

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

Table 1: (s,s) block.

No.	multipole	matrix
1	symmetry	1
	$Q_0^{(a)}(A_{1g})$	$\begin{bmatrix} 1 \end{bmatrix}$

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

Table 2: (s,p) block.

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

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

Table 3: (s,d) block.

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

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

Table 4: (s,f) block.

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

continued ...

Table 4

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

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

Table 5: (p,p) block.

No.	multipole	matrix
32	symmetry	1
	$\mathbb{Q}_0^{(a)}(A_{1g})$	$\begin{bmatrix} \frac{\sqrt{3}}{3} & 0 & 0 \\ 0 & \frac{\sqrt{3}}{3} & 0 \\ 0 & 0 & \frac{\sqrt{3}}{3} \end{bmatrix}$
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	$\sqrt{3}yz$
	$\mathbb{Q}_{2,1}^{(a)}(E_{1g})$	$\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{2}}{2} \\ 0 & \frac{\sqrt{2}}{2} & 0 \end{bmatrix}$
35	symmetry	$-\sqrt{3}xz$
	$\mathbb{Q}_{2,2}^{(a)}(E_{1g})$	$\begin{bmatrix} 0 & 0 & -\frac{\sqrt{2}}{2} \\ 0 & 0 & 0 \\ -\frac{\sqrt{2}}{2} & 0 & 0 \end{bmatrix}$
36	symmetry	$\frac{\sqrt{3}(x-y)(x+y)}{2}$
	$\mathbb{Q}_{2,1}^{(a)}(E_{2g})$	$\begin{bmatrix} \frac{\sqrt{2}}{2} & 0 & 0 \\ 0 & -\frac{\sqrt{2}}{2} & 0 \\ 0 & 0 & 0 \end{bmatrix}$

continued ...

Table 5

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

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

Table 6: (p,d) block.

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

continued ...

Table 6

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

continued ...

Table 6

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

continued ...

Table 6

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

continued ...

Table 6

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

continued ...

Table 6

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

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

Table 7: (p,f) block.

No.	multipole	matrix
71	symmetry	$-\frac{x^2}{2} - \frac{y^2}{2} + z^2$
	$\mathbb{Q}_2^{(a)}(A_{1g})$	$\begin{bmatrix} 0 & 0 & 0 & 0 & \frac{\sqrt{7}}{7} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{7}}{7} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{42}}{14} \end{bmatrix}$
72	symmetry	$\sqrt{3}yz$
	$\mathbb{Q}_{2,1}^{(a)}(E_{1g})$	$\begin{bmatrix} 0 & 0 & 0 & \frac{\sqrt{210}}{42} & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{210}}{42} & 0 & 0 & 0 & -\frac{\sqrt{14}}{14} \\ 0 & 0 & 0 & 0 & 0 & \frac{2\sqrt{21}}{21} & 0 \end{bmatrix}$
73	symmetry	$-\sqrt{3}xz$
	$\mathbb{Q}_{2,2}^{(a)}(E_{1g})$	$\begin{bmatrix} 0 & 0 & -\frac{\sqrt{210}}{42} & 0 & 0 & 0 & \frac{\sqrt{14}}{14} \\ 0 & 0 & 0 & -\frac{\sqrt{210}}{42} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{2\sqrt{21}}{21} & 0 & 0 \end{bmatrix}$
74	symmetry	$\frac{\sqrt{3}(x-y)(x+y)}{2}$
	$\mathbb{Q}_{2,1}^{(a)}(E_{2g})$	$\begin{bmatrix} \frac{\sqrt{35}}{14} & 0 & 0 & 0 & -\frac{\sqrt{21}}{42} & 0 & 0 \\ 0 & \frac{\sqrt{35}}{14} & 0 & 0 & 0 & \frac{\sqrt{21}}{42} & 0 \\ 0 & 0 & \frac{\sqrt{210}}{42} & 0 & 0 & 0 & 0 \end{bmatrix}$
75	symmetry	$-\sqrt{3}xy$

continued ...

Table 7

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

continued ...

Table 7

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

continued ...

Table 7

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

continued ...

Table 7

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

continued ...

