

PG No. 8 D_{2h} mmm [orthorhombic] (lg basis)

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

Table 1: (s,s) block.

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

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

Table 2: (s,p) block.

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

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	$-\frac{x^2}{2} - \frac{y^2}{2} + z^2$
	$\mathbb{Q}_2^{(a)}(A_g, 1)$	$\begin{bmatrix} 0 & 0 & 0 & 0 & \frac{\sqrt{2}}{2} \end{bmatrix}$
9	symmetry	$\frac{\sqrt{3}(x-y)(x+y)}{2}$
	$\mathbb{Q}_2^{(a)}(A_g, 2)$	$\begin{bmatrix} \frac{\sqrt{2}}{2} & 0 & 0 & 0 & 0 \end{bmatrix}$
10	symmetry	$\sqrt{3}xy$
	$\mathbb{Q}_2^{(a)}(B_{1g})$	$\begin{bmatrix} 0 & \frac{\sqrt{2}}{2} & 0 & 0 & 0 \end{bmatrix}$
11	symmetry	$\sqrt{3}xz$
	$\mathbb{Q}_2^{(a)}(B_{2g})$	$\begin{bmatrix} 0 & 0 & \frac{\sqrt{2}}{2} & 0 & 0 \end{bmatrix}$
12	symmetry	$\sqrt{3}yz$
	$\mathbb{Q}_2^{(a)}(B_{3g})$	$\begin{bmatrix} 0 & 0 & 0 & \frac{\sqrt{2}}{2} & 0 \end{bmatrix}$
13	symmetry	$-\frac{x^2}{2} - \frac{y^2}{2} + z^2$
	$\mathbb{T}_2^{(a)}(A_g, 1)$	$\begin{bmatrix} 0 & 0 & 0 & 0 & \frac{\sqrt{2}i}{2} \end{bmatrix}$
14	symmetry	$\frac{\sqrt{3}(x-y)(x+y)}{2}$
	$\mathbb{T}_2^{(a)}(A_g, 2)$	$\begin{bmatrix} \frac{\sqrt{2}i}{2} & 0 & 0 & 0 & 0 \end{bmatrix}$
15	symmetry	$\sqrt{3}xy$
	$\mathbb{T}_2^{(a)}(B_{1g})$	$\begin{bmatrix} 0 & \frac{\sqrt{2}i}{2} & 0 & 0 & 0 \end{bmatrix}$
16	symmetry	$\sqrt{3}xz$
	$\mathbb{T}_2^{(a)}(B_{2g})$	$\begin{bmatrix} 0 & 0 & \frac{\sqrt{2}i}{2} & 0 & 0 \end{bmatrix}$
17	symmetry	$\sqrt{3}yz$
	$\mathbb{T}_2^{(a)}(B_{3g})$	$\begin{bmatrix} 0 & 0 & 0 & \frac{\sqrt{2}i}{2} & 0 \end{bmatrix}$

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	$\sqrt{15}xyz$
	$\mathbb{Q}_3^{(a)}(A_u)$	$\begin{bmatrix} 0 & 0 & 0 & \frac{\sqrt{2}}{2} & 0 & 0 & 0 \end{bmatrix}$
19	symmetry	$-\frac{z(3x^2+3y^2-2z^2)}{2}$
	$\mathbb{Q}_3^{(a)}(B_{1u}, 1)$	$\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{2}}{2} \end{bmatrix}$
20	symmetry	$\frac{\sqrt{15}z(x-y)(x+y)}{2}$
	$\mathbb{Q}_3^{(a)}(B_{1u}, 2)$	$\begin{bmatrix} 0 & 0 & \frac{\sqrt{2}}{2} & 0 & 0 & 0 & 0 \end{bmatrix}$
21	symmetry	$-\frac{y(3x^2-2y^2+3z^2)}{2}$
	$\mathbb{Q}_3^{(a)}(B_{2u}, 1)$	$\begin{bmatrix} 0 & -\frac{\sqrt{5}}{4} & 0 & 0 & 0 & -\frac{\sqrt{3}}{4} & 0 \end{bmatrix}$
22	symmetry	$-\frac{\sqrt{15}y(x-z)(x+z)}{2}$
	$\mathbb{Q}_3^{(a)}(B_{2u}, 2)$	$\begin{bmatrix} 0 & -\frac{\sqrt{3}}{4} & 0 & 0 & 0 & \frac{\sqrt{5}}{4} & 0 \end{bmatrix}$
23	symmetry	$\frac{x(2x^2-3y^2-3z^2)}{2}$
	$\mathbb{Q}_3^{(a)}(B_{3u}, 1)$	$\begin{bmatrix} \frac{\sqrt{5}}{4} & 0 & 0 & 0 & -\frac{\sqrt{3}}{4} & 0 & 0 \end{bmatrix}$
24	symmetry	$\frac{\sqrt{15}x(y-z)(y+z)}{2}$
	$\mathbb{Q}_3^{(a)}(B_{3u}, 2)$	$\begin{bmatrix} -\frac{\sqrt{3}}{4} & 0 & 0 & 0 & -\frac{\sqrt{5}}{4} & 0 & 0 \end{bmatrix}$
25	symmetry	$\sqrt{15}xyz$
	$\mathbb{T}_3^{(a)}(A_u)$	$\begin{bmatrix} 0 & 0 & 0 & \frac{\sqrt{2}i}{2} & 0 & 0 & 0 \end{bmatrix}$
26	symmetry	$-\frac{z(3x^2+3y^2-2z^2)}{2}$
	$\mathbb{T}_3^{(a)}(B_{1u}, 1)$	$\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{2}i}{2} \end{bmatrix}$
27	symmetry	$\frac{\sqrt{15}z(x-y)(x+y)}{2}$
	$\mathbb{T}_3^{(a)}(B_{1u}, 2)$	$\begin{bmatrix} 0 & 0 & \frac{\sqrt{2}i}{2} & 0 & 0 & 0 & 0 \end{bmatrix}$
28	symmetry	$-\frac{y(3x^2-2y^2+3z^2)}{2}$
	$\mathbb{T}_3^{(a)}(B_{2u}, 1)$	$\begin{bmatrix} 0 & -\frac{\sqrt{5}i}{4} & 0 & 0 & 0 & -\frac{\sqrt{3}i}{4} & 0 \end{bmatrix}$
29	symmetry	$-\frac{\sqrt{15}y(x-z)(x+z)}{2}$
	$\mathbb{T}_3^{(a)}(B_{2u}, 2)$	$\begin{bmatrix} 0 & -\frac{\sqrt{3}i}{4} & 0 & 0 & 0 & \frac{\sqrt{5}i}{4} & 0 \end{bmatrix}$
30	symmetry	$\frac{x(2x^2-3y^2-3z^2)}{2}$
	$\mathbb{T}_3^{(a)}(B_{3u}, 1)$	$\begin{bmatrix} \frac{\sqrt{5}i}{4} & 0 & 0 & 0 & -\frac{\sqrt{3}i}{4} & 0 & 0 \end{bmatrix}$
31	symmetry	$\frac{\sqrt{15}x(y-z)(y+z)}{2}$

continued ...

Table 4

No.	multipole	matrix
	$\mathbb{T}_3^{(a)}(B_{3u}, 2)$	$\begin{bmatrix} -\frac{\sqrt{3}i}{4} & 0 & 0 & 0 & -\frac{\sqrt{5}i}{4} & 0 & 0 \end{bmatrix}$

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

continued ...

Table 5

No.	multipole	matrix
37	symmetry	$\sqrt{3}yz$
	$\mathbb{Q}_2^{(a)}(B_{3g})$	$\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{2}}{2} \\ 0 & \frac{\sqrt{2}}{2} & 0 \end{bmatrix}$
38	symmetry	z
	$\mathbb{M}_1^{(a)}(B_{1g})$	$\begin{bmatrix} 0 & -\frac{\sqrt{2}i}{2} & 0 \\ \frac{\sqrt{2}i}{2} & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$
39	symmetry	y
	$\mathbb{M}_1^{(a)}(B_{2g})$	$\begin{bmatrix} 0 & 0 & \frac{\sqrt{2}i}{2} \\ 0 & 0 & 0 \\ -\frac{\sqrt{2}i}{2} & 0 & 0 \end{bmatrix}$
40	symmetry	x
	$\mathbb{M}_1^{(a)}(B_{3g})$	$\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{2}i}{2} \\ 0 & \frac{\sqrt{2}i}{2} & 0 \end{bmatrix}$

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
	$\mathbb{Q}_1^{(a)}(B_{1u})$	$\begin{bmatrix} 0 & 0 & \frac{\sqrt{15}}{10} & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{15}}{10} & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{5}}{5} \end{bmatrix}$
42	symmetry	y

continued ...

Table 6

No.	multipole	matrix
	$\mathbb{Q}_1^{(a)}(B_{2u})$	$\begin{bmatrix} 0 & \frac{\sqrt{15}}{10} & 0 & 0 & 0 \\ -\frac{\sqrt{15}}{10} & 0 & 0 & 0 & -\frac{\sqrt{5}}{10} \\ 0 & 0 & 0 & \frac{\sqrt{15}}{10} & 0 \end{bmatrix}$
43	symmetry	x
	$\mathbb{Q}_1^{(a)}(B_{3u})$	$\begin{bmatrix} \frac{\sqrt{15}}{10} & 0 & 0 & 0 & -\frac{\sqrt{5}}{10} \\ 0 & \frac{\sqrt{15}}{10} & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{15}}{10} & 0 & 0 \end{bmatrix}$
44	symmetry	$\sqrt{15}xyz$
	$\mathbb{Q}_3^{(a)}(A_u)$	$\begin{bmatrix} 0 & 0 & 0 & \frac{\sqrt{6}}{6} & 0 \\ 0 & 0 & \frac{\sqrt{6}}{6} & 0 & 0 \\ 0 & \frac{\sqrt{6}}{6} & 0 & 0 & 0 \end{bmatrix}$
45	symmetry	$-\frac{z(3x^2+3y^2-2z^2)}{2}$
	$\mathbb{Q}_3^{(a)}(B_{1u}, 1)$	$\begin{bmatrix} 0 & 0 & -\frac{\sqrt{10}}{10} & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{10}}{10} & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{30}}{10} \end{bmatrix}$
46	symmetry	$\frac{\sqrt{15}z(x-y)(x+y)}{2}$
	$\mathbb{Q}_3^{(a)}(B_{1u}, 2)$	$\begin{bmatrix} 0 & 0 & \frac{\sqrt{6}}{6} & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{6}}{6} & 0 \\ \frac{\sqrt{6}}{6} & 0 & 0 & 0 & 0 \end{bmatrix}$
47	symmetry	$-\frac{y(3x^2-2y^2+3z^2)}{2}$
	$\mathbb{Q}_3^{(a)}(B_{2u}, 1)$	$\begin{bmatrix} 0 & -\frac{\sqrt{10}}{10} & 0 & 0 & 0 \\ -\frac{3\sqrt{10}}{20} & 0 & 0 & 0 & -\frac{\sqrt{30}}{20} \\ 0 & 0 & 0 & -\frac{\sqrt{10}}{10} & 0 \end{bmatrix}$
48	symmetry	$-\frac{\sqrt{15}y(x-z)(x+z)}{2}$
	$\mathbb{Q}_3^{(a)}(B_{2u}, 2)$	$\begin{bmatrix} 0 & -\frac{\sqrt{6}}{6} & 0 & 0 & 0 \\ -\frac{\sqrt{6}}{12} & 0 & 0 & 0 & \frac{\sqrt{2}}{4} \\ 0 & 0 & 0 & \frac{\sqrt{6}}{6} & 0 \end{bmatrix}$
49	symmetry	$\frac{x(2x^2-3y^2-3z^2)}{2}$

continued ...

Table 6

No.	multipole	matrix
	$\mathbb{Q}_3^{(a)}(B_{3u}, 1)$	$\begin{bmatrix} \frac{3\sqrt{10}}{20} & 0 & 0 & 0 & -\frac{\sqrt{30}}{20} \\ 0 & -\frac{\sqrt{10}}{10} & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{10}}{10} & 0 & 0 \end{bmatrix}$
50	symmetry	$\frac{\sqrt{15}x(y-z)(y+z)}{2}$
	$\mathbb{Q}_3^{(a)}(B_{3u}, 2)$	$\begin{bmatrix} -\frac{\sqrt{6}}{12} & 0 & 0 & 0 & -\frac{\sqrt{2}}{4} \\ 0 & \frac{\sqrt{6}}{6} & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{6}}{6} & 0 & 0 \end{bmatrix}$
51	symmetry	$-\frac{x^2}{2} - \frac{y^2}{2} + z^2$
	$\mathbb{G}_2^{(a)}(A_u, 1)$	$\begin{bmatrix} 0 & 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & -\frac{1}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}$
52	symmetry	$\frac{\sqrt{3}(x-y)(x+y)}{2}$
	$\mathbb{G}_2^{(a)}(A_u, 2)$	$\begin{bmatrix} 0 & 0 & 0 & \frac{\sqrt{3}}{6} & 0 \\ 0 & 0 & \frac{\sqrt{3}}{6} & 0 & 0 \\ 0 & -\frac{\sqrt{3}}{3} & 0 & 0 & 0 \end{bmatrix}$
53	symmetry	$\sqrt{3}xy$
	$\mathbb{G}_2^{(a)}(B_{1u})$	$\begin{bmatrix} 0 & 0 & -\frac{\sqrt{3}}{6} & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{3}}{6} & 0 \\ \frac{\sqrt{3}}{3} & 0 & 0 & 0 & 0 \end{bmatrix}$
54	symmetry	$\sqrt{3}xz$
	$\mathbb{G}_2^{(a)}(B_{2u})$	$\begin{bmatrix} 0 & \frac{\sqrt{3}}{6} & 0 & 0 & 0 \\ -\frac{\sqrt{3}}{6} & 0 & 0 & 0 & \frac{1}{2} \\ 0 & 0 & 0 & -\frac{\sqrt{3}}{6} & 0 \end{bmatrix}$
55	symmetry	$\sqrt{3}yz$
	$\mathbb{G}_2^{(a)}(B_{3u})$	$\begin{bmatrix} -\frac{\sqrt{3}}{6} & 0 & 0 & 0 & -\frac{1}{2} \\ 0 & -\frac{\sqrt{3}}{6} & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{3}}{6} & 0 & 0 \end{bmatrix}$
56	symmetry	z

continued ...

