

# Model for “Mn3Sn”

Generated on 2026-02-01 12:28:23 by MultiPie 2.0.8

---

## General Condition

- Basis type: **1g**
- SAMB selection:
  - Type: **[Q, G]**
  - Rank: **[0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11]**
  - Irrep.: **[A<sub>1g</sub>, A<sub>2g</sub>, B<sub>1g</sub>, B<sub>2g</sub>, E<sub>1g</sub>, E<sub>2g</sub>, A<sub>1u</sub>, A<sub>2u</sub>, B<sub>1u</sub>, B<sub>2u</sub>, E<sub>1u</sub>, E<sub>2u</sub>]**
  - Spin (s): **[0, 1]**
- Atomic selection:
  - Type: **[Q, G, M, T]**
  - Rank: **[0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11]**
  - Irrep.: **[A<sub>1g</sub>, A<sub>2g</sub>, B<sub>1g</sub>, B<sub>2g</sub>, E<sub>1g</sub>, E<sub>2g</sub>, A<sub>1u</sub>, A<sub>2u</sub>, B<sub>1u</sub>, B<sub>2u</sub>, E<sub>1u</sub>, E<sub>2u</sub>]**
  - Spin (s): **[0, 1]**
- Site-cluster selection:
  - Rank: **[0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11]**
  - Irrep.: **[A<sub>1g</sub>, A<sub>2g</sub>, B<sub>1g</sub>, B<sub>2g</sub>, E<sub>1g</sub>, E<sub>2g</sub>, A<sub>1u</sub>, A<sub>2u</sub>, B<sub>1u</sub>, B<sub>2u</sub>, E<sub>1u</sub>, E<sub>2u</sub>]**
- Bond-cluster selection:
  - Type: **[Q, G, M, T]**
  - Rank: **[0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11]**
  - Irrep.: **[A<sub>1g</sub>, A<sub>2g</sub>, B<sub>1g</sub>, B<sub>2g</sub>, E<sub>1g</sub>, E<sub>2g</sub>, A<sub>1u</sub>, A<sub>2u</sub>, B<sub>1u</sub>, B<sub>2u</sub>, E<sub>1u</sub>, E<sub>2u</sub>]**
- Max. neighbor: **10**
- Search cell range: **(-2, 3), (-2, 3), (-2, 3)**
- Toroidal priority: **false**

---

## Group and Unit Cell

- Group: SG No. 194  $D_{6h}^4$   $P6_3/mmc$  [ hexagonal ]
- Associated point group: PG No. 194  $D_{6h}$   $6/mmm$  [ hexagonal ]
- Unit cell:
  - $a = 1.00000$ ,  $b = 1.00000$ ,  $c = 1.00000$ ,  $\alpha = 90.0$ ,  $\beta = 90.0$ ,  $\gamma = 120.0$
- Lattice vectors (conventional cell):
  - $\mathbf{a}_1 = [ 1.00000, 0.00000, 0.00000 ]$
  - $\mathbf{a}_2 = [ -0.50000, 0.86603, 0.00000 ]$
  - $\mathbf{a}_3 = [ 0.00000, 0.00000, 1.00000 ]$

---

**Symmetry Operation**


---

Table 1: Symmetry operation

#	SO	#	SO	#	SO	#	SO	#	SO
1	$\{1 0\}$	2	$\{3_{001}^+ 0\}$	3	$\{3_{001}^- 0\}$	4	$\{2_{001} 00\frac{1}{2}\}$	5	$\{6_{001}^- 00\frac{1}{2}\}$
6	$\{6_{001}^+ 00\frac{1}{2}\}$	7	$\{2_{110} 0\}$	8	$\{2_{100} 0\}$	9	$\{2_{010} 0\}$	10	$\{2_{1-10} 00\frac{1}{2}\}$
11	$\{2_{120} 00\frac{1}{2}\}$	12	$\{2_{210} 00\frac{1}{2}\}$	13	$\{-1 0\}$	14	$\{-3_{001}^+ 0\}$	15	$\{-3_{001}^- 0\}$
16	$\{m_{001} 00\frac{1}{2}\}$	17	$\{-6_{001}^- 00\frac{1}{2}\}$	18	$\{-6_{001}^+ 00\frac{1}{2}\}$	19	$\{m_{110} 0\}$	20	$\{m_{100} 0\}$
21	$\{m_{010} 0\}$	22	$\{m_{1-10} 00\frac{1}{2}\}$	23	$\{m_{120} 00\frac{1}{2}\}$	24	$\{m_{210} 00\frac{1}{2}\}$		