Table 7

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

continued ...

Table 7

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

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

Table 8: (d,d) block.

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

continued ...

Table 8

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

continued ...

Table 8

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

continued ...

Table 8

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

continued ...

Table 8

No.	multipole	matrix
	$Q_{4,1}^{(a)}(E_{2g}, 2)$	$\begin{bmatrix} 0 & 0 & 0 & 0 & \frac{\sqrt{42}}{14} \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{14}}{7} & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{14}}{7} & 0 \\ \frac{\sqrt{42}}{14} & 0 & 0 & 0 & 0 \end{bmatrix}$
127	symmetry	$\frac{\sqrt{5}xy(x^2+y^2-6z^2)}{2}$
	$Q_{4,2}^{(a)}(E_{2g}, 2)$	$\begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{42}}{14} \\ 0 & 0 & 0 & -\frac{\sqrt{14}}{7} & 0 \\ 0 & 0 & -\frac{\sqrt{14}}{7} & 0 & 0 \\ 0 & -\frac{\sqrt{42}}{14} & 0 & 0 & 0 \end{bmatrix}$
128	symmetry	z
	$M_1^{(a)}(A_{2g})$	$\begin{bmatrix} 0 & -\frac{\sqrt{10}i}{5} & 0 & 0 & 0 \\ \frac{\sqrt{10}i}{5} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{10}i}{10} & 0 \\ 0 & 0 & \frac{\sqrt{10}i}{10} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}$
129	symmetry	x
	$M_{1,1}^{(a)}(E_{1g})$	$\begin{bmatrix} 0 & 0 & 0 & \frac{\sqrt{10}i}{10} & 0 \\ 0 & 0 & -\frac{\sqrt{10}i}{10} & 0 & 0 \\ 0 & \frac{\sqrt{10}i}{10} & 0 & 0 & 0 \\ -\frac{\sqrt{10}i}{10} & 0 & 0 & 0 & -\frac{\sqrt{30}i}{10} \\ 0 & 0 & 0 & \frac{\sqrt{30}i}{10} & 0 \end{bmatrix}$
130	symmetry	y

continued ...

Table 8

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

continued ...

Table 8

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

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

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

Table 9: (d,f) block.

No.	multipole	matrix
138	symmetry	z $\mathbb{Q}_1^{(a)}(A_{2u}) \begin{bmatrix} 0 & 0 & \frac{\sqrt{14}}{14} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{14}}{14} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{2\sqrt{35}}{35} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{2\sqrt{35}}{35} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{3\sqrt{70}}{70} \end{bmatrix}$
139	symmetry	x $\mathbb{Q}_{1,1}^{(a)}(E_{1u}) \begin{bmatrix} \frac{\sqrt{21}}{14} & 0 & 0 & 0 & -\frac{\sqrt{35}}{70} & 0 & 0 \\ 0 & \frac{\sqrt{21}}{14} & 0 & 0 & 0 & -\frac{\sqrt{35}}{70} & 0 \\ 0 & 0 & \frac{\sqrt{14}}{14} & 0 & 0 & 0 & -\frac{\sqrt{210}}{70} \\ 0 & 0 & 0 & \frac{\sqrt{14}}{14} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{105}}{35} & 0 & 0 \end{bmatrix}$
140	symmetry	y $\mathbb{Q}_{1,2}^{(a)}(E_{1u}) \begin{bmatrix} 0 & \frac{\sqrt{21}}{14} & 0 & 0 & 0 & \frac{\sqrt{35}}{70} & 0 \\ -\frac{\sqrt{21}}{14} & 0 & 0 & 0 & -\frac{\sqrt{35}}{70} & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{14}}{14} & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{14}}{14} & 0 & 0 & 0 & -\frac{\sqrt{210}}{70} \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{105}}{35} & 0 \end{bmatrix}$
141	symmetry	$-\frac{z(3x^2+3y^2-2z^2)}{2}$ $\mathbb{Q}_3^{(a)}(A_{2u}) \begin{bmatrix} 0 & 0 & -\frac{\sqrt{6}}{6} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{6}}{6} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{15}}{30} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{15}}{30} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{30}}{15} \end{bmatrix}$
142	symmetry	$\frac{\sqrt{10}y(3x^2-y^2)}{4}$

continued ...