Table 6

No.	multipole	matrix
	$\mathbb{T}_1^{(a)}(B_{1u})$	$\begin{bmatrix} 0 & 0 & \frac{\sqrt{15}i}{10} & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{15}i}{10} & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{5}i}{5} \end{bmatrix}$
57	symmetry	y $\mathbb{T}_1^{(a)}(B_{2u}) \begin{bmatrix} 0 & \frac{\sqrt{15}i}{10} & 0 & 0 & 0 \\ -\frac{\sqrt{15}i}{10} & 0 & 0 & 0 & -\frac{\sqrt{5}i}{10} \\ 0 & 0 & 0 & \frac{\sqrt{15}i}{10} & 0 \end{bmatrix}$
58	symmetry	x $\mathbb{T}_1^{(a)}(B_{3u}) \begin{bmatrix} \frac{\sqrt{15}i}{10} & 0 & 0 & 0 & -\frac{\sqrt{5}i}{10} \\ 0 & \frac{\sqrt{15}i}{10} & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{15}i}{10} & 0 & 0 \end{bmatrix}$
59	symmetry	$\sqrt{15}xyz$ $\mathbb{T}_3^{(a)}(A_u) \begin{bmatrix} 0 & 0 & 0 & \frac{\sqrt{6}i}{6} & 0 \\ 0 & 0 & \frac{\sqrt{6}i}{6} & 0 & 0 \\ 0 & \frac{\sqrt{6}i}{6} & 0 & 0 & 0 \end{bmatrix}$
60	symmetry	$-\frac{z(3x^2+3y^2-2z^2)}{2}$ $\mathbb{T}_3^{(a)}(B_{1u}, 1) \begin{bmatrix} 0 & 0 & -\frac{\sqrt{10}i}{10} & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{10}i}{10} & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{30}i}{10} \end{bmatrix}$
61	symmetry	$\frac{\sqrt{15}z(x-y)(x+y)}{2}$ $\mathbb{T}_3^{(a)}(B_{1u}, 2) \begin{bmatrix} 0 & 0 & \frac{\sqrt{6}i}{6} & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{6}i}{6} & 0 \\ \frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 \end{bmatrix}$
62	symmetry	$-\frac{y(3x^2-2y^2+3z^2)}{2}$ $\mathbb{T}_3^{(a)}(B_{2u}, 1) \begin{bmatrix} 0 & -\frac{\sqrt{10}i}{10} & 0 & 0 & 0 \\ -\frac{3\sqrt{10}i}{20} & 0 & 0 & 0 & -\frac{\sqrt{30}i}{20} \\ 0 & 0 & 0 & -\frac{\sqrt{10}i}{10} & 0 \end{bmatrix}$
63	symmetry	$-\frac{\sqrt{15}y(x-z)(x+z)}{2}$

continued ...

Table 6

No.	multipole	matrix
	$\mathbb{T}_3^{(a)}(B_{2u}, 2)$	$\begin{bmatrix} 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 & 0 \\ -\frac{\sqrt{6}i}{12} & 0 & 0 & 0 & \frac{\sqrt{2}i}{4} \\ 0 & 0 & 0 & \frac{\sqrt{6}i}{6} & 0 \end{bmatrix}$
64	symmetry	$\frac{x(2x^2-3y^2-3z^2)}{2}$
	$\mathbb{T}_3^{(a)}(B_{3u}, 1)$	$\begin{bmatrix} \frac{3\sqrt{10}i}{20} & 0 & 0 & 0 & -\frac{\sqrt{30}i}{20} \\ 0 & -\frac{\sqrt{10}i}{10} & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{10}i}{10} & 0 & 0 \end{bmatrix}$
65	symmetry	$\frac{\sqrt{15}x(y-z)(y+z)}{2}$
	$\mathbb{T}_3^{(a)}(B_{3u}, 2)$	$\begin{bmatrix} -\frac{\sqrt{6}i}{12} & 0 & 0 & 0 & -\frac{\sqrt{2}i}{4} \\ 0 & \frac{\sqrt{6}i}{6} & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 \end{bmatrix}$
66	symmetry	$-\frac{x^2}{2} - \frac{y^2}{2} + z^2$
	$\mathbb{M}_2^{(a)}(A_u, 1)$	$\begin{bmatrix} 0 & 0 & 0 & -\frac{i}{2} & 0 \\ 0 & 0 & \frac{i}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}$
67	symmetry	$\frac{\sqrt{3}(x-y)(x+y)}{2}$
	$\mathbb{M}_2^{(a)}(A_u, 2)$	$\begin{bmatrix} 0 & 0 & 0 & -\frac{\sqrt{3}i}{6} & 0 \\ 0 & 0 & -\frac{\sqrt{3}i}{6} & 0 & 0 \\ 0 & \frac{\sqrt{3}i}{3} & 0 & 0 & 0 \end{bmatrix}$
68	symmetry	$\sqrt{3}xy$
	$\mathbb{M}_2^{(a)}(B_{1u})$	$\begin{bmatrix} 0 & 0 & \frac{\sqrt{3}i}{6} & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{3}i}{6} & 0 \\ -\frac{\sqrt{3}i}{3} & 0 & 0 & 0 & 0 \end{bmatrix}$
69	symmetry	$\sqrt{3}xz$
	$\mathbb{M}_2^{(a)}(B_{2u})$	$\begin{bmatrix} 0 & -\frac{\sqrt{3}i}{6} & 0 & 0 & 0 \\ \frac{\sqrt{3}i}{6} & 0 & 0 & 0 & -\frac{i}{2} \\ 0 & 0 & 0 & \frac{\sqrt{3}i}{6} & 0 \end{bmatrix}$
70	symmetry	$\sqrt{3}yz$

continued ...

Table 6

No.	multipole	matrix				
		$\frac{\sqrt{3}i}{6}$	0	0	0	$\frac{i}{2}$
		0	$\frac{\sqrt{3}i}{6}$	0	0	0
		0	0	$-\frac{\sqrt{3}i}{6}$	0	0

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

Table 7: (p,f) block.

No.	multipole	matrix						
71	symmetry	$-\frac{x^2}{2} - \frac{y^2}{2} + z^2$						
	$\mathbb{Q}_2^{(a)}(A_g, 1)$	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	$\frac{\sqrt{42}}{14}$
72	symmetry	$\frac{\sqrt{3}(x-y)(x+y)}{2}$						
	$\mathbb{Q}_2^{(a)}(A_g, 2)$	$\frac{\sqrt{35}}{14}$	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
73	symmetry	$\sqrt{3}xy$						
	$\mathbb{Q}_2^{(a)}(B_{1g})$	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
74	symmetry	$\sqrt{3}xz$						
	$\mathbb{Q}_2^{(a)}(B_{2g})$	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
75	symmetry	$\sqrt{3}yz$						

continued ...

Table 7

No.	multipole	matrix
	$\mathbb{Q}_2^{(a)}(B_{3g})$	$\begin{bmatrix} 0 & 0 & 0 & \frac{\sqrt{210}}{42} & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{210}}{42} & 0 & 0 & 0 & -\frac{\sqrt{14}}{14} \\ 0 & 0 & 0 & 0 & 0 & \frac{2\sqrt{21}}{21} & 0 \end{bmatrix}$
76	symmetry	$\frac{\sqrt{21}(x^4-3x^2y^2-3x^2z^2+y^4-3y^2z^2+z^4)}{6}$
	$\mathbb{Q}_4^{(a)}(A_g, 1)$	$\begin{bmatrix} \frac{\sqrt{15}}{12} & 0 & 0 & 0 & -\frac{1}{4} & 0 & 0 \\ 0 & -\frac{\sqrt{15}}{12} & 0 & 0 & 0 & -\frac{1}{4} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{6}}{6} \end{bmatrix}$
77	symmetry	$-\frac{\sqrt{15}(x^4-12x^2y^2+6x^2z^2+y^4+6y^2z^2-2z^4)}{12}$
	$\mathbb{Q}_4^{(a)}(A_g, 2)$	$\begin{bmatrix} -\frac{\sqrt{21}}{12} & 0 & 0 & 0 & -\frac{\sqrt{35}}{28} & 0 & 0 \\ 0 & \frac{\sqrt{21}}{12} & 0 & 0 & 0 & -\frac{\sqrt{35}}{28} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{210}}{42} \end{bmatrix}$
78	symmetry	$\frac{\sqrt{5}(x-y)(x+y)(x^2+y^2-6z^2)}{4}$
	$\mathbb{Q}_4^{(a)}(A_g, 3)$	$\begin{bmatrix} \frac{\sqrt{7}}{28} & 0 & 0 & 0 & -\frac{\sqrt{105}}{28} & 0 & 0 \\ 0 & \frac{\sqrt{7}}{28} & 0 & 0 & 0 & \frac{\sqrt{105}}{28} & 0 \\ 0 & 0 & -\frac{\sqrt{42}}{14} & 0 & 0 & 0 & 0 \end{bmatrix}$
79	symmetry	$\frac{\sqrt{35}xy(x-y)(x+y)}{2}$
	$\mathbb{Q}_4^{(a)}(B_{1g}, 1)$	$\begin{bmatrix} 0 & \frac{1}{2} & 0 & 0 & 0 & 0 & 0 \\ \frac{1}{2} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$
80	symmetry	$-\frac{\sqrt{5}xy(x^2+y^2-6z^2)}{2}$
	$\mathbb{Q}_4^{(a)}(B_{1g}, 2)$	$\begin{bmatrix} 0 & -\frac{\sqrt{7}}{28} & 0 & 0 & 0 & \frac{\sqrt{105}}{28} & 0 \\ \frac{\sqrt{7}}{28} & 0 & 0 & 0 & \frac{\sqrt{105}}{28} & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{42}}{14} & 0 & 0 & 0 \end{bmatrix}$
81	symmetry	$-\frac{\sqrt{35}xz(x-z)(x+z)}{2}$
	$\mathbb{Q}_4^{(a)}(B_{2g}, 1)$	$\begin{bmatrix} 0 & 0 & -\frac{\sqrt{6}}{8} & 0 & 0 & 0 & \frac{\sqrt{10}}{8} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -\frac{1}{8} & 0 & 0 & 0 & \frac{\sqrt{15}}{8} & 0 & 0 \end{bmatrix}$
82	symmetry	$-\frac{\sqrt{5}xz(x^2-6y^2+z^2)}{2}$

continued ...

Table 7

No.	multipole	matrix
	$\mathbb{Q}_4^{(a)}(B_{2g}, 2)$	$\begin{bmatrix} 0 & 0 & -\frac{3\sqrt{42}}{56} & 0 & 0 & 0 & -\frac{\sqrt{70}}{56} \\ 0 & 0 & 0 & \frac{\sqrt{42}}{14} & 0 & 0 & 0 \\ -\frac{\sqrt{7}}{8} & 0 & 0 & 0 & -\frac{\sqrt{105}}{56} & 0 & 0 \end{bmatrix}$
83	symmetry	$\frac{\sqrt{35}yz(y-z)(y+z)}{2}$
	$\mathbb{Q}_4^{(a)}(B_{3g}, 1)$	$\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{6}}{8} & 0 & 0 & 0 & -\frac{\sqrt{10}}{8} \\ 0 & -\frac{1}{8} & 0 & 0 & 0 & -\frac{\sqrt{15}}{8} & 0 \end{bmatrix}$
84	symmetry	$\frac{\sqrt{5}yz(6x^2-y^2-z^2)}{2}$
	$\mathbb{Q}_4^{(a)}(B_{3g}, 2)$	$\begin{bmatrix} 0 & 0 & 0 & \frac{\sqrt{42}}{14} & 0 & 0 & 0 \\ 0 & 0 & \frac{3\sqrt{42}}{56} & 0 & 0 & 0 & -\frac{\sqrt{70}}{56} \\ 0 & \frac{\sqrt{7}}{8} & 0 & 0 & 0 & -\frac{\sqrt{105}}{56} & 0 \end{bmatrix}$
85	symmetry	$\sqrt{15}xyz$
	$\mathbb{G}_3^{(a)}(A_g)$	$\begin{bmatrix} -\frac{1}{4} & 0 & 0 & 0 & -\frac{\sqrt{15}}{12} & 0 & 0 \\ 0 & -\frac{1}{4} & 0 & 0 & 0 & \frac{\sqrt{15}}{12} & 0 \\ 0 & 0 & \frac{\sqrt{6}}{6} & 0 & 0 & 0 & 0 \end{bmatrix}$
86	symmetry	$-\frac{z(3x^2+3y^2-2z^2)}{2}$
	$\mathbb{G}_3^{(a)}(B_{1g}, 1)$	$\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & 0 & -\frac{1}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$
87	symmetry	$\frac{\sqrt{15}z(x-y)(x+y)}{2}$
	$\mathbb{G}_3^{(a)}(B_{1g}, 2)$	$\begin{bmatrix} 0 & \frac{1}{4} & 0 & 0 & 0 & \frac{\sqrt{15}}{12} & 0 \\ -\frac{1}{4} & 0 & 0 & 0 & \frac{\sqrt{15}}{12} & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{6}}{6} & 0 & 0 & 0 \end{bmatrix}$
88	symmetry	$-\frac{y(3x^2-2y^2+3z^2)}{2}$
	$\mathbb{G}_3^{(a)}(B_{2g}, 1)$	$\begin{bmatrix} 0 & 0 & \frac{\sqrt{10}}{8} & 0 & 0 & 0 & \frac{\sqrt{6}}{8} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -\frac{\sqrt{15}}{8} & 0 & 0 & 0 & -\frac{1}{8} & 0 & 0 \end{bmatrix}$
89	symmetry	$-\frac{\sqrt{15}y(x-z)(x+z)}{2}$

continued ...

Table 7

No.	multipole	matrix
	$\mathbb{G}_3^{(a)}(B_{2g}, 2)$	$\begin{bmatrix} 0 & 0 & -\frac{\sqrt{6}}{24} & 0 & 0 & 0 & -\frac{\sqrt{10}}{8} \\ 0 & 0 & 0 & -\frac{\sqrt{6}}{6} & 0 & 0 & 0 \\ -\frac{3}{8} & 0 & 0 & 0 & \frac{\sqrt{15}}{24} & 0 & 0 \end{bmatrix}$
90	symmetry	$\frac{x(2x^2-3y^2-3z^2)}{2}$
	$\mathbb{G}_3^{(a)}(B_{3g}, 1)$	$\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{10}}{8} & 0 & 0 & 0 & -\frac{\sqrt{6}}{8} \\ 0 & -\frac{\sqrt{15}}{8} & 0 & 0 & 0 & \frac{1}{8} & 0 \end{bmatrix}$
91	symmetry	$\frac{\sqrt{15}x(y-z)(y+z)}{2}$
	$\mathbb{G}_3^{(a)}(B_{3g}, 2)$	$\begin{bmatrix} 0 & 0 & 0 & -\frac{\sqrt{6}}{6} & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{6}}{24} & 0 & 0 & 0 & -\frac{\sqrt{10}}{8} \\ 0 & \frac{3}{8} & 0 & 0 & 0 & \frac{\sqrt{15}}{24} & 0 \end{bmatrix}$
92	symmetry	$-\frac{x^2}{2} - \frac{y^2}{2} + z^2$
	$\mathbb{T}_2^{(a)}(A_g, 1)$	$\begin{bmatrix} 0 & 0 & 0 & 0 & \frac{\sqrt{7}i}{7} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{7}i}{7} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{42}i}{14} \end{bmatrix}$
93	symmetry	$\frac{\sqrt{3}(x-y)(x+y)}{2}$
	$\mathbb{T}_2^{(a)}(A_g, 2)$	$\begin{bmatrix} \frac{\sqrt{35}i}{14} & 0 & 0 & 0 & -\frac{\sqrt{21}i}{42} & 0 & 0 \\ 0 & \frac{\sqrt{35}i}{14} & 0 & 0 & 0 & \frac{\sqrt{21}i}{42} & 0 \\ 0 & 0 & \frac{\sqrt{210}i}{42} & 0 & 0 & 0 & 0 \end{bmatrix}$
94	symmetry	$\sqrt{3}xy$
	$\mathbb{T}_2^{(a)}(B_{1g})$	$\begin{bmatrix} 0 & \frac{\sqrt{35}i}{14} & 0 & 0 & 0 & -\frac{\sqrt{21}i}{42} & 0 \\ -\frac{\sqrt{35}i}{14} & 0 & 0 & 0 & -\frac{\sqrt{21}i}{42} & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{210}i}{42} & 0 & 0 & 0 \end{bmatrix}$
95	symmetry	$\sqrt{3}xz$
	$\mathbb{T}_2^{(a)}(B_{2g})$	$\begin{bmatrix} 0 & 0 & \frac{\sqrt{210}i}{42} & 0 & 0 & 0 & -\frac{\sqrt{14}i}{14} \\ 0 & 0 & 0 & \frac{\sqrt{210}i}{42} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{2\sqrt{21}i}{21} & 0 & 0 \end{bmatrix}$
96	symmetry	$\sqrt{3}yz$

continued ...