---

**Harmonics**


---

Table 2: Harmonics

#	symbol	irrep.	rank	X	multiplicity	component	symmetry
1	$\mathbb{Q}_0(A_{1g})$	$A_{1g}$	0	$Q, T$	-	-	1
2	$\mathbb{Q}_2(A_{1g})$	$A_{1g}$	2	$Q, T$	-	-	$-\frac{x^2}{2} - \frac{y^2}{2} + z^2$
3	$\mathbb{Q}_4(A_{1g})$	$A_{1g}$	4	$Q, T$	-	-	$\frac{3x^4}{8} + \frac{3x^2y^2}{4} - 3x^2z^2 + \frac{3y^4}{8} - 3y^2z^2 + z^4$
4	$\mathbb{Q}_6(A_{1g}, 2)$	$A_{1g}$	6	$Q, T$	2	-	$\frac{\sqrt{462}(x-y)(x+y)(x^2-4xy+y^2)(x^2+4xy+y^2)}{32}$
5	$\mathbb{G}_0(A_{1u})$	$A_{1u}$	0	$G, M$	-	-	1
6	$\mathbb{G}_2(A_{1u})$	$A_{1u}$	2	$G, M$	-	-	$-\frac{x^2}{2} - \frac{y^2}{2} + z^2$

*continued ...*

Table 2

#	symbol	irrep.	rank	X	multiplicity	component	symmetry
7	$\mathbb{G}_4(A_{1u})$	$A_{1u}$	4	$G, M$	-	-	$\frac{3x^4}{8} + \frac{3x^2y^2}{4} - 3x^2z^2 + \frac{3y^4}{8} - 3y^2z^2 + z^4$
8	$\mathbb{G}_6(A_{1u}, 2)$	$A_{1u}$	6	$G, M$	2	-	$\frac{\sqrt{462}(x-y)(x+y)(x^2-4xy+y^2)(x^2+4xy+y^2)}{32}$
9	$\mathbb{Q}_7(A_{1u})$	$A_{1u}$	7	$Q, T$	-	-	$\frac{\sqrt{6006}xyz(x^2-3y^2)(3x^2-y^2)}{16}$
10	$\mathbb{G}_1(A_{2g})$	$A_{2g}$	1	$G, M$	-	-	$z$
11	$\mathbb{G}_3(A_{2g})$	$A_{2g}$	3	$G, M$	-	-	$-\frac{z(3x^2+3y^2-2z^2)}{2}$
12	$\mathbb{G}_5(A_{2g})$	$A_{2g}$	5	$G, M$	-	-	$\frac{z(15x^4+30x^2y^2-40x^2z^2+15y^4-40y^2z^2+8z^4)}{8}$
13	$\mathbb{Q}_6(A_{2g})$	$A_{2g}$	6	$Q, T$	-	-	$\frac{\sqrt{462}xy(x^2-3y^2)(3x^2-y^2)}{16}$
14	$\mathbb{Q}_1(A_{2u})$	$A_{2u}$	1	$Q, T$	-	-	$z$
15	$\mathbb{Q}_3(A_{2u})$	$A_{2u}$	3	$Q, T$	-	-	$-\frac{z(3x^2+3y^2-2z^2)}{2}$
16	$\mathbb{G}_6(A_{2u})$	$A_{2u}$	6	$G, M$	-	-	$\frac{\sqrt{462}xy(x^2-3y^2)(3x^2-y^2)}{16}$
17	$\mathbb{Q}_7(A_{2u}, 2)$	$A_{2u}$	7	$Q, T$	2	-	$\frac{\sqrt{6006}z(x-y)(x+y)(x^2-4xy+y^2)(x^2+4xy+y^2)}{32}$