Table 9

No.	multipole	matrix
	$\mathbb{Q}_3^{(a)}(B_{1u})$	$\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{6}}{12} & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{6}}{12} & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{15}}{12} & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{15}}{12} & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{30}}{12} & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$
143	symmetry	$\frac{\sqrt{10}x(x^2-3y^2)}{4}$
	$\mathbb{Q}_3^{(a)}(B_{2u})$	$\begin{bmatrix} 0 & 0 & 0 & 0 & -\frac{\sqrt{6}}{12} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{6}}{12} & 0 \\ 0 & 0 & \frac{\sqrt{15}}{12} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{15}}{12} & 0 & 0 & 0 \\ -\frac{\sqrt{30}}{12} & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$
144	symmetry	$-\frac{\sqrt{6}x(x^2+y^2-4z^2)}{4}$
	$\mathbb{Q}_{3,1}^{(a)}(E_{1u})$	$\begin{bmatrix} -\frac{\sqrt{6}}{12} & 0 & 0 & 0 & \frac{\sqrt{10}}{10} & 0 & 0 \\ 0 & -\frac{\sqrt{6}}{12} & 0 & 0 & 0 & \frac{\sqrt{10}}{10} & 0 \\ 0 & 0 & \frac{1}{4} & 0 & 0 & 0 & \frac{\sqrt{15}}{30} \\ 0 & 0 & 0 & \frac{1}{4} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{30}}{20} & 0 & 0 \end{bmatrix}$
145	symmetry	$-\frac{\sqrt{6}y(x^2+y^2-4z^2)}{4}$
	$\mathbb{Q}_{3,2}^{(a)}(E_{1u})$	$\begin{bmatrix} 0 & -\frac{\sqrt{6}}{12} & 0 & 0 & 0 & -\frac{\sqrt{10}}{10} & 0 \\ \frac{\sqrt{6}}{12} & 0 & 0 & 0 & \frac{\sqrt{10}}{10} & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{4} & 0 & 0 & 0 \\ 0 & 0 & -\frac{1}{4} & 0 & 0 & 0 & \frac{\sqrt{15}}{30} \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{30}}{20} & 0 \end{bmatrix}$
146	symmetry	$\sqrt{15}xyz$

continued ...

Table 9

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

continued ...

Table 9

No.	multipole	matrix
	$\mathbb{Q}_5^{(a)}(B_{2u})$	$\begin{bmatrix} 0 & 0 & 0 & 0 & \frac{\sqrt{3}}{6} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{3}}{6} & 0 \\ 0 & 0 & \frac{\sqrt{30}}{15} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{30}}{15} & 0 & 0 & 0 \\ \frac{\sqrt{15}}{15} & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$
151	symmetry	$\frac{3\sqrt{14}x(x^4-10x^2y^2+5y^4)}{16}$
	$\mathbb{Q}_{5,1}^{(a)}(E_{1u}, 1)$	$\begin{bmatrix} \frac{1}{2} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{1}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$
152	symmetry	$-\frac{3\sqrt{14}y(5x^4-10x^2y^2+y^4)}{16}$
	$\mathbb{Q}_{5,2}^{(a)}(E_{1u}, 1)$	$\begin{bmatrix} 0 & -\frac{1}{2} & 0 & 0 & 0 & 0 & 0 \\ -\frac{1}{2} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$
153	symmetry	$\frac{\sqrt{15}x(x^4+2x^2y^2-12x^2z^2+y^4-12y^2z^2+8z^4)}{8}$
	$\mathbb{Q}_{5,1}^{(a)}(E_{1u}, 2)$	$\begin{bmatrix} \frac{\sqrt{210}}{420} & 0 & 0 & 0 & -\frac{\sqrt{14}}{28} & 0 & 0 \\ 0 & \frac{\sqrt{210}}{420} & 0 & 0 & 0 & -\frac{\sqrt{14}}{28} & 0 \\ 0 & 0 & -\frac{\sqrt{35}}{35} & 0 & 0 & 0 & \frac{2\sqrt{21}}{21} \\ 0 & 0 & 0 & -\frac{\sqrt{35}}{35} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{42}}{14} & 0 & 0 \end{bmatrix}$
154	symmetry	$\frac{\sqrt{15}y(x^4+2x^2y^2-12x^2z^2+y^4-12y^2z^2+8z^4)}{8}$

continued ...