Table 7

No.	multipole	matrix
	$\mathbb{T}_2^{(a)}(B_{3g})$	$\begin{bmatrix} 0 & 0 & 0 & \frac{\sqrt{210}i}{42} & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{210}i}{42} & 0 & 0 & 0 & -\frac{\sqrt{14}i}{14} \\ 0 & 0 & 0 & 0 & 0 & \frac{2\sqrt{21}i}{21} & 0 \end{bmatrix}$
97	symmetry	$\frac{\sqrt{21}(x^4-3x^2y^2-3x^2z^2+y^4-3y^2z^2+z^4)}{6}$
	$\mathbb{T}_4^{(a)}(A_g, 1)$	$\begin{bmatrix} \frac{\sqrt{15}i}{12} & 0 & 0 & 0 & -\frac{i}{4} & 0 & 0 \\ 0 & -\frac{\sqrt{15}i}{12} & 0 & 0 & 0 & -\frac{i}{4} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{6}i}{6} \end{bmatrix}$
98	symmetry	$-\frac{\sqrt{15}(x^4-12x^2y^2+6x^2z^2+y^4+6y^2z^2-2z^4)}{12}$
	$\mathbb{T}_4^{(a)}(A_g, 2)$	$\begin{bmatrix} -\frac{\sqrt{21}i}{12} & 0 & 0 & 0 & -\frac{\sqrt{35}i}{28} & 0 & 0 \\ 0 & \frac{\sqrt{21}i}{12} & 0 & 0 & 0 & -\frac{\sqrt{35}i}{28} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{210}i}{42} \end{bmatrix}$
99	symmetry	$\frac{\sqrt{5}(x-y)(x+y)(x^2+y^2-6z^2)}{4}$
	$\mathbb{T}_4^{(a)}(A_g, 3)$	$\begin{bmatrix} \frac{\sqrt{7}i}{28} & 0 & 0 & 0 & -\frac{\sqrt{105}i}{28} & 0 & 0 \\ 0 & \frac{\sqrt{7}i}{28} & 0 & 0 & 0 & \frac{\sqrt{105}i}{28} & 0 \\ 0 & 0 & -\frac{\sqrt{42}i}{14} & 0 & 0 & 0 & 0 \end{bmatrix}$
100	symmetry	$\frac{\sqrt{35}xy(x-y)(x+y)}{2}$
	$\mathbb{T}_4^{(a)}(B_{1g}, 1)$	$\begin{bmatrix} 0 & \frac{i}{2} & 0 & 0 & 0 & 0 & 0 \\ \frac{i}{2} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$
101	symmetry	$-\frac{\sqrt{5}xy(x^2+y^2-6z^2)}{2}$
	$\mathbb{T}_4^{(a)}(B_{1g}, 2)$	$\begin{bmatrix} 0 & -\frac{\sqrt{7}i}{28} & 0 & 0 & 0 & \frac{\sqrt{105}i}{28} & 0 \\ \frac{\sqrt{7}i}{28} & 0 & 0 & 0 & \frac{\sqrt{105}i}{28} & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{42}i}{14} & 0 & 0 & 0 \end{bmatrix}$
102	symmetry	$-\frac{\sqrt{35}xz(x-z)(x+z)}{2}$
	$\mathbb{T}_4^{(a)}(B_{2g}, 1)$	$\begin{bmatrix} 0 & 0 & -\frac{\sqrt{6}i}{8} & 0 & 0 & 0 & \frac{\sqrt{10}i}{8} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -\frac{i}{8} & 0 & 0 & 0 & \frac{\sqrt{15}i}{8} & 0 & 0 \end{bmatrix}$
103	symmetry	$-\frac{\sqrt{5}xz(x^2-6y^2+z^2)}{2}$

continued ...

Table 7

No.	multipole	matrix
	$\mathbb{T}_4^{(a)}(B_{2g}, 2)$	$\begin{bmatrix} 0 & 0 & -\frac{3\sqrt{42}i}{56} & 0 & 0 & 0 & -\frac{\sqrt{70}i}{56} \\ 0 & 0 & 0 & \frac{\sqrt{42}i}{14} & 0 & 0 & 0 \\ -\frac{\sqrt{7}i}{8} & 0 & 0 & 0 & -\frac{\sqrt{105}i}{56} & 0 & 0 \end{bmatrix}$
104	symmetry	$\frac{\sqrt{35}yz(y-z)(y+z)}{2}$
	$\mathbb{T}_4^{(a)}(B_{3g}, 1)$	$\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{6}i}{8} & 0 & 0 & 0 & -\frac{\sqrt{10}i}{8} \\ 0 & -\frac{i}{8} & 0 & 0 & 0 & -\frac{\sqrt{15}i}{8} & 0 \end{bmatrix}$
105	symmetry	$\frac{\sqrt{5}yz(6x^2-y^2-z^2)}{2}$
	$\mathbb{T}_4^{(a)}(B_{3g}, 2)$	$\begin{bmatrix} 0 & 0 & 0 & \frac{\sqrt{42}i}{14} & 0 & 0 & 0 \\ 0 & 0 & \frac{3\sqrt{42}i}{56} & 0 & 0 & 0 & -\frac{\sqrt{70}i}{56} \\ 0 & \frac{\sqrt{7}i}{8} & 0 & 0 & 0 & -\frac{\sqrt{105}i}{56} & 0 \end{bmatrix}$
106	symmetry	$\sqrt{15}xyz$
	$\mathbb{M}_3^{(a)}(A_g)$	$\begin{bmatrix} \frac{i}{4} & 0 & 0 & 0 & \frac{\sqrt{15}i}{12} & 0 & 0 \\ 0 & \frac{i}{4} & 0 & 0 & 0 & -\frac{\sqrt{15}i}{12} & 0 \\ 0 & 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 \end{bmatrix}$
107	symmetry	$-\frac{z(3x^2+3y^2-2z^2)}{2}$
	$\mathbb{M}_3^{(a)}(B_{1g}, 1)$	$\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & -\frac{i}{2} & 0 \\ 0 & 0 & 0 & 0 & \frac{i}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$
108	symmetry	$\frac{\sqrt{15}z(x-y)(x+y)}{2}$
	$\mathbb{M}_3^{(a)}(B_{1g}, 2)$	$\begin{bmatrix} 0 & -\frac{i}{4} & 0 & 0 & 0 & -\frac{\sqrt{15}i}{12} & 0 \\ \frac{i}{4} & 0 & 0 & 0 & -\frac{\sqrt{15}i}{12} & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{6}i}{6} & 0 & 0 & 0 \end{bmatrix}$
109	symmetry	$-\frac{y(3x^2-2y^2+3z^2)}{2}$
	$\mathbb{M}_3^{(a)}(B_{2g}, 1)$	$\begin{bmatrix} 0 & 0 & -\frac{\sqrt{10}i}{8} & 0 & 0 & 0 & -\frac{\sqrt{6}i}{8} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{\sqrt{15}i}{8} & 0 & 0 & 0 & \frac{i}{8} & 0 & 0 \end{bmatrix}$
110	symmetry	$-\frac{\sqrt{15}y(x-z)(x+z)}{2}$

continued ...

Table 7

No.	multipole	matrix
	$\mathbb{M}_3^{(a)}(B_{2g}, 2)$	$\begin{bmatrix} 0 & 0 & \frac{\sqrt{6}i}{24} & 0 & 0 & 0 & \frac{\sqrt{10}i}{8} \\ 0 & 0 & 0 & \frac{\sqrt{6}i}{6} & 0 & 0 & 0 \\ \frac{3i}{8} & 0 & 0 & 0 & -\frac{\sqrt{15}i}{24} & 0 & 0 \end{bmatrix}$
111	symmetry	$\frac{x(2x^2-3y^2-3z^2)}{2}$
	$\mathbb{M}_3^{(a)}(B_{3g}, 1)$	$\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{10}i}{8} & 0 & 0 & 0 & \frac{\sqrt{6}i}{8} \\ 0 & \frac{\sqrt{15}i}{8} & 0 & 0 & 0 & -\frac{i}{8} & 0 \end{bmatrix}$
112	symmetry	$\frac{\sqrt{15}x(y-z)(y+z)}{2}$
	$\mathbb{M}_3^{(a)}(B_{3g}, 2)$	$\begin{bmatrix} 0 & 0 & 0 & \frac{\sqrt{6}i}{6} & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{6}i}{24} & 0 & 0 & 0 & \frac{\sqrt{10}i}{8} \\ 0 & -\frac{3i}{8} & 0 & 0 & 0 & -\frac{\sqrt{15}i}{24} & 0 \end{bmatrix}$

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
	$\mathbb{Q}_0^{(a)}(A_g)$	$\begin{bmatrix} \frac{\sqrt{5}}{5} & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{5}}{5} & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{5}}{5} & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{5}}{5} & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{5}}{5} \end{bmatrix}$
114	symmetry	$-\frac{x^2}{2} - \frac{y^2}{2} + z^2$

continued ...

Table 8

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

continued ...

Table 8

No.	multipole	matrix
	$\mathbb{Q}_2^{(a)}(B_{3g})$	$\begin{bmatrix} 0 & 0 & 0 & -\frac{\sqrt{42}}{14} & 0 \\ 0 & 0 & \frac{\sqrt{42}}{14} & 0 & 0 \\ 0 & \frac{\sqrt{42}}{14} & 0 & 0 & 0 \\ -\frac{\sqrt{42}}{14} & 0 & 0 & 0 & \frac{\sqrt{14}}{14} \\ 0 & 0 & 0 & \frac{\sqrt{14}}{14} & 0 \end{bmatrix}$
119	symmetry	$\frac{\sqrt{21}(x^4 - 3x^2y^2 - 3x^2z^2 + y^4 - 3y^2z^2 + z^4)}{6}$
	$\mathbb{Q}_4^{(a)}(A_g, 1)$	$\begin{bmatrix} \frac{\sqrt{30}}{10} & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{30}}{15} & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{30}}{15} & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{30}}{15} & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{30}}{10} \end{bmatrix}$
120	symmetry	$-\frac{\sqrt{15}(x^4 - 12x^2y^2 + 6x^2z^2 + y^4 + 6y^2z^2 - 2z^4)}{12}$
	$\mathbb{Q}_4^{(a)}(A_g, 2)$	$\begin{bmatrix} -\frac{\sqrt{42}}{14} & 0 & 0 & 0 & 0 \\ 0 & \frac{2\sqrt{42}}{21} & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{42}}{21} & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{42}}{21} & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{42}}{14} \end{bmatrix}$
121	symmetry	$\frac{\sqrt{5}(x-y)(x+y)(x^2+y^2-6z^2)}{4}$
	$\mathbb{Q}_4^{(a)}(A_g, 3)$	$\begin{bmatrix} 0 & 0 & 0 & 0 & -\frac{\sqrt{42}}{14} \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{14}}{7} & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{14}}{7} & 0 \\ -\frac{\sqrt{42}}{14} & 0 & 0 & 0 & 0 \end{bmatrix}$
122	symmetry	$\frac{\sqrt{35}xy(x-y)(x+y)}{2}$

continued ...

Table 8

No.	multipole	matrix
	$\mathbb{Q}_4^{(a)}(B_{1g}, 1)$	$\begin{bmatrix} 0 & \frac{\sqrt{2}}{2} & 0 & 0 & 0 \\ \frac{\sqrt{2}}{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}$
123	symmetry	$-\frac{\sqrt{5}xy(x^2+y^2-6z^2)}{2}$
	$\mathbb{Q}_4^{(a)}(B_{1g}, 2)$	$\begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{42}}{14} \\ 0 & 0 & 0 & \frac{\sqrt{14}}{7} & 0 \\ 0 & 0 & \frac{\sqrt{14}}{7} & 0 & 0 \\ 0 & \frac{\sqrt{42}}{14} & 0 & 0 & 0 \end{bmatrix}$
124	symmetry	$-\frac{\sqrt{35}xz(x-z)(x+z)}{2}$
	$\mathbb{Q}_4^{(a)}(B_{2g}, 1)$	$\begin{bmatrix} 0 & 0 & -\frac{\sqrt{2}}{4} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ -\frac{\sqrt{2}}{4} & 0 & 0 & 0 & \frac{\sqrt{6}}{4} \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{6}}{4} & 0 & 0 \end{bmatrix}$
125	symmetry	$-\frac{\sqrt{5}xz(x^2-6y^2+z^2)}{2}$
	$\mathbb{Q}_4^{(a)}(B_{2g}, 2)$	$\begin{bmatrix} 0 & 0 & -\frac{3\sqrt{14}}{28} & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{14}}{7} & 0 \\ -\frac{3\sqrt{14}}{28} & 0 & 0 & 0 & -\frac{\sqrt{42}}{28} \\ 0 & \frac{\sqrt{14}}{7} & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{42}}{28} & 0 & 0 \end{bmatrix}$
126	symmetry	$\frac{\sqrt{35}yz(y-z)(y+z)}{2}$

continued ...

Table 8

No.	multipole	matrix
	$\mathbb{Q}_4^{(a)}(B_{3g}, 1)$	$\begin{bmatrix} 0 & 0 & 0 & -\frac{\sqrt{2}}{4} & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ -\frac{\sqrt{2}}{4} & 0 & 0 & 0 & -\frac{\sqrt{6}}{4} \\ 0 & 0 & 0 & -\frac{\sqrt{6}}{4} & 0 \end{bmatrix}$
127	symmetry	$\frac{\sqrt{5}yz(6x^2-y^2-z^2)}{2}$
	$\mathbb{Q}_4^{(a)}(B_{3g}, 2)$	$\begin{bmatrix} 0 & 0 & 0 & \frac{3\sqrt{14}}{28} & 0 \\ 0 & 0 & \frac{\sqrt{14}}{7} & 0 & 0 \\ 0 & \frac{\sqrt{14}}{7} & 0 & 0 & 0 \\ \frac{3\sqrt{14}}{28} & 0 & 0 & 0 & -\frac{\sqrt{42}}{28} \\ 0 & 0 & 0 & -\frac{\sqrt{42}}{28} & 0 \end{bmatrix}$
128	symmetry	z
	$\mathbb{M}_1^{(a)}(B_{1g})$	$\begin{bmatrix} 0 & -\frac{\sqrt{10}i}{5} & 0 & 0 & 0 \\ \frac{\sqrt{10}i}{5} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{10}i}{10} & 0 \\ 0 & 0 & \frac{\sqrt{10}i}{10} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}$
129	symmetry	y
	$\mathbb{M}_1^{(a)}(B_{2g})$	$\begin{bmatrix} 0 & 0 & \frac{\sqrt{10}i}{10} & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{10}i}{10} & 0 \\ -\frac{\sqrt{10}i}{10} & 0 & 0 & 0 & \frac{\sqrt{30}i}{10} \\ 0 & -\frac{\sqrt{10}i}{10} & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{30}i}{10} & 0 & 0 \end{bmatrix}$
130	symmetry	x

continued ...

