}i}{12} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{35}i}{28} & 0 & 0 & -\frac{\sqrt{21}i}{42} \\ 0 & 0 & -\frac{\sqrt{35}i}{28} & 0 & 0 & \frac{5\sqrt{21}i}{84} & 0 \\ \frac{\sqrt{35}i}{28} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{5\sqrt{21}i}{84} & 0 & 0 & \frac{\sqrt{35}i}{14} \\ 0 & 0 & \frac{\sqrt{21}i}{42} & 0 & 0 & -\frac{\sqrt{35}i}{14} & 0 \end{bmatrix}$ |
| 252 | symmetry  | $\frac{\sqrt{15}y(x^4+2x^2y^2-12x^2z^2+y^4-12y^2z^2+8z^4)}{8}$  |
|     |           | $\begin{bmatrix} 0 & 0 & \frac{\sqrt{21}i}{12} & 0 & 0 & -\frac{\sqrt{35}i}{28} & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{35}i}{28} & 0 & 0 & -\frac{\sqrt{21}i}{42} \\ -\frac{\sqrt{21}i}{12} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{35}i}{28} & 0 & 0 & \frac{5\sqrt{21}i}{84} & 0 & 0 \\ 0 & 0 & 0 & -\frac{5\sqrt{21}i}{84} & 0 & 0 & -\frac{\sqrt{35}i}{14} \\ \frac{\sqrt{35}i}{28} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{21}i}{42} & 0 & 0 & \frac{\sqrt{35}i}{14} & 0 & 0 \end{bmatrix}$ |
| 253 | symmetry  | $-\frac{3\sqrt{35}xyz(x-y)(x+y)}{2}$  |
|     |           | $\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{i}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{i}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{i}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{i}{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$   |
| 254 | symmetry  | $\frac{3\sqrt{35}z(x^2-2xy-y^2)(x^2+2xy-y^2)}{8}$   |

continued ...

Table 10

| No. | multipole                           | matrix  |
|-----|-------------------------------------|---|
|     | $\mathbb{M}_{5,1}^{(a)}(E_{2g}, 1)$ | $\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{15}i}{8} & 0 & 0 & -\frac{i}{8} & 0 \\ 0 & -\frac{\sqrt{15}i}{8} & 0 & 0 & -\frac{i}{8} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{i}{8} & 0 & 0 & \frac{\sqrt{15}i}{8} & 0 \\ 0 & \frac{i}{8} & 0 & 0 & -\frac{\sqrt{15}i}{8} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$ |
| 255 | symmetry                            | $-\frac{\sqrt{105}xyz(x^2+y^2-2z^2)}{2}$  |
|     | $\mathbb{M}_{5,0}^{(a)}(E_{2g}, 2)$ | $\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{3}i}{6} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{3}i}{6} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{3}i}{3} \\ 0 & -\frac{\sqrt{3}i}{6} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{3}i}{6} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{3}i}{3} & 0 & 0 & 0 \end{bmatrix}$          |
| 256 | symmetry                            | $-\frac{\sqrt{105}z(x-y)(x+y)(x^2+y^2-2z^2)}{4}$  |
|     | $\mathbb{M}_{5,1}^{(a)}(E_{2g}, 2)$ | $\begin{bmatrix} 0 & 0 & 0 & -\frac{\sqrt{3}i}{3} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{3}i}{6} & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{3}i}{6} & 0 & 0 \\ \frac{\sqrt{3}i}{3} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{3}i}{6} & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{3}i}{6} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$          |