Table 9

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

continued ...

Table 9

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

continued ...

Table 9

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

continued ...

Table 9

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

continued ...

Table 9

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

continued ...

Table 9

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

continued ...

Table 9

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

continued ...

Table 9

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

continued ...

Table 9

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

continued ...

Table 9

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

continued ...

Table 9

No.	multipole	matrix
	$\mathbb{M}_2^{(a)}(A_{1u})$	$\begin{bmatrix} 0 & 0 & 0 & -\frac{\sqrt{35}i}{14} & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{35}i}{14} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{14}i}{14} & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{14}i}{14} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$
195	symmetry	$\sqrt{3}yz$
	$\mathbb{M}_{2,1}^{(a)}(E_{1u})$	$\begin{bmatrix} \frac{\sqrt{70}i}{28} & 0 & 0 & 0 & \frac{\sqrt{42}i}{28} & 0 & 0 \\ 0 & \frac{\sqrt{70}i}{28} & 0 & 0 & 0 & \frac{\sqrt{42}i}{28} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{7}i}{7} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{14}i}{14} & 0 & 0 \end{bmatrix}$
196	symmetry	$-\sqrt{3}xz$
	$\mathbb{M}_{2,2}^{(a)}(E_{1u})$	$\begin{bmatrix} 0 & \frac{\sqrt{70}i}{28} & 0 & 0 & 0 & -\frac{\sqrt{42}i}{28} & 0 \\ -\frac{\sqrt{70}i}{28} & 0 & 0 & 0 & \frac{\sqrt{42}i}{28} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{7}i}{7} \\ 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{14}i}{14} & 0 \end{bmatrix}$
197	symmetry	$\frac{\sqrt{3}(x-y)(x+y)}{2}$
	$\mathbb{M}_{2,1}^{(a)}(E_{2u})$	$\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{7}i}{14} \\ 0 & \frac{\sqrt{70}i}{28} & 0 & 0 & 0 & -\frac{\sqrt{42}i}{28} & 0 \\ -\frac{\sqrt{70}i}{28} & 0 & 0 & 0 & -\frac{\sqrt{42}i}{28} & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{35}i}{14} & 0 & 0 & 0 \end{bmatrix}$
198	symmetry	$-\sqrt{3}xy$

continued ...

Table 9

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

continued ...

Table 9

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

continued ...

Table 9

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

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

Table 10: (f,f) block.

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

continued ...

Table 10

No.	multipole	matrix
	$\mathbb{Q}_2^{(a)}(A_{1g})$	$\begin{bmatrix} -\frac{5\sqrt{21}}{42} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{5\sqrt{21}}{42} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{21}}{14} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{21}}{14} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{2\sqrt{21}}{21} \end{bmatrix}$
210	symmetry	$\begin{matrix} \sqrt{3}yz \\ \mathbb{Q}_{2,1}^{(a)}(E_{1g}) \end{matrix} \begin{bmatrix} 0 & 0 & 0 & -\frac{5\sqrt{42}}{84} & 0 & 0 & 0 \\ 0 & 0 & \frac{5\sqrt{42}}{84} & 0 & 0 & 0 & 0 \\ 0 & \frac{5\sqrt{42}}{84} & 0 & 0 & 0 & -\frac{\sqrt{70}}{28} & 0 \\ -\frac{5\sqrt{42}}{84} & 0 & 0 & 0 & \frac{\sqrt{70}}{28} & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{70}}{28} & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{70}}{28} & 0 & 0 & 0 & \frac{\sqrt{42}}{42} \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{42}}{42} & 0 \end{bmatrix}$
211	symmetry	$\begin{matrix} -\sqrt{3}xz \\ \mathbb{Q}_{2,2}^{(a)}(E_{1g}) \end{matrix} \begin{bmatrix} 0 & 0 & -\frac{5\sqrt{42}}{84} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{5\sqrt{42}}{84} & 0 & 0 & 0 \\ -\frac{5\sqrt{42}}{84} & 0 & 0 & 0 & -\frac{\sqrt{70}}{28} & 0 & 0 \\ 0 & -\frac{5\sqrt{42}}{84} & 0 & 0 & 0 & -\frac{\sqrt{70}}{28} & 0 \\ 0 & 0 & -\frac{\sqrt{70}}{28} & 0 & 0 & 0 & -\frac{\sqrt{42}}{42} \\ 0 & 0 & 0 & -\frac{\sqrt{70}}{28} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{42}}{42} & 0 & 0 \end{bmatrix}$
212	symmetry	$\frac{\sqrt{3}(x-y)(x+y)}{2}$