Table 8

No.	multipole	matrix
	$\mathbb{M}_1^{(a)}(B_{3g})$	$\begin{bmatrix} 0 & 0 & 0 & \frac{\sqrt{10}i}{10} & 0 \\ 0 & 0 & -\frac{\sqrt{10}i}{10} & 0 & 0 \\ 0 & \frac{\sqrt{10}i}{10} & 0 & 0 & 0 \\ -\frac{\sqrt{10}i}{10} & 0 & 0 & 0 & -\frac{\sqrt{30}i}{10} \\ 0 & 0 & 0 & \frac{\sqrt{30}i}{10} & 0 \end{bmatrix}$
131	symmetry	$\sqrt{15}xyz$ $\mathbb{M}_3^{(a)}(A_g) = \begin{bmatrix} 0 & 0 & 0 & 0 & \frac{\sqrt{2}i}{2} \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ -\frac{\sqrt{2}i}{2} & 0 & 0 & 0 & 0 \end{bmatrix}$
132	symmetry	$-\frac{z(3x^2+3y^2-2z^2)}{2}$ $\mathbb{M}_3^{(a)}(B_{1g}, 1) = \begin{bmatrix} 0 & \frac{\sqrt{10}i}{10} & 0 & 0 & 0 \\ -\frac{\sqrt{10}i}{10} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{10}i}{5} & 0 \\ 0 & 0 & \frac{\sqrt{10}i}{5} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}$
133	symmetry	$\frac{\sqrt{15}z(x-y)(x+y)}{2}$ $\mathbb{M}_3^{(a)}(B_{1g}, 2) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{2}i}{2} \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{2}i}{2} & 0 & 0 & 0 \end{bmatrix}$
134	symmetry	$-\frac{y(3x^2-2y^2+3z^2)}{2}$

continued ...

Table 8

No.	multipole	matrix
	$\mathbb{M}_3^{(a)}(B_{2g}, 1)$	$\begin{bmatrix} 0 & 0 & -\frac{\sqrt{10}i}{20} & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{10}i}{5} & 0 \\ \frac{\sqrt{10}i}{20} & 0 & 0 & 0 & -\frac{\sqrt{30}i}{20} \\ 0 & -\frac{\sqrt{10}i}{5} & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{30}i}{20} & 0 & 0 \end{bmatrix}$
135	symmetry	$-\frac{\sqrt{15}y(x-z)(x+z)}{2}$ $\mathbb{M}_3^{(a)}(B_{2g}, 2) = \begin{bmatrix} 0 & 0 & -\frac{\sqrt{6}i}{4} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ \frac{\sqrt{6}i}{4} & 0 & 0 & 0 & \frac{\sqrt{2}i}{4} \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{2}i}{4} & 0 & 0 \end{bmatrix}$
136	symmetry	$\frac{x(2x^2-3y^2-3z^2)}{2}$ $\mathbb{M}_3^{(a)}(B_{3g}, 1) = \begin{bmatrix} 0 & 0 & 0 & -\frac{\sqrt{10}i}{20} & 0 \\ 0 & 0 & -\frac{\sqrt{10}i}{5} & 0 & 0 \\ 0 & \frac{\sqrt{10}i}{5} & 0 & 0 & 0 \\ \frac{\sqrt{10}i}{20} & 0 & 0 & 0 & \frac{\sqrt{30}i}{20} \\ 0 & 0 & 0 & -\frac{\sqrt{30}i}{20} & 0 \end{bmatrix}$
137	symmetry	$\frac{\sqrt{15}x(y-z)(y+z)}{2}$ $\mathbb{M}_3^{(a)}(B_{3g}, 2) = \begin{bmatrix} 0 & 0 & 0 & \frac{\sqrt{6}i}{4} & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ -\frac{\sqrt{6}i}{4} & 0 & 0 & 0 & \frac{\sqrt{2}i}{4} \\ 0 & 0 & 0 & -\frac{\sqrt{2}i}{4} & 0 \end{bmatrix}$

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 $\mathbb{Q}_1^{(a)}(B_{1u}) \begin{bmatrix} 0 & 0 & \frac{\sqrt{14}}{14} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{14}}{14} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{2\sqrt{35}}{35} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{2\sqrt{35}}{35} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{3\sqrt{70}}{70} \end{bmatrix}$
139	symmetry	y $\mathbb{Q}_1^{(a)}(B_{2u}) \begin{bmatrix} 0 & \frac{\sqrt{21}}{14} & 0 & 0 & 0 & \frac{\sqrt{35}}{70} & 0 \\ -\frac{\sqrt{21}}{14} & 0 & 0 & 0 & -\frac{\sqrt{35}}{70} & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{14}}{14} & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{14}}{14} & 0 & 0 & 0 & -\frac{\sqrt{210}}{70} \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{105}}{35} & 0 \end{bmatrix}$
140	symmetry	x $\mathbb{Q}_1^{(a)}(B_{3u}) \begin{bmatrix} \frac{\sqrt{21}}{14} & 0 & 0 & 0 & -\frac{\sqrt{35}}{70} & 0 & 0 \\ 0 & \frac{\sqrt{21}}{14} & 0 & 0 & 0 & -\frac{\sqrt{35}}{70} & 0 \\ 0 & 0 & \frac{\sqrt{14}}{14} & 0 & 0 & 0 & -\frac{\sqrt{210}}{70} \\ 0 & 0 & 0 & \frac{\sqrt{14}}{14} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{105}}{35} & 0 & 0 \end{bmatrix}$
141	symmetry	$\sqrt{15}xyz$ $\mathbb{Q}_3^{(a)}(A_u) \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{6}}{6} \\ 0 & \frac{\sqrt{15}}{12} & 0 & 0 & 0 & \frac{1}{4} & 0 \\ -\frac{\sqrt{15}}{12} & 0 & 0 & 0 & \frac{1}{4} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$
142	symmetry	$-\frac{z(3x^2+3y^2-2z^2)}{2}$

continued ...

Table 9

No.	multipole	matrix
	$\mathbb{Q}_3^{(a)}(B_{1u}, 1)$	$\begin{bmatrix} 0 & 0 & -\frac{\sqrt{6}}{6} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{6}}{6} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{15}}{30} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{15}}{30} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{30}}{15} \end{bmatrix}$
143	symmetry	$\frac{\sqrt{15}z(x-y)(x+y)}{2}$ $\mathbb{Q}_3^{(a)}(B_{1u}, 2) \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{6}}{6} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{\sqrt{15}}{12} & 0 & 0 & 0 & \frac{1}{4} & 0 & 0 \\ 0 & \frac{\sqrt{15}}{12} & 0 & 0 & 0 & -\frac{1}{4} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$
144	symmetry	$-\frac{y(3x^2-2y^2+3z^2)}{2}$ $\mathbb{Q}_3^{(a)}(B_{2u}, 1) \begin{bmatrix} 0 & \frac{1}{8} & 0 & 0 & 0 & \frac{11\sqrt{15}}{120} & 0 \\ -\frac{1}{8} & 0 & 0 & 0 & -\frac{\sqrt{15}}{120} & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{6}}{6} & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{6}}{24} & 0 & 0 & 0 & -\frac{\sqrt{10}}{40} \\ 0 & \frac{5\sqrt{3}}{24} & 0 & 0 & 0 & -\frac{3\sqrt{5}}{40} & 0 \end{bmatrix}$
145	symmetry	$-\frac{\sqrt{15}y(x-z)(x+z)}{2}$ $\mathbb{Q}_3^{(a)}(B_{2u}, 2) \begin{bmatrix} 0 & -\frac{\sqrt{15}}{24} & 0 & 0 & 0 & -\frac{1}{8} & 0 \\ \frac{\sqrt{15}}{24} & 0 & 0 & 0 & \frac{3}{8} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{10}}{8} & 0 & 0 & 0 & \frac{\sqrt{6}}{24} \\ 0 & \frac{\sqrt{5}}{8} & 0 & 0 & 0 & \frac{\sqrt{3}}{8} & 0 \end{bmatrix}$
146	symmetry	$\frac{x(2x^2-3y^2-3z^2)}{2}$

continued ...

Table 9

No.	multipole	matrix
	$\mathbb{Q}_3^{(a)}(B_{3u}, 1)$	$\begin{bmatrix} \frac{1}{8} & 0 & 0 & 0 & -\frac{11\sqrt{15}}{120} & 0 & 0 \\ 0 & \frac{1}{8} & 0 & 0 & 0 & -\frac{\sqrt{15}}{120} & 0 \\ 0 & 0 & \frac{\sqrt{6}}{24} & 0 & 0 & 0 & -\frac{\sqrt{10}}{40} \\ 0 & 0 & 0 & -\frac{\sqrt{6}}{6} & 0 & 0 & 0 \\ -\frac{5\sqrt{3}}{24} & 0 & 0 & 0 & -\frac{3\sqrt{5}}{40} & 0 & 0 \end{bmatrix}$
147	symmetry	$\frac{\sqrt{15}x(y-z)(y+z)}{2}$ $\mathbb{Q}_3^{(a)}(B_{3u}, 2) \begin{bmatrix} \frac{\sqrt{15}}{24} & 0 & 0 & 0 & -\frac{1}{8} & 0 & 0 \\ 0 & \frac{\sqrt{15}}{24} & 0 & 0 & 0 & -\frac{3}{8} & 0 \\ 0 & 0 & -\frac{\sqrt{10}}{8} & 0 & 0 & 0 & -\frac{\sqrt{6}}{24} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{\sqrt{5}}{8} & 0 & 0 & 0 & -\frac{\sqrt{3}}{8} & 0 & 0 \end{bmatrix}$
148	symmetry	$\frac{3\sqrt{35}xyz(x-y)(x+y)}{2}$ $\mathbb{Q}_5^{(a)}(A_u, 1) \begin{bmatrix} 0 & 0 & 0 & \frac{\sqrt{15}}{10} & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{15}}{10} & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{10}}{10} & 0 & 0 & 0 & 0 & 0 \\ \frac{\sqrt{10}}{10} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$
149	symmetry	$\frac{\sqrt{105}xyz(x^2+y^2-2z^2)}{2}$ $\mathbb{Q}_5^{(a)}(A_u, 2) \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{3}}{6} \\ 0 & \frac{\sqrt{30}}{60} & 0 & 0 & 0 & -\frac{\sqrt{2}}{4} & 0 \\ -\frac{\sqrt{30}}{60} & 0 & 0 & 0 & -\frac{\sqrt{2}}{4} & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{15}}{10} & 0 & 0 & 0 \end{bmatrix}$
150	symmetry	$\frac{z(15x^4+30x^2y^2-40x^2z^2+15y^4-40y^2z^2+8z^4)}{8}$

continued ...

Table 9

No.	multipole	matrix
	$\mathbb{Q}_5^{(a)}(B_{1u}, 1)$	$\begin{bmatrix} 0 & 0 & \frac{\sqrt{21}}{42} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{21}}{42} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{210}}{42} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{210}}{42} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{105}}{21} \end{bmatrix}$
151	symmetry	$\frac{3\sqrt{35}z(x^2-2xy-y^2)(x^2+2xy-y^2)}{8}$
	$\mathbb{Q}_5^{(a)}(B_{1u}, 2)$	$\begin{bmatrix} 0 & 0 & \frac{\sqrt{15}}{10} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{15}}{10} & 0 & 0 & 0 \\ \frac{\sqrt{10}}{10} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{10}}{10} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$
152	symmetry	$-\frac{\sqrt{105}z(x-y)(x+y)(x^2+y^2-2z^2)}{4}$
	$\mathbb{Q}_5^{(a)}(B_{1u}, 3)$	$\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{3}}{6} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -\frac{\sqrt{30}}{60} & 0 & 0 & 0 & \frac{\sqrt{2}}{4} & 0 & 0 \\ 0 & -\frac{\sqrt{30}}{60} & 0 & 0 & 0 & -\frac{\sqrt{2}}{4} & 0 \\ 0 & 0 & \frac{\sqrt{15}}{10} & 0 & 0 & 0 & 0 \end{bmatrix}$
153	symmetry	$\frac{y(15x^4-40x^2y^2+30x^2z^2+8y^4-40y^2z^2+15z^4)}{8}$
	$\mathbb{Q}_5^{(a)}(B_{2u}, 1)$	$\begin{bmatrix} 0 & \frac{11\sqrt{14}}{112} & 0 & 0 & 0 & \frac{5\sqrt{210}}{336} & 0 \\ \frac{5\sqrt{14}}{56} & 0 & 0 & 0 & \frac{\sqrt{210}}{168} & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{21}}{42} & 0 & 0 & 0 \\ 0 & 0 & \frac{5\sqrt{21}}{84} & 0 & 0 & 0 & \frac{\sqrt{35}}{28} \\ 0 & \frac{\sqrt{42}}{48} & 0 & 0 & 0 & \frac{3\sqrt{70}}{112} & 0 \end{bmatrix}$
154	symmetry	$\frac{3\sqrt{35}y(x^2-2xz-z^2)(x^2+2xz-z^2)}{8}$

continued ...

Table 9

No.	multipole	matrix
	$\mathbb{Q}_5^{(a)}(B_{2u}, 2)$	$\begin{bmatrix} 0 & \frac{3\sqrt{10}}{80} & 0 & 0 & 0 & -\frac{\sqrt{6}}{16} & 0 \\ \frac{\sqrt{10}}{40} & 0 & 0 & 0 & -\frac{\sqrt{6}}{8} & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{15}}{10} & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{15}}{20} & 0 & 0 & 0 & \frac{1}{4} \\ 0 & -\frac{3\sqrt{30}}{80} & 0 & 0 & 0 & \frac{3\sqrt{2}}{16} & 0 \end{bmatrix}$
155	symmetry	$\frac{\sqrt{105}y(x-z)(x+z)(x^2-2y^2+z^2)}{4}$
	$\mathbb{Q}_5^{(a)}(B_{2u}, 3)$	$\begin{bmatrix} 0 & \frac{7\sqrt{30}}{120} & 0 & 0 & 0 & -\frac{\sqrt{2}}{8} & 0 \\ \frac{\sqrt{30}}{15} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{5}}{10} & 0 & 0 & 0 & -\frac{\sqrt{3}}{6} \\ 0 & -\frac{\sqrt{10}}{40} & 0 & 0 & 0 & -\frac{\sqrt{6}}{8} & 0 \end{bmatrix}$
156	symmetry	$\frac{x(8x^4-40x^2y^2-40x^2z^2+15y^4+30y^2z^2+15z^4)}{8}$
	$\mathbb{Q}_5^{(a)}(B_{3u}, 1)$	$\begin{bmatrix} \frac{11\sqrt{14}}{112} & 0 & 0 & 0 & -\frac{5\sqrt{210}}{336} & 0 & 0 \\ 0 & -\frac{5\sqrt{14}}{56} & 0 & 0 & 0 & \frac{\sqrt{210}}{168} & 0 \\ 0 & 0 & -\frac{5\sqrt{21}}{84} & 0 & 0 & 0 & \frac{\sqrt{35}}{28} \\ 0 & 0 & 0 & \frac{\sqrt{21}}{42} & 0 & 0 & 0 \\ -\frac{\sqrt{42}}{48} & 0 & 0 & 0 & \frac{3\sqrt{70}}{112} & 0 & 0 \end{bmatrix}$
157	symmetry	$\frac{3\sqrt{35}x(y^2-2yz-z^2)(y^2+2yz-z^2)}{8}$
	$\mathbb{Q}_5^{(a)}(B_{3u}, 2)$	$\begin{bmatrix} \frac{3\sqrt{10}}{80} & 0 & 0 & 0 & \frac{\sqrt{6}}{16} & 0 & 0 \\ 0 & -\frac{\sqrt{10}}{40} & 0 & 0 & 0 & -\frac{\sqrt{6}}{8} & 0 \\ 0 & 0 & \frac{\sqrt{15}}{20} & 0 & 0 & 0 & \frac{1}{4} \\ 0 & 0 & 0 & -\frac{\sqrt{15}}{10} & 0 & 0 & 0 \\ \frac{3\sqrt{30}}{80} & 0 & 0 & 0 & \frac{3\sqrt{2}}{16} & 0 & 0 \end{bmatrix}$
158	symmetry	$\frac{\sqrt{105}x(y-z)(y+z)(2x^2-y^2-z^2)}{4}$

continued ...