continued ...

Table 10

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

continued ...

Table 10

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

continued ...

Table 10

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

continued ...

Table 10

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

continued ...

Table 10

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

continued ...

Table 10

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

continued ...

Table 10

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

continued ...

Table 10

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

continued ...

Table 10

No.	multipole	matrix
	$M_1^{(a)}(A_{2g})$	$\begin{bmatrix} 0 & -\frac{3\sqrt{7}i}{14} & 0 & 0 & 0 & 0 & 0 \\ \frac{3\sqrt{7}i}{14} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{7}i}{7} & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{7}i}{7} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{7}i}{14} & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{7}i}{14} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$
237	symmetry	$\begin{array}{c} x \\ \left[\begin{array}{ccccccc} 0 & 0 & 0 & \frac{\sqrt{42}i}{28} & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{42}i}{28} & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{42}i}{28} & 0 & 0 & 0 & \frac{\sqrt{70}i}{28} & 0 \\ -\frac{\sqrt{42}i}{28} & 0 & 0 & 0 & -\frac{\sqrt{70}i}{28} & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{70}i}{28} & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{70}i}{28} & 0 & 0 & 0 & -\frac{\sqrt{42}i}{14} \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{42}i}{14} & 0 \end{array} \right] \end{array}$
	$M_{1,1}^{(a)}(E_{1g})$	
238	symmetry	$\begin{array}{c} y \\ \left[\begin{array}{ccccccc} 0 & 0 & \frac{\sqrt{42}i}{28} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{42}i}{28} & 0 & 0 & 0 \\ -\frac{\sqrt{42}i}{28} & 0 & 0 & 0 & \frac{\sqrt{70}i}{28} & 0 & 0 \\ 0 & -\frac{\sqrt{42}i}{28} & 0 & 0 & 0 & \frac{\sqrt{70}i}{28} & 0 \\ 0 & 0 & -\frac{\sqrt{70}i}{28} & 0 & 0 & 0 & \frac{\sqrt{42}i}{14} \\ 0 & 0 & 0 & -\frac{\sqrt{70}i}{28} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{42}i}{14} & 0 & 0 \end{array} \right] \end{array}$
	$M_{1,2}^{(a)}(E_{1g})$	
239	symmetry	$-\frac{z(3x^2+3y^2-2z^2)}{2}$

continued ...

Table 10

No.	multipole	matrix
	$M_3^{(a)}(A_{2g})$	$\begin{bmatrix} 0 & \frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 & 0 \\ -\frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{6}i}{6} & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{6}i}{6} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$
240	symmetry	$\frac{\sqrt{10}y(3x^2-y^2)}{4}$ $\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{6}i}{6} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{6}i}{6} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{6}i}{6} & 0 \\ 0 & 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{6}i}{6} & 0 & 0 & 0 \\ \frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$
241	symmetry	$\frac{\sqrt{10}x(x^2-3y^2)}{4}$ $\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{6}i}{6} \\ 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{6}i}{6} & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{6}i}{6} & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$
242	symmetry	$-\frac{\sqrt{6}x(x^2+y^2-4z^2)}{4}$

continued ...

Table 10

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

continued ...

Table 10

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

continued ...

Table 10

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

continued ...

Table 10

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

continued ...

Table 10

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