Table 9

No.	multipole	matrix
	$\mathbb{Q}_5^{(a)}(B_{3u}, 3)$	$\begin{bmatrix} -\frac{7\sqrt{30}}{120} & 0 & 0 & 0 & -\frac{\sqrt{2}}{8} & 0 & 0 \\ 0 & \frac{\sqrt{30}}{15} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{5}}{10} & 0 & 0 & 0 & \frac{\sqrt{3}}{6} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -\frac{\sqrt{10}}{40} & 0 & 0 & 0 & \frac{\sqrt{6}}{8} & 0 & 0 \end{bmatrix}$
159	symmetry	$-\frac{x^2}{2} - \frac{y^2}{2} + z^2$
	$\mathbb{G}_2^{(a)}(A_u, 1)$	$\begin{bmatrix} 0 & 0 & 0 & \frac{\sqrt{35}}{14} & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{35}}{14} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{14}}{14} & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{14}}{14} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$
160	symmetry	$\frac{\sqrt{3}(x-y)(x+y)}{2}$
	$\mathbb{G}_2^{(a)}(A_u, 2)$	$\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{7}}{14} \\ 0 & -\frac{\sqrt{70}}{28} & 0 & 0 & 0 & \frac{\sqrt{42}}{28} & 0 \\ \frac{\sqrt{70}}{28} & 0 & 0 & 0 & \frac{\sqrt{42}}{28} & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{35}}{14} & 0 & 0 & 0 \end{bmatrix}$
161	symmetry	$\sqrt{3}xy$
	$\mathbb{G}_2^{(a)}(B_{1u})$	$\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{7}}{14} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{\sqrt{70}}{28} & 0 & 0 & 0 & -\frac{\sqrt{42}}{28} & 0 & 0 \\ 0 & \frac{\sqrt{70}}{28} & 0 & 0 & 0 & \frac{\sqrt{42}}{28} & 0 \\ 0 & 0 & \frac{\sqrt{35}}{14} & 0 & 0 & 0 & 0 \end{bmatrix}$
162	symmetry	$\sqrt{3}xz$

continued ...

Table 9

No.	multipole	matrix
	$\mathbb{G}_2^{(a)}(B_{2u})$	$\begin{bmatrix} 0 & \frac{\sqrt{70}}{28} & 0 & 0 & 0 & -\frac{\sqrt{42}}{28} & 0 \\ -\frac{\sqrt{70}}{28} & 0 & 0 & 0 & \frac{\sqrt{42}}{28} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{7}}{7} \\ 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{14}}{14} & 0 \end{bmatrix}$
163	symmetry	$\sqrt{3}yz$ $\mathbb{G}_2^{(a)}(B_{3u}) \begin{bmatrix} -\frac{\sqrt{70}}{28} & 0 & 0 & 0 & -\frac{\sqrt{42}}{28} & 0 & 0 \\ 0 & -\frac{\sqrt{70}}{28} & 0 & 0 & 0 & -\frac{\sqrt{42}}{28} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{7}}{7} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{14}}{14} & 0 & 0 \end{bmatrix}$
164	symmetry	$\frac{\sqrt{21}(x^4 - 3x^2y^2 - 3x^2z^2 + y^4 - 3y^2z^2 + z^4)}{6}$ $\mathbb{G}_4^{(a)}(A_u, 1) \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{6}}{6} & 0 & 0 & 0 & 0 \\ 0 & -\frac{1}{4} & 0 & 0 & 0 & \frac{\sqrt{15}}{12} & 0 \\ -\frac{1}{4} & 0 & 0 & 0 & -\frac{\sqrt{15}}{12} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$
165	symmetry	$-\frac{\sqrt{15}(x^4 - 12x^2y^2 + 6x^2z^2 + y^4 + 6y^2z^2 - 2z^4)}{12}$ $\mathbb{G}_4^{(a)}(A_u, 2) \begin{bmatrix} 0 & 0 & 0 & -\frac{\sqrt{210}}{35} & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{210}}{210} & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{35}}{20} & 0 & 0 & 0 & \frac{5\sqrt{21}}{84} & 0 \\ \frac{\sqrt{35}}{20} & 0 & 0 & 0 & -\frac{5\sqrt{21}}{84} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$
166	symmetry	$\frac{\sqrt{5}(x-y)(x+y)(x^2+y^2-6z^2)}{4}$

continued ...

Table 9

No.	multipole	matrix
	$\mathbb{G}_4^{(a)}(A_u, 3)$	$\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{42}}{14} & 0 \\ 0 & -\frac{3\sqrt{105}}{140} & 0 & 0 & 0 & -\frac{\sqrt{7}}{28} & 0 & 0 \\ \frac{3\sqrt{105}}{140} & 0 & 0 & 0 & -\frac{\sqrt{7}}{28} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{210}}{35} & 0 & 0 & 0 & 0 \end{bmatrix}$
167	symmetry	$\frac{\sqrt{35}xy(x-y)(x+y)}{2}$ $\mathbb{G}_4^{(a)}(B_{1u}, 1) \begin{bmatrix} 0 & 0 & -\frac{\sqrt{10}}{10} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{10}}{10} & 0 & 0 & 0 & 0 \\ \frac{\sqrt{15}}{10} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{15}}{10} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$
168	symmetry	$-\frac{\sqrt{5}xy(x^2+y^2-6z^2)}{2}$ $\mathbb{G}_4^{(a)}(B_{1u}, 2) \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{42}}{14} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -\frac{3\sqrt{105}}{140} & 0 & 0 & 0 & -\frac{\sqrt{7}}{28} & 0 & 0 & 0 \\ 0 & -\frac{3\sqrt{105}}{140} & 0 & 0 & 0 & \frac{\sqrt{7}}{28} & 0 & 0 \\ 0 & 0 & \frac{\sqrt{210}}{35} & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$
169	symmetry	$-\frac{\sqrt{35}xz(x-z)(x+z)}{2}$ $\mathbb{G}_4^{(a)}(B_{2u}, 1) \begin{bmatrix} 0 & -\frac{\sqrt{15}}{40} & 0 & 0 & 0 & \frac{1}{8} & 0 & 0 \\ \frac{\sqrt{15}}{40} & 0 & 0 & 0 & -\frac{3}{8} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{10}}{10} & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{3\sqrt{10}}{40} & 0 & 0 & 0 & \frac{\sqrt{6}}{8} & 0 \\ 0 & \frac{3\sqrt{5}}{40} & 0 & 0 & 0 & -\frac{\sqrt{3}}{8} & 0 & 0 \end{bmatrix}$
170	symmetry	$-\frac{\sqrt{5}xz(x^2-6y^2+z^2)}{2}$

continued ...

Table 9

No.	multipole	matrix
	$\mathbb{G}_4^{(a)}(B_{2u}, 2)$	$\begin{bmatrix} 0 & \frac{\sqrt{105}}{280} & 0 & 0 & 0 & -\frac{9\sqrt{7}}{56} & 0 \\ -\frac{\sqrt{105}}{280} & 0 & 0 & 0 & -\frac{5\sqrt{7}}{56} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{70}}{40} & 0 & 0 & 0 & -\frac{\sqrt{42}}{56} \\ 0 & \frac{3\sqrt{35}}{40} & 0 & 0 & 0 & \frac{\sqrt{21}}{56} & 0 \end{bmatrix}$
171	symmetry	$\frac{\sqrt{35}yz(y-z)(y+z)}{2}$ $\mathbb{G}_4^{(a)}(B_{3u}, 1) \begin{bmatrix} -\frac{\sqrt{15}}{40} & 0 & 0 & 0 & -\frac{1}{8} & 0 & 0 \\ 0 & -\frac{\sqrt{15}}{40} & 0 & 0 & 0 & -\frac{3}{8} & 0 \\ 0 & 0 & \frac{3\sqrt{10}}{40} & 0 & 0 & 0 & \frac{\sqrt{6}}{8} \\ 0 & 0 & 0 & \frac{\sqrt{10}}{10} & 0 & 0 & 0 \\ -\frac{3\sqrt{5}}{40} & 0 & 0 & 0 & -\frac{\sqrt{3}}{8} & 0 & 0 \end{bmatrix}$
172	symmetry	$\frac{\sqrt{5}yz(6x^2-y^2-z^2)}{2}$ $\mathbb{G}_4^{(a)}(B_{3u}, 2) \begin{bmatrix} -\frac{\sqrt{105}}{280} & 0 & 0 & 0 & -\frac{9\sqrt{7}}{56} & 0 & 0 \\ 0 & -\frac{\sqrt{105}}{280} & 0 & 0 & 0 & \frac{5\sqrt{7}}{56} & 0 \\ 0 & 0 & \frac{\sqrt{70}}{40} & 0 & 0 & 0 & \frac{\sqrt{42}}{56} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{3\sqrt{35}}{40} & 0 & 0 & 0 & -\frac{\sqrt{21}}{56} & 0 & 0 \end{bmatrix}$
173	symmetry	z $\mathbb{T}_1^{(a)}(B_{1u}) \begin{bmatrix} 0 & 0 & \frac{\sqrt{14}i}{14} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{14}i}{14} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{2\sqrt{35}i}{35} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{2\sqrt{35}i}{35} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{3\sqrt{70}i}{70} \end{bmatrix}$
174	symmetry	y

continued ...

Table 9

No.	multipole	matrix
	$\mathbb{T}_1^{(a)}(B_{2u})$	$\begin{bmatrix} 0 & \frac{\sqrt{21}i}{14} & 0 & 0 & 0 & \frac{\sqrt{35}i}{70} & 0 \\ -\frac{\sqrt{21}i}{14} & 0 & 0 & 0 & -\frac{\sqrt{35}i}{70} & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{14}i}{14} & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{14}i}{14} & 0 & 0 & 0 & -\frac{\sqrt{210}i}{70} \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{105}i}{35} & 0 \end{bmatrix}$
175	symmetry	$\begin{matrix} x \\ \mathbb{T}_1^{(a)}(B_{3u}) \end{matrix} \begin{bmatrix} \frac{\sqrt{21}i}{14} & 0 & 0 & 0 & -\frac{\sqrt{35}i}{70} & 0 & 0 \\ 0 & \frac{\sqrt{21}i}{14} & 0 & 0 & 0 & -\frac{\sqrt{35}i}{70} & 0 \\ 0 & 0 & \frac{\sqrt{14}i}{14} & 0 & 0 & 0 & -\frac{\sqrt{210}i}{70} \\ 0 & 0 & 0 & \frac{\sqrt{14}i}{14} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{105}i}{35} & 0 & 0 \end{bmatrix}$
176	symmetry	$\begin{matrix} \sqrt{15}xyz \\ \mathbb{T}_3^{(a)}(A_u) \end{matrix} \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{6}i}{6} \\ 0 & \frac{\sqrt{15}i}{12} & 0 & 0 & 0 & \frac{i}{4} & 0 \\ -\frac{\sqrt{15}i}{12} & 0 & 0 & 0 & \frac{i}{4} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$
177	symmetry	$\begin{matrix} -\frac{z(3x^2+3y^2-2z^2)}{2} \\ \mathbb{T}_3^{(a)}(B_{1u}, 1) \end{matrix} \begin{bmatrix} 0 & 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{15}i}{30} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{15}i}{30} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{30}i}{15} \end{bmatrix}$
178	symmetry	$\frac{\sqrt{15}z(x-y)(x+y)}{2}$

continued ...

Table 9

No.	multipole	matrix
	$\mathbb{T}_3^{(a)}(B_{1u}, 2)$	$\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{6}i}{6} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{\sqrt{15}i}{12} & 0 & 0 & 0 & \frac{i}{4} & 0 & 0 \\ 0 & \frac{\sqrt{15}i}{12} & 0 & 0 & 0 & -\frac{i}{4} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$
179	symmetry	$-\frac{y(3x^2-2y^2+3z^2)}{2}$
	$\mathbb{T}_3^{(a)}(B_{2u}, 1)$	$\begin{bmatrix} 0 & \frac{i}{8} & 0 & 0 & 0 & \frac{11\sqrt{15}i}{120} & 0 \\ -\frac{i}{8} & 0 & 0 & 0 & -\frac{\sqrt{15}i}{120} & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{6}i}{24} & 0 & 0 & 0 & -\frac{\sqrt{10}i}{40} \\ 0 & \frac{5\sqrt{3}i}{24} & 0 & 0 & 0 & -\frac{3\sqrt{5}i}{40} & 0 \end{bmatrix}$
180	symmetry	$-\frac{\sqrt{15}y(x-z)(x+z)}{2}$
	$\mathbb{T}_3^{(a)}(B_{2u}, 2)$	$\begin{bmatrix} 0 & -\frac{\sqrt{15}i}{24} & 0 & 0 & 0 & -\frac{i}{8} & 0 \\ \frac{\sqrt{15}i}{24} & 0 & 0 & 0 & \frac{3i}{8} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{10}i}{8} & 0 & 0 & 0 & \frac{\sqrt{6}i}{24} \\ 0 & \frac{\sqrt{5}i}{8} & 0 & 0 & 0 & \frac{\sqrt{3}i}{8} & 0 \end{bmatrix}$
181	symmetry	$\frac{x(2x^2-3y^2-3z^2)}{2}$
	$\mathbb{T}_3^{(a)}(B_{3u}, 1)$	$\begin{bmatrix} \frac{i}{8} & 0 & 0 & 0 & -\frac{11\sqrt{15}i}{120} & 0 & 0 \\ 0 & \frac{i}{8} & 0 & 0 & 0 & -\frac{\sqrt{15}i}{120} & 0 \\ 0 & 0 & \frac{\sqrt{6}i}{24} & 0 & 0 & 0 & -\frac{\sqrt{10}i}{40} \\ 0 & 0 & 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 & 0 \\ -\frac{5\sqrt{3}i}{24} & 0 & 0 & 0 & -\frac{3\sqrt{5}i}{40} & 0 & 0 \end{bmatrix}$
182	symmetry	$\frac{\sqrt{15}x(y-z)(y+z)}{2}$

continued ...

Table 9

No.	multipole	matrix
	$\mathbb{T}_3^{(a)}(B_{3u}, 2)$	$\begin{bmatrix} \frac{\sqrt{15}i}{24} & 0 & 0 & 0 & -\frac{i}{8} & 0 & 0 \\ 0 & \frac{\sqrt{15}i}{24} & 0 & 0 & 0 & -\frac{3i}{8} & 0 \\ 0 & 0 & -\frac{\sqrt{10}i}{8} & 0 & 0 & 0 & -\frac{\sqrt{6}i}{24} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{\sqrt{5}i}{8} & 0 & 0 & 0 & -\frac{\sqrt{3}i}{8} & 0 & 0 \end{bmatrix}$
183	symmetry	$\frac{3\sqrt{35}xyz(x-y)(x+y)}{2}$ $\mathbb{T}_5^{(a)}(A_u, 1) \begin{bmatrix} 0 & 0 & 0 & \frac{\sqrt{15}i}{10} & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{15}i}{10} & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{10}i}{10} & 0 & 0 & 0 & 0 & 0 \\ \frac{\sqrt{10}i}{10} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$
184	symmetry	$\frac{\sqrt{105}xyz(x^2+y^2-2z^2)}{2}$ $\mathbb{T}_5^{(a)}(A_u, 2) \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{3}i}{6} \\ 0 & \frac{\sqrt{30}i}{60} & 0 & 0 & 0 & -\frac{\sqrt{2}i}{4} & 0 \\ -\frac{\sqrt{30}i}{60} & 0 & 0 & 0 & -\frac{\sqrt{2}i}{4} & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{15}i}{10} & 0 & 0 & 0 \end{bmatrix}$
185	symmetry	$\frac{z(15x^4+30x^2y^2-40x^2z^2+15y^4-40y^2z^2+8z^4)}{8}$ $\mathbb{T}_5^{(a)}(B_{1u}, 1) \begin{bmatrix} 0 & 0 & \frac{\sqrt{21}i}{42} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{21}i}{42} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{210}i}{42} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{210}i}{42} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{105}i}{21} \end{bmatrix}$
186	symmetry	$\frac{3\sqrt{35}z(x^2-2xy-y^2)(x^2+2xy-y^2)}{8}$

continued ...

Table 9

No.	multipole	matrix
	$\mathbb{T}_5^{(a)}(B_{1u}, 2)$	$\begin{bmatrix} 0 & 0 & \frac{\sqrt{15}i}{10} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{15}i}{10} & 0 & 0 & 0 \\ \frac{\sqrt{10}i}{10} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{10}i}{10} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$
187	symmetry	$-\frac{\sqrt{105}z(x-y)(x+y)(x^2+y^2-2z^2)}{4}$
	$\mathbb{T}_5^{(a)}(B_{1u}, 3)$	$\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{3}i}{6} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -\frac{\sqrt{30}i}{60} & 0 & 0 & 0 & \frac{\sqrt{2}i}{4} & 0 & 0 \\ 0 & -\frac{\sqrt{30}i}{60} & 0 & 0 & 0 & -\frac{\sqrt{2}i}{4} & 0 \\ 0 & 0 & \frac{\sqrt{15}i}{10} & 0 & 0 & 0 & 0 \end{bmatrix}$
188	symmetry	$\frac{y(15x^4-40x^2y^2+30x^2z^2+8y^4-40y^2z^2+15z^4)}{8}$
	$\mathbb{T}_5^{(a)}(B_{2u}, 1)$	$\begin{bmatrix} 0 & \frac{11\sqrt{14}i}{112} & 0 & 0 & 0 & \frac{5\sqrt{210}i}{336} & 0 \\ \frac{5\sqrt{14}i}{56} & 0 & 0 & 0 & \frac{\sqrt{210}i}{168} & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{21}i}{42} & 0 & 0 & 0 \\ 0 & 0 & \frac{5\sqrt{21}i}{84} & 0 & 0 & 0 & \frac{\sqrt{35}i}{28} \\ 0 & \frac{\sqrt{42}i}{48} & 0 & 0 & 0 & \frac{3\sqrt{70}i}{112} & 0 \end{bmatrix}$
189	symmetry	$\frac{3\sqrt{35}y(x^2-2xz-z^2)(x^2+2xz-z^2)}{8}$
	$\mathbb{T}_5^{(a)}(B_{2u}, 2)$	$\begin{bmatrix} 0 & \frac{3\sqrt{10}i}{80} & 0 & 0 & 0 & -\frac{\sqrt{6}i}{16} & 0 \\ \frac{\sqrt{10}i}{40} & 0 & 0 & 0 & -\frac{\sqrt{6}i}{8} & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{15}i}{10} & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{15}i}{20} & 0 & 0 & 0 & \frac{i}{4} \\ 0 & -\frac{3\sqrt{30}i}{80} & 0 & 0 & 0 & \frac{3\sqrt{2}i}{16} & 0 \end{bmatrix}$
190	symmetry	$\frac{\sqrt{105}y(x-z)(x+z)(x^2-2y^2+z^2)}{4}$

continued ...

Table 9

No.	multipole	matrix
	$\mathbb{T}_5^{(a)}(B_{2u}, 3)$	$\begin{bmatrix} 0 & \frac{7\sqrt{30}i}{120} & 0 & 0 & 0 & -\frac{\sqrt{2}i}{8} & 0 \\ \frac{\sqrt{30}i}{15} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{5}i}{10} & 0 & 0 & 0 & -\frac{\sqrt{3}i}{6} \\ 0 & -\frac{\sqrt{10}i}{40} & 0 & 0 & 0 & -\frac{\sqrt{6}i}{8} & 0 \end{bmatrix}$
191	symmetry	$\frac{x(8x^4 - 40x^2y^2 - 40x^2z^2 + 15y^4 + 30y^2z^2 + 15z^4)}{8}$
	$\mathbb{T}_5^{(a)}(B_{3u}, 1)$	$\begin{bmatrix} \frac{11\sqrt{14}i}{112} & 0 & 0 & 0 & -\frac{5\sqrt{210}i}{336} & 0 & 0 \\ 0 & -\frac{5\sqrt{14}i}{56} & 0 & 0 & 0 & \frac{\sqrt{210}i}{168} & 0 \\ 0 & 0 & -\frac{5\sqrt{21}i}{84} & 0 & 0 & 0 & \frac{\sqrt{35}i}{28} \\ 0 & 0 & 0 & \frac{\sqrt{21}i}{42} & 0 & 0 & 0 \\ -\frac{\sqrt{42}i}{48} & 0 & 0 & 0 & \frac{3\sqrt{70}i}{112} & 0 & 0 \end{bmatrix}$
192	symmetry	$\frac{3\sqrt{35}x(y^2 - 2yz - z^2)(y^2 + 2yz - z^2)}{8}$
	$\mathbb{T}_5^{(a)}(B_{3u}, 2)$	$\begin{bmatrix} \frac{3\sqrt{10}i}{80} & 0 & 0 & 0 & \frac{\sqrt{6}i}{16} & 0 & 0 \\ 0 & -\frac{\sqrt{10}i}{40} & 0 & 0 & 0 & -\frac{\sqrt{6}i}{8} & 0 \\ 0 & 0 & \frac{\sqrt{15}i}{20} & 0 & 0 & 0 & \frac{i}{4} \\ 0 & 0 & 0 & -\frac{\sqrt{15}i}{10} & 0 & 0 & 0 \\ \frac{3\sqrt{30}i}{80} & 0 & 0 & 0 & \frac{3\sqrt{2}i}{16} & 0 & 0 \end{bmatrix}$
193	symmetry	$\frac{\sqrt{105}x(y-z)(y+z)(2x^2 - y^2 - z^2)}{4}$
	$\mathbb{T}_5^{(a)}(B_{3u}, 3)$	$\begin{bmatrix} -\frac{7\sqrt{30}i}{120} & 0 & 0 & 0 & -\frac{\sqrt{2}i}{8} & 0 & 0 \\ 0 & \frac{\sqrt{30}i}{15} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{5}i}{10} & 0 & 0 & 0 & \frac{\sqrt{3}i}{6} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -\frac{\sqrt{10}i}{40} & 0 & 0 & 0 & \frac{\sqrt{6}i}{8} & 0 & 0 \end{bmatrix}$
194	symmetry	$-\frac{x^2}{2} - \frac{y^2}{2} + z^2$

continued ...

Table 9

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

continued ...

Table 9

No.	multipole	matrix
	$\mathbb{M}_2^{(a)}(B_{3u})$	$\begin{bmatrix} \frac{\sqrt{70}i}{28} & 0 & 0 & 0 & \frac{\sqrt{42}i}{28} & 0 & 0 \\ 0 & \frac{\sqrt{70}i}{28} & 0 & 0 & 0 & \frac{\sqrt{42}i}{28} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{7}i}{7} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{14}i}{14} & 0 & 0 \end{bmatrix}$
199	symmetry	$\frac{\sqrt{21}(x^4 - 3x^2y^2 - 3x^2z^2 + y^4 - 3y^2z^2 + z^4)}{6}$
	$\mathbb{M}_4^{(a)}(A_u, 1)$	$\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 \\ 0 & \frac{i}{4} & 0 & 0 & 0 & -\frac{\sqrt{15}i}{12} & 0 \\ \frac{i}{4} & 0 & 0 & 0 & \frac{\sqrt{15}i}{12} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$
200	symmetry	$-\frac{\sqrt{15}(x^4 - 12x^2y^2 + 6x^2z^2 + y^4 + 6y^2z^2 - 2z^4)}{12}$
	$\mathbb{M}_4^{(a)}(A_u, 2)$	$\begin{bmatrix} 0 & 0 & 0 & \frac{\sqrt{210}i}{35} & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{210}i}{210} & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{35}i}{20} & 0 & 0 & 0 & -\frac{5\sqrt{21}i}{84} & 0 \\ -\frac{\sqrt{35}i}{20} & 0 & 0 & 0 & \frac{5\sqrt{21}i}{84} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$
201	symmetry	$\frac{\sqrt{5}(x-y)(x+y)(x^2+y^2-6z^2)}{4}$
	$\mathbb{M}_4^{(a)}(A_u, 3)$	$\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{42}i}{14} \\ 0 & \frac{3\sqrt{105}i}{140} & 0 & 0 & 0 & \frac{\sqrt{7}i}{28} & 0 \\ -\frac{3\sqrt{105}i}{140} & 0 & 0 & 0 & \frac{\sqrt{7}i}{28} & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{210}i}{35} & 0 & 0 & 0 \end{bmatrix}$
202	symmetry	$\frac{\sqrt{35}xy(x-y)(x+y)}{2}$

continued ...

Table 9

No.	multipole	matrix
	$\mathbb{M}_4^{(a)}(B_{1u}, 1)$	$\begin{bmatrix} 0 & 0 & \frac{\sqrt{10}i}{10} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{10}i}{10} & 0 & 0 & 0 \\ -\frac{\sqrt{15}i}{10} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{15}i}{10} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$
203	symmetry	$-\frac{\sqrt{5}xy(x^2+y^2-6z^2)}{2}$
	$\mathbb{M}_4^{(a)}(B_{1u}, 2)$	$\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{42}i}{14} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{3\sqrt{105}i}{140} & 0 & 0 & 0 & \frac{\sqrt{7}i}{28} & 0 & 0 \\ 0 & \frac{3\sqrt{105}i}{140} & 0 & 0 & 0 & -\frac{\sqrt{7}i}{28} & 0 \\ 0 & 0 & -\frac{\sqrt{210}i}{35} & 0 & 0 & 0 & 0 \end{bmatrix}$
204	symmetry	$-\frac{\sqrt{35}xz(x-z)(x+z)}{2}$
	$\mathbb{M}_4^{(a)}(B_{2u}, 1)$	$\begin{bmatrix} 0 & \frac{\sqrt{15}i}{40} & 0 & 0 & 0 & -\frac{i}{8} & 0 \\ -\frac{\sqrt{15}i}{40} & 0 & 0 & 0 & \frac{3i}{8} & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{10}i}{10} & 0 & 0 & 0 \\ 0 & 0 & \frac{3\sqrt{10}i}{40} & 0 & 0 & 0 & -\frac{\sqrt{6}i}{8} \\ 0 & -\frac{3\sqrt{5}i}{40} & 0 & 0 & 0 & \frac{\sqrt{3}i}{8} & 0 \end{bmatrix}$
205	symmetry	$-\frac{\sqrt{5}xz(x^2-6y^2+z^2)}{2}$
	$\mathbb{M}_4^{(a)}(B_{2u}, 2)$	$\begin{bmatrix} 0 & -\frac{\sqrt{105}i}{280} & 0 & 0 & 0 & \frac{9\sqrt{7}i}{56} & 0 \\ \frac{\sqrt{105}i}{280} & 0 & 0 & 0 & \frac{5\sqrt{7}i}{56} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{70}i}{40} & 0 & 0 & 0 & \frac{\sqrt{42}i}{56} \\ 0 & -\frac{3\sqrt{35}i}{40} & 0 & 0 & 0 & -\frac{\sqrt{21}i}{56} & 0 \end{bmatrix}$
206	symmetry	$\frac{\sqrt{35}yz(y-z)(y+z)}{2}$

continued ...

Table 9

No.	multipole	matrix							
		$\begin{bmatrix} \frac{\sqrt{15}i}{40} & 0 & 0 & 0 & \frac{i}{8} & 0 & 0 \\ 0 & \frac{\sqrt{15}i}{40} & 0 & 0 & 0 & \frac{3i}{8} & 0 \\ 0 & 0 & -\frac{3\sqrt{10}i}{40} & 0 & 0 & 0 & -\frac{\sqrt{6}i}{8} \\ 0 & 0 & 0 & -\frac{\sqrt{10}i}{10} & 0 & 0 & 0 \\ \frac{3\sqrt{5}i}{40} & 0 & 0 & 0 & \frac{\sqrt{3}i}{8} & 0 & 0 \end{bmatrix}$							
207	symmetry	$\frac{\sqrt{5}yz(6x^2-y^2-z^2)}{2}$							
		$\begin{bmatrix} \frac{\sqrt{105}i}{280} & 0 & 0 & 0 & \frac{9\sqrt{7}i}{56} & 0 & 0 \\ 0 & \frac{\sqrt{105}i}{280} & 0 & 0 & 0 & -\frac{5\sqrt{7}i}{56} & 0 \\ 0 & 0 & -\frac{\sqrt{70}i}{40} & 0 & 0 & 0 & -\frac{\sqrt{42}i}{56} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -\frac{3\sqrt{35}i}{40} & 0 & 0 & 0 & \frac{\sqrt{21}i}{56} & 0 & 0 \end{bmatrix}$							

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	$\begin{bmatrix} 1 \\ \frac{\sqrt{7}}{7} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{7}}{7} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{7}}{7} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{7}}{7} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{7}}{7} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{7}}{7} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{7}}{7} \end{bmatrix}$							
209	symmetry	$-\frac{x^2}{2} - \frac{y^2}{2} + z^2$							

continued ...

Table 10

No.	multipole	matrix
	$\mathbb{Q}_2^{(a)}(A_g, 1)$	$ \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{array}{c} \frac{\sqrt{3}(x-y)(x+y)}{2} \\ \mathbb{Q}_2^{(a)}(A_g, 2) \end{array} \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} $
211	symmetry	$ \begin{array}{c} \sqrt{3}xy \\ \mathbb{Q}_2^{(a)}(B_{1g}) \end{array} \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} $
212	symmetry	$\sqrt{3}xz$

continued ...

Table 10

No.	multipole	matrix							
	$\mathbb{Q}_2^{(a)}(B_{2g})$	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	
213	symmetry	$\sqrt{3}yz$							
	$\mathbb{Q}_2^{(a)}(B_{3g})$	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	
214	symmetry	$\frac{\sqrt{21}(x^4-3x^2y^2-3x^2z^2+y^4-3y^2z^2+z^4)}{6}$							
	$\mathbb{Q}_4^{(a)}(A_g, 1)$	$\frac{\sqrt{66}}{44}$	0	0	0	$-\frac{\sqrt{110}}{44}$	0	0	
		0	$\frac{\sqrt{66}}{44}$	0	0	0	$\frac{\sqrt{110}}{44}$	0	
		0	0	$-\frac{\sqrt{66}}{66}$	0	0	0	0	
		0	0	0	$-\frac{\sqrt{66}}{11}$	0	0	0	
		$-\frac{\sqrt{110}}{44}$	0	0	0	$\frac{\sqrt{66}}{132}$	0	0	
		0	$\frac{\sqrt{110}}{44}$	0	0	0	$\frac{\sqrt{66}}{132}$	0	
		0	0	0	0	0	0	$\frac{\sqrt{66}}{22}$	
215	symmetry	$-\frac{\sqrt{15}(x^4-12x^2y^2+6x^2z^2+y^4+6y^2z^2-2z^4)}{12}$							

continued ...

Table 10

No.	multipole	matrix						
	$\mathbb{Q}_4^{(a)}(A_g, 2)$	$\begin{bmatrix} \frac{\sqrt{2310}}{308} & 0 & 0 & 0 & \frac{\sqrt{154}}{44} & 0 & 0 \\ 0 & \frac{\sqrt{2310}}{308} & 0 & 0 & 0 & -\frac{\sqrt{154}}{44} & 0 \\ 0 & 0 & -\frac{\sqrt{2310}}{66} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{\sqrt{154}}{44} & 0 & 0 & 0 & \frac{\sqrt{2310}}{924} & 0 & 0 \\ 0 & -\frac{\sqrt{154}}{44} & 0 & 0 & 0 & \frac{\sqrt{2310}}{924} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{2310}}{154} \end{bmatrix}$						
216	symmetry	$\frac{\sqrt{5}(x-y)(x+y)(x^2+y^2-6z^2)}{4}$						
	$\mathbb{Q}_4^{(a)}(A_g, 3)$	$\begin{bmatrix} 0 & 0 & 0 & 0 & -\frac{3\sqrt{462}}{154} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{3\sqrt{462}}{154} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{462}}{154} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -\frac{3\sqrt{462}}{154} & 0 & 0 & 0 & -\frac{\sqrt{770}}{77} & 0 & 0 \\ 0 & -\frac{3\sqrt{462}}{154} & 0 & 0 & 0 & \frac{\sqrt{770}}{77} & 0 \\ 0 & 0 & \frac{\sqrt{462}}{154} & 0 & 0 & 0 & 0 \end{bmatrix}$						
217	symmetry	$\frac{\sqrt{35}xy(x-y)(x+y)}{2}$						
	$\mathbb{Q}_4^{(a)}(B_{1g}, 1)$	$\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{66}}{22} & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{66}}{22} & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{110}}{22} & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{110}}{22} & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{66}}{22} & 0 & 0 & 0 & 0 & 0 \\ -\frac{\sqrt{66}}{22} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$						
218	symmetry	$-\frac{\sqrt{5}xy(x^2+y^2-6z^2)}{2}$						

continued ...

Table 10

No.	multipole	matrix						
	$\mathbb{Q}_4^{(a)}(B_{1g}, 2)$	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
219	symmetry	$-\frac{\sqrt{35}xz(x-z)(x+z)}{2}$						
	$\mathbb{Q}_4^{(a)}(B_{2g}, 1)$	0	0	$-\frac{\sqrt{165}}{44}$	0	0	0	$\frac{3\sqrt{11}}{44}$
		0	0	0	$-\frac{\sqrt{165}}{44}$	0	0	0
		$-\frac{\sqrt{165}}{44}$	0	0	0	$\frac{3\sqrt{11}}{44}$	0	0
		0	$-\frac{\sqrt{165}}{44}$	0	0	0	$\frac{5\sqrt{11}}{44}$	0
		0	0	$\frac{3\sqrt{11}}{44}$	0	0	0	$\frac{\sqrt{165}}{44}$
		0	0	0	$\frac{5\sqrt{11}}{44}$	0	0	0
		$\frac{3\sqrt{11}}{44}$	0	0	0	$\frac{\sqrt{165}}{44}$	0	0
220	symmetry	$-\frac{\sqrt{5}xz(x^2-6y^2+z^2)}{2}$						
	$\mathbb{Q}_4^{(a)}(B_{2g}, 2)$	0	0	$\frac{\sqrt{1155}}{308}$	0	0	0	$\frac{3\sqrt{77}}{44}$
		0	0	0	$\frac{\sqrt{1155}}{308}$	0	0	0
		$\frac{\sqrt{1155}}{308}$	0	0	0	$-\frac{\sqrt{77}}{28}$	0	0
		0	$\frac{\sqrt{1155}}{308}$	0	0	0	$\frac{3\sqrt{77}}{308}$	0
		0	0	$-\frac{\sqrt{77}}{28}$	0	0	0	$-\frac{\sqrt{1155}}{308}$
		0	0	0	$\frac{3\sqrt{77}}{308}$	0	0	0
		$\frac{3\sqrt{77}}{44}$	0	0	0	$-\frac{\sqrt{1155}}{308}$	0	0
221	symmetry	$\frac{\sqrt{35}yz(y-z)(y+z)}{2}$						

continued ...

Table 10

No.	multipole	matrix
	$\mathbb{Q}_4^{(a)}(B_{3g}, 1)$	$\begin{bmatrix} 0 & 0 & 0 & -\frac{\sqrt{165}}{44} & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{165}}{44} & 0 & 0 & 0 & \frac{3\sqrt{11}}{44} \\ 0 & \frac{\sqrt{165}}{44} & 0 & 0 & 0 & \frac{3\sqrt{11}}{44} & 0 \\ -\frac{\sqrt{165}}{44} & 0 & 0 & 0 & -\frac{5\sqrt{11}}{44} & 0 & 0 \\ 0 & 0 & 0 & -\frac{5\sqrt{11}}{44} & 0 & 0 & 0 \\ 0 & 0 & \frac{3\sqrt{11}}{44} & 0 & 0 & 0 & -\frac{\sqrt{165}}{44} \\ 0 & \frac{3\sqrt{11}}{44} & 0 & 0 & 0 & -\frac{\sqrt{165}}{44} & 0 \end{bmatrix}$
222	symmetry	$\frac{\sqrt{5}yz(6x^2-y^2-z^2)}{2}$
	$\mathbb{Q}_4^{(a)}(B_{3g}, 2)$	$\begin{bmatrix} 0 & 0 & 0 & -\frac{\sqrt{1155}}{308} & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{1155}}{308} & 0 & 0 & 0 & -\frac{3\sqrt{77}}{44} \\ 0 & \frac{\sqrt{1155}}{308} & 0 & 0 & 0 & \frac{\sqrt{77}}{28} & 0 \\ -\frac{\sqrt{1155}}{308} & 0 & 0 & 0 & \frac{3\sqrt{77}}{308} & 0 & 0 \\ 0 & 0 & 0 & \frac{3\sqrt{77}}{308} & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{77}}{28} & 0 & 0 & 0 & -\frac{\sqrt{1155}}{308} \\ 0 & -\frac{3\sqrt{77}}{44} & 0 & 0 & 0 & -\frac{\sqrt{1155}}{308} & 0 \end{bmatrix}$
223	symmetry	$\frac{\sqrt{2}(2x^6-15x^4y^2-15x^4z^2-15x^2y^4+180x^2y^2z^2-15x^2z^4+2y^6-15y^4z^2-15y^2z^4+2z^6)}{8}$
	$\mathbb{Q}_6^{(a)}(A_g, 1)$	$\begin{bmatrix} -\frac{\sqrt{462}}{1848} & 0 & 0 & 0 & -\frac{\sqrt{770}}{88} & 0 & 0 \\ 0 & -\frac{\sqrt{462}}{1848} & 0 & 0 & 0 & \frac{\sqrt{770}}{88} & 0 \\ 0 & 0 & -\frac{3\sqrt{462}}{154} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{2\sqrt{462}}{77} & 0 & 0 & 0 \\ -\frac{\sqrt{770}}{88} & 0 & 0 & 0 & -\frac{5\sqrt{462}}{616} & 0 & 0 \\ 0 & \frac{\sqrt{770}}{88} & 0 & 0 & 0 & -\frac{5\sqrt{462}}{616} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{5\sqrt{462}}{462} \end{bmatrix}$
224	symmetry	$-\frac{\sqrt{2310}(x-y)(x+y)(x-z)(x+z)(y-z)(y+z)}{8}$

continued ...

Table 10

No.	multipole	matrix
	$\mathbb{Q}_6^{(a)}(A_g, 2)$	$\begin{bmatrix} \frac{\sqrt{10}}{8} & 0 & 0 & 0 & \frac{\sqrt{6}}{24} & 0 & 0 \\ 0 & -\frac{\sqrt{10}}{8} & 0 & 0 & 0 & \frac{\sqrt{6}}{24} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{6}}{6} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{\sqrt{6}}{24} & 0 & 0 & 0 & -\frac{\sqrt{10}}{8} & 0 & 0 \\ 0 & \frac{\sqrt{6}}{24} & 0 & 0 & 0 & \frac{\sqrt{10}}{8} & 0 \\ 0 & 0 & -\frac{\sqrt{6}}{6} & 0 & 0 & 0 & 0 \end{bmatrix}$
225	symmetry	$-\frac{\sqrt{14}(x^6-15x^4z^2+15x^2z^4+y^6-15y^4z^2+15y^2z^4-2z^6)}{8}$
	$\mathbb{Q}_6^{(a)}(A_g, 3)$	$\begin{bmatrix} -\frac{\sqrt{66}}{264} & 0 & 0 & 0 & \frac{\sqrt{110}}{88} & 0 & 0 \\ 0 & -\frac{\sqrt{66}}{264} & 0 & 0 & 0 & -\frac{\sqrt{110}}{88} & 0 \\ 0 & 0 & \frac{\sqrt{66}}{22} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{\sqrt{110}}{88} & 0 & 0 & 0 & -\frac{5\sqrt{66}}{88} & 0 & 0 \\ 0 & -\frac{\sqrt{110}}{88} & 0 & 0 & 0 & -\frac{5\sqrt{66}}{88} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{5\sqrt{66}}{66} \end{bmatrix}$
226	symmetry	$\frac{\sqrt{42}(x-y)(x+y)(x^4-9x^2y^2-5x^2z^2+y^4-5y^2z^2+5z^4)}{8}$
	$\mathbb{Q}_6^{(a)}(A_g, 4)$	$\begin{bmatrix} \frac{\sqrt{22}}{8} & 0 & 0 & 0 & -\frac{\sqrt{330}}{264} & 0 & 0 \\ 0 & -\frac{\sqrt{22}}{8} & 0 & 0 & 0 & -\frac{\sqrt{330}}{264} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{330}}{66} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -\frac{\sqrt{330}}{264} & 0 & 0 & 0 & \frac{5\sqrt{22}}{88} & 0 & 0 \\ 0 & -\frac{\sqrt{330}}{264} & 0 & 0 & 0 & -\frac{5\sqrt{22}}{88} & 0 \\ 0 & 0 & \frac{\sqrt{330}}{66} & 0 & 0 & 0 & 0 \end{bmatrix}$
227	symmetry	$-\frac{3\sqrt{7}xy(x-y)(x+y)(x^2+y^2-10z^2)}{4}$

continued ...

Table 10

No.	multipole	matrix
	$\mathbb{Q}_6^{(a)}(B_{1g}, 1)$	$\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{55}}{22} & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{55}}{22} & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{33}}{11} & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{33}}{11} & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{55}}{22} & 0 & 0 & 0 & 0 & 0 \\ \frac{\sqrt{55}}{22} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$
228	symmetry	$\frac{\sqrt{462}xy(x^2-3y^2)(3x^2-y^2)}{16}$ $\begin{bmatrix} 0 & \frac{\sqrt{2}}{2} & 0 & 0 & 0 & 0 & 0 \\ \frac{\sqrt{2}}{2} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$
	$\mathbb{Q}_6^{(a)}(B_{1g}, 2)$	
229	symmetry	$\frac{\sqrt{210}xy(x^4+2x^2y^2-16x^2z^2+y^4-16y^2z^2+16z^4)}{16}$ $\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{66}}{66} & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{66}}{66} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{2\sqrt{66}}{33} \\ 0 & -\frac{\sqrt{66}}{66} & 0 & 0 & 0 & \frac{\sqrt{110}}{22} & 0 \\ \frac{\sqrt{66}}{66} & 0 & 0 & 0 & \frac{\sqrt{110}}{22} & 0 & 0 \\ 0 & 0 & 0 & \frac{2\sqrt{66}}{33} & 0 & 0 & 0 \end{bmatrix}$
	$\mathbb{Q}_6^{(a)}(B_{1g}, 3)$	
230	symmetry	$\frac{3\sqrt{7}xz(x-z)(x+z)(x^2-10y^2+z^2)}{4}$

continued ...

Table 10

No.	multipole	matrix						
	$\mathbb{Q}_6^{(a)}(B_{2g}, 1)$	0	0	$\frac{5\sqrt{22}}{88}$	0	0	0	$-\frac{\sqrt{330}}{88}$
		0	0	0	$-\frac{3\sqrt{22}}{44}$	0	0	0
		$\frac{5\sqrt{22}}{88}$	0	0	0	$-\frac{\sqrt{330}}{88}$	0	0
		0	$-\frac{3\sqrt{22}}{44}$	0	0	0	$\frac{\sqrt{330}}{44}$	0
		0	0	$-\frac{\sqrt{330}}{88}$	0	0	0	$-\frac{5\sqrt{22}}{88}$
		0	0	0	$\frac{\sqrt{330}}{44}$	0	0	0
		$-\frac{\sqrt{330}}{88}$	0	0	0	$-\frac{5\sqrt{22}}{88}$	0	0
231	symmetry	$\frac{\sqrt{462}xz(x^2-3z^2)(3x^2-z^2)}{16}$						
	$\mathbb{Q}_6^{(a)}(B_{2g}, 2)$	0	0	$\frac{\sqrt{3}}{16}$	0	0	0	$-\frac{\sqrt{5}}{16}$
		0	0	0	0	0	0	0
		$\frac{\sqrt{3}}{16}$	0	0	0	$-\frac{3\sqrt{5}}{16}$	0	0
		0	0	0	0	0	0	0
		0	0	$-\frac{3\sqrt{5}}{16}$	0	0	0	$\frac{5\sqrt{3}}{16}$
		0	0	0	0	0	0	0
		$-\frac{\sqrt{5}}{16}$	0	0	0	$\frac{5\sqrt{3}}{16}$	0	0
232	symmetry	$\frac{\sqrt{210}xz(x^4-16x^2y^2+2x^2z^2+16y^4-16y^2z^2+z^4)}{16}$						
	$\mathbb{Q}_6^{(a)}(B_{2g}, 3)$	0	0	$\frac{17\sqrt{165}}{528}$	0	0	0	$\frac{9\sqrt{11}}{176}$
		0	0	0	$-\frac{\sqrt{165}}{33}$	0	0	0
		$\frac{17\sqrt{165}}{528}$	0	0	0	$\frac{\sqrt{11}}{16}$	0	0
		0	$-\frac{\sqrt{165}}{33}$	0	0	0	$-\frac{\sqrt{11}}{11}$	0
		0	0	$\frac{\sqrt{11}}{16}$	0	0	0	$\frac{5\sqrt{165}}{528}$
		0	0	0	$-\frac{\sqrt{11}}{11}$	0	0	0
		$\frac{9\sqrt{11}}{176}$	0	0	0	$\frac{5\sqrt{165}}{528}$	0	0
233	symmetry	$\frac{3\sqrt{7}yz(y-z)(y+z)(10x^2-y^2-z^2)}{4}$						

continued ...

Table 10

No.	multipole	matrix						
	$\mathbb{Q}_6^{(a)}(B_{3g}, 1)$	0	0	0	$-\frac{3\sqrt{22}}{44}$	0	0	0
		0	0	$-\frac{5\sqrt{22}}{88}$	0	0	0	$-\frac{\sqrt{330}}{88}$
		0	$-\frac{5\sqrt{22}}{88}$	0	0	0	$-\frac{\sqrt{330}}{88}$	0
		$-\frac{3\sqrt{22}}{44}$	0	0	0	$-\frac{\sqrt{330}}{44}$	0	0
		0	0	0	$-\frac{\sqrt{330}}{44}$	0	0	0
		0	0	$-\frac{\sqrt{330}}{88}$	0	0	0	$\frac{5\sqrt{22}}{88}$
		0	$-\frac{\sqrt{330}}{88}$	0	0	0	$\frac{5\sqrt{22}}{88}$	0
234	symmetry	$\frac{\sqrt{462}yz(y^2-3z^2)(3y^2-z^2)}{16}$						
	$\mathbb{Q}_6^{(a)}(B_{3g}, 2)$	0	0	0	0	0	0	0
		0	0	$\frac{\sqrt{3}}{16}$	0	0	0	$\frac{\sqrt{5}}{16}$
		0	$\frac{\sqrt{3}}{16}$	0	0	0	$\frac{3\sqrt{5}}{16}$	0
		0	0	0	0	0	0	0
		0	0	0	0	0	0	0
		0	0	$\frac{3\sqrt{5}}{16}$	0	0	0	$\frac{5\sqrt{3}}{16}$
		0	$\frac{\sqrt{5}}{16}$	0	0	0	$\frac{5\sqrt{3}}{16}$	0
235	symmetry	$\frac{\sqrt{210}yz(16x^4-16x^2y^2-16x^2z^2+y^4+2y^2z^2+z^4)}{16}$						
	$\mathbb{Q}_6^{(a)}(B_{3g}, 3)$	0	0	0	$\frac{\sqrt{165}}{33}$	0	0	0
		0	0	$\frac{17\sqrt{165}}{528}$	0	0	0	$-\frac{9\sqrt{11}}{176}$
		0	$\frac{17\sqrt{165}}{528}$	0	0	0	$-\frac{\sqrt{11}}{16}$	0
		$\frac{\sqrt{165}}{33}$	0	0	0	$-\frac{\sqrt{11}}{11}$	0	0
		0	0	0	$-\frac{\sqrt{11}}{11}$	0	0	0
		0	0	$-\frac{\sqrt{11}}{16}$	0	0	0	$\frac{5\sqrt{165}}{528}$
		0	$-\frac{9\sqrt{11}}{176}$	0	0	0	$\frac{5\sqrt{165}}{528}$	0
236	symmetry	z						

continued ...

Table 10

No.	multipole	matrix
	$\mathbb{M}_1^{(a)}(B_{1g})$	$\begin{bmatrix} 0 & -\frac{3\sqrt{7}i}{14} & 0 & 0 & 0 & 0 & 0 \\ \frac{3\sqrt{7}i}{14} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{7}i}{7} & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{7}i}{7} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{7}i}{14} & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{7}i}{14} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$
237	symmetry	y $\mathbb{M}_1^{(a)}(B_{2g})$ $\begin{bmatrix} 0 & 0 & \frac{\sqrt{42}i}{28} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{42}i}{28} & 0 & 0 & 0 \\ -\frac{\sqrt{42}i}{28} & 0 & 0 & 0 & \frac{\sqrt{70}i}{28} & 0 & 0 \\ 0 & -\frac{\sqrt{42}i}{28} & 0 & 0 & 0 & \frac{\sqrt{70}i}{28} & 0 \\ 0 & 0 & -\frac{\sqrt{70}i}{28} & 0 & 0 & 0 & \frac{\sqrt{42}i}{14} \\ 0 & 0 & 0 & -\frac{\sqrt{70}i}{28} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{42}i}{14} & 0 & 0 \end{bmatrix}$
238	symmetry	x $\mathbb{M}_1^{(a)}(B_{3g})$ $\begin{bmatrix} 0 & 0 & 0 & \frac{\sqrt{42}i}{28} & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{42}i}{28} & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{42}i}{28} & 0 & 0 & 0 & \frac{\sqrt{70}i}{28} & 0 \\ -\frac{\sqrt{42}i}{28} & 0 & 0 & 0 & -\frac{\sqrt{70}i}{28} & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{70}i}{28} & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{70}i}{28} & 0 & 0 & 0 & -\frac{\sqrt{42}i}{14} \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{42}i}{14} & 0 \end{bmatrix}$
239	symmetry	$\sqrt{15}xyz$

continued ...

Table 10

No.	multipole	matrix
	$\mathbb{M}_3^{(a)}(A_g)$	$ \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} $
240	symmetry	$ -\frac{z(3x^2+3y^2-2z^2)}{2} $ $ \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} $
241	symmetry	$ \frac{\sqrt{15}z(x-y)(x+y)}{2} $ $ \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{6}i}{6} & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{6}i}{6} \\ 0 & \frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 & 0 \\ -\frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{6}i}{6} & 0 & 0 & 0 \end{bmatrix} $
242	symmetry	$ -\frac{y(3x^2-2y^2+3z^2)}{2} $

continued ...

Table 10

No.	multipole	matrix						
		$\begin{bmatrix} 0 & 0 & \frac{i}{4} & 0 & 0 & 0 & \frac{\sqrt{15}i}{12} \\ 0 & 0 & 0 & \frac{i}{4} & 0 & 0 & 0 \\ -\frac{i}{4} & 0 & 0 & 0 & -\frac{\sqrt{15}i}{12} & 0 & 0 \\ 0 & -\frac{i}{4} & 0 & 0 & 0 & \frac{\sqrt{15}i}{12} & 0 \\ 0 & 0 & \frac{\sqrt{15}i}{12} & 0 & 0 & 0 & -\frac{i}{4} \\ 0 & 0 & 0 & -\frac{\sqrt{15}i}{12} & 0 & 0 & 0 \\ -\frac{\sqrt{15}i}{12} & 0 & 0 & 0 & \frac{i}{4} & 0 & 0 \end{bmatrix}$						
243	symmetry	$-\frac{\sqrt{15}y(x-z)(x+z)}{2}$ $\begin{bmatrix} 0 & 0 & -\frac{\sqrt{15}i}{12} & 0 & 0 & 0 & \frac{i}{4} \\ 0 & 0 & 0 & -\frac{\sqrt{15}i}{12} & 0 & 0 & 0 \\ \frac{\sqrt{15}i}{12} & 0 & 0 & 0 & -\frac{i}{4} & 0 & 0 \\ 0 & \frac{\sqrt{15}i}{12} & 0 & 0 & 0 & \frac{i}{4} & 0 \\ 0 & 0 & \frac{i}{4} & 0 & 0 & 0 & \frac{\sqrt{15}i}{12} \\ 0 & 0 & 0 & -\frac{i}{4} & 0 & 0 & 0 \\ -\frac{i}{4} & 0 & 0 & 0 & -\frac{\sqrt{15}i}{12} & 0 & 0 \end{bmatrix}$						
244	symmetry	$\frac{x(2x^2-3y^2-3z^2)}{2}$ $\begin{bmatrix} 0 & 0 & 0 & \frac{i}{4} & 0 & 0 & 0 \\ 0 & 0 & -\frac{i}{4} & 0 & 0 & 0 & \frac{\sqrt{15}i}{12} \\ 0 & \frac{i}{4} & 0 & 0 & 0 & -\frac{\sqrt{15}i}{12} & 0 \\ -\frac{i}{4} & 0 & 0 & 0 & -\frac{\sqrt{15}i}{12} & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{15}i}{12} & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{15}i}{12} & 0 & 0 & 0 & \frac{i}{4} \\ 0 & -\frac{\sqrt{15}i}{12} & 0 & 0 & 0 & -\frac{i}{4} & 0 \end{bmatrix}$						
245	symmetry	$\frac{\sqrt{15}x(y-z)(y+z)}{2}$						

continued ...

Table 10

No.	multipole	matrix
	$\mathbb{M}_3^{(a)}(B_{3g}, 2)$	$ \begin{bmatrix} 0 & 0 & 0 & \frac{\sqrt{15}i}{12} & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{15}i}{12} & 0 & 0 & 0 & 0 & -\frac{i}{4} \\ 0 & \frac{\sqrt{15}i}{12} & 0 & 0 & 0 & 0 & \frac{i}{4} & 0 \\ -\frac{\sqrt{15}i}{12} & 0 & 0 & 0 & \frac{i}{4} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{i}{4} & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{i}{4} & 0 & 0 & 0 & 0 & \frac{\sqrt{15}i}{12} \\ 0 & \frac{i}{4} & 0 & 0 & 0 & -\frac{\sqrt{15}i}{12} & 0 & 0 \end{bmatrix} $
246	symmetry	$ \frac{3\sqrt{35}xyz(x-y)(x+y)}{2} $ $ \begin{bmatrix} 0 & 0 & 0 & 0 & \frac{i}{2} & 0 & 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 \\ -\frac{i}{2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{i}{2} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} $
247	symmetry	$ \frac{\sqrt{105}xyz(x^2+y^2-2z^2)}{2} $ $ \begin{bmatrix} 0 & 0 & 0 & 0 & \frac{\sqrt{3}i}{6} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{3}i}{6} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{3}i}{3} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -\frac{\sqrt{3}i}{6} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{3}i}{6} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{3}i}{3} & 0 & 0 & 0 & 0 & 0 \end{bmatrix} $
248	symmetry	$ \frac{z(15x^4+30x^2y^2-40x^2z^2+15y^4-40y^2z^2+8z^4)}{8} $

continued ...

Table 10

No.	multipole	matrix
	$\mathbb{M}_5^{(a)}(B_{1g}, 1)$	$\begin{bmatrix} 0 & -\frac{\sqrt{21}i}{42} & 0 & 0 & 0 & 0 & 0 \\ \frac{\sqrt{21}i}{42} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{2\sqrt{21}i}{21} & 0 & 0 & 0 \\ 0 & 0 & -\frac{2\sqrt{21}i}{21} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{5\sqrt{21}i}{42} & 0 \\ 0 & 0 & 0 & 0 & \frac{5\sqrt{21}i}{42} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$
249	symmetry	$\frac{3\sqrt{35}z(x^2-2xy-y^2)(x^2+2xy-y^2)}{8}$ $\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & -\frac{i}{2} & 0 \\ 0 & 0 & 0 & 0 & -\frac{i}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{i}{2} & 0 & 0 & 0 & 0 & 0 \\ \frac{i}{2} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$
250	symmetry	$-\frac{\sqrt{105}z(x-y)(x+y)(x^2+y^2-2z^2)}{4}$ $\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{3}i}{6} & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{3}i}{6} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{3}i}{3} \\ 0 & -\frac{\sqrt{3}i}{6} & 0 & 0 & 0 & 0 & 0 \\ \frac{\sqrt{3}i}{6} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{3}i}{3} & 0 & 0 & 0 \end{bmatrix}$
251	symmetry	$\frac{y(15x^4-40x^2y^2+30x^2z^2+8y^4-40y^2z^2+15z^4)}{8}$

continued ...

Table 10

No.	multipole	matrix						
	$M_5^{(a)}(B_{2g}, 1)$	0	0	$\frac{13\sqrt{14}i}{112}$	0	0	0	$\frac{\sqrt{210}i}{48}$
		0	0	0	$-\frac{\sqrt{14}i}{14}$	0	0	0
		$-\frac{13\sqrt{14}i}{112}$	0	0	0	$-\frac{\sqrt{210}i}{336}$	0	0
		0	$\frac{\sqrt{14}i}{14}$	0	0	0	$-\frac{\sqrt{210}i}{42}$	0
		0	0	$\frac{\sqrt{210}i}{336}$	0	0	0	$\frac{5\sqrt{14}i}{112}$
		0	0	0	$\frac{\sqrt{210}i}{42}$	0	0	0
		$-\frac{\sqrt{210}i}{48}$	0	0	0	$-\frac{5\sqrt{14}i}{112}$	0	0
252	symmetry	$\frac{3\sqrt{35}y(x^2-2xz-z^2)(x^2+2xz-z^2)}{8}$						
	$M_5^{(a)}(B_{2g}, 2)$	0	0	$\frac{\sqrt{10}i}{16}$	0	0	0	$-\frac{3\sqrt{6}i}{16}$
		0	0	0	0	0	0	0
		$-\frac{\sqrt{10}i}{16}$	0	0	0	$-\frac{3\sqrt{6}i}{16}$	0	0
		0	0	0	0	0	0	0
		0	0	$\frac{3\sqrt{6}i}{16}$	0	0	0	$\frac{\sqrt{10}i}{16}$
		0	0	0	0	0	0	0
		$\frac{3\sqrt{6}i}{16}$	0	0	0	$-\frac{\sqrt{10}i}{16}$	0	0
253	symmetry	$\frac{\sqrt{105}y(x-z)(x+z)(x^2-2y^2+z^2)}{4}$						
	$M_5^{(a)}(B_{2g}, 3)$	0	0	$\frac{\sqrt{30}i}{24}$	0	0	0	$-\frac{\sqrt{2}i}{8}$
		0	0	0	$-\frac{\sqrt{30}i}{12}$	0	0	0
		$-\frac{\sqrt{30}i}{24}$	0	0	0	$\frac{\sqrt{2}i}{8}$	0	0
		0	$\frac{\sqrt{30}i}{12}$	0	0	0	$\frac{\sqrt{2}i}{4}$	0
		0	0	$-\frac{\sqrt{2}i}{8}$	0	0	0	$-\frac{\sqrt{30}i}{24}$
		0	0	0	$-\frac{\sqrt{2}i}{4}$	0	0	0
		$\frac{\sqrt{2}i}{8}$	0	0	0	$\frac{\sqrt{30}i}{24}$	0	0
254	symmetry	$\frac{x(8x^4-40x^2y^2-40x^2z^2+15y^4+30y^2z^2+15z^4)}{8}$						

continued ...

Table 10

No.	multipole	matrix						
		0	0	0	$-\frac{\sqrt{14}i}{14}$	0	0	0
		0	0	$-\frac{13\sqrt{14}i}{112}$	0	0	0	$\frac{\sqrt{210}i}{48}$
		0	$\frac{13\sqrt{14}i}{112}$	0	0	0	$-\frac{\sqrt{210}i}{336}$	0
	$M_5^{(a)}(B_{3g}, 1)$	$\frac{\sqrt{14}i}{14}$	0	0	0	$\frac{\sqrt{210}i}{42}$	0	0
		0	0	0	$-\frac{\sqrt{210}i}{42}$	0	0	0
		0	0	$\frac{\sqrt{210}i}{336}$	0	0	0	$-\frac{5\sqrt{14}i}{112}$
		0	$-\frac{\sqrt{210}i}{48}$	0	0	0	$\frac{5\sqrt{14}i}{112}$	0
255	symmetry	$\frac{3\sqrt{35}x(y^2-2yz-z^2)(y^2+2yz-z^2)}{8}$						
		0	0	0	0	0	0	0
		0	0	$-\frac{\sqrt{10}i}{16}$	0	0	0	$-\frac{3\sqrt{6}i}{16}$
		0	$\frac{\sqrt{10}i}{16}$	0	0	0	$-\frac{3\sqrt{6}i}{16}$	0
	$M_5^{(a)}(B_{3g}, 2)$	0	0	0	0	0	0	0
		0	0	0	0	0	0	0
		0	0	$\frac{3\sqrt{6}i}{16}$	0	0	0	$-\frac{\sqrt{10}i}{16}$
		0	$\frac{3\sqrt{6}i}{16}$	0	0	0	$\frac{\sqrt{10}i}{16}$	0
256	symmetry	$\frac{\sqrt{105}x(y-z)(y+z)(2x^2-y^2-z^2)}{4}$						
		0	0	0	$\frac{\sqrt{30}i}{12}$	0	0	0
		0	0	$\frac{\sqrt{30}i}{24}$	0	0	0	$\frac{\sqrt{2}i}{8}$
		0	$-\frac{\sqrt{30}i}{24}$	0	0	0	$-\frac{\sqrt{2}i}{8}$	0
	$M_5^{(a)}(B_{3g}, 3)$	$-\frac{\sqrt{30}i}{12}$	0	0	0	$\frac{\sqrt{2}i}{4}$	0	0
		0	0	0	$-\frac{\sqrt{2}i}{4}$	0	0	0
		0	0	$\frac{\sqrt{2}i}{8}$	0	0	0	$-\frac{\sqrt{30}i}{24}$
		0	$-\frac{\sqrt{2}i}{8}$	0	0	0	$\frac{\sqrt{30}i}{24}$	0