18	$\mathbb{G}_3(B_{1g})$	$B_{1g}$	3	$G, M$	-	-	$\frac{\sqrt{10}y(3x^2-y^2)}{4}$
19	$\mathbb{Q}_4(B_{1g})$	$B_{1g}$	4	$Q, T$	-	-	$\frac{\sqrt{70}xz(x^2-3y^2)}{4}$
20	$\mathbb{Q}_6(B_{1g})$	$B_{1g}$	6	$Q, T$	-	-	$-\frac{\sqrt{210}xz(x^2-3y^2)(3x^2+3y^2-8z^2)}{16}$
21	$\mathbb{Q}_3(B_{1u})$	$B_{1u}$	3	$Q, T$	-	-	$\frac{\sqrt{10}y(3x^2-y^2)}{4}$
22	$\mathbb{G}_4(B_{1u})$	$B_{1u}$	4	$G, M$	-	-	$\frac{\sqrt{70}xz(x^2-3y^2)}{4}$
23	$\mathbb{Q}_5(B_{1u})$	$B_{1u}$	5	$Q, T$	-	-	$-\frac{\sqrt{70}y(3x^2-y^2)(x^2+y^2-8z^2)}{16}$
24	$\mathbb{Q}_9(B_{1u}, 1)$	$B_{1u}$	9	$Q, T$	1	-	$\frac{\sqrt{24310}y(3x^2-y^2)(3x^6-27x^4y^2+33x^2y^4-y^6)}{256}$
25	$\mathbb{G}_3(B_{2g})$	$B_{2g}$	3	$G, M$	-	-	$\frac{\sqrt{10}x(x^2-3y^2)}{4}$
26	$\mathbb{Q}_4(B_{2g})$	$B_{2g}$	4	$Q, T$	-	-	$\frac{\sqrt{70}yz(3x^2-y^2)}{4}$
27	$\mathbb{Q}_6(B_{2g})$	$B_{2g}$	6	$Q, T$	-	-	$-\frac{\sqrt{210}yz(3x^2-y^2)(3x^2+3y^2-8z^2)}{16}$

continued ...

Table 2

#	symbol	irrep.	rank	X	multiplicity	component	symmetry
28	$\mathbb{Q}_3(B_{2u})$	$B_{2u}$	3	$Q, T$	-	-	$\frac{\sqrt{10}x(x^2-3y^2)}{4}$
29	$\mathbb{G}_4(B_{2u})$	$B_{2u}$	4	$G, M$	-	-	$\frac{\sqrt{70}yz(3x^2-y^2)}{4}$
30	$\mathbb{Q}_5(B_{2u})$	$B_{2u}$	5	$Q, T$	-	-	$-\frac{\sqrt{70}x(x^2-3y^2)(x^2+y^2-8z^2)}{16}$
31	$\mathbb{Q}_9(B_{2u}, 1)$	$B_{2u}$	9	$Q, T$	1	-	$\frac{\sqrt{24310}x(x^2-3y^2)(x^6-33x^4y^2+27x^2y^4-3y^6)}{256}$
32	$\mathbb{G}_{1,1}(E_{1g})$	$E_{1g}$	1	$G, M$	-	1	$x$
33	$\mathbb{G}_{1,2}(E_{1g})$					2	$y$
34	$\mathbb{Q}_{2,1}(E_{1g})$	$E_{1g}$	2	$Q, T$	-	1	$\sqrt{3}yz$
35	$\mathbb{Q}_{2,2}(E_{1g})$					2	$-\sqrt{3}xz$
36	$\mathbb{G}_{3,1}(E_{1g})$	$E_{1g}$	3	$G, M$	-	1	$-\frac{\sqrt{6}x(x^2+y^2-4z^2)}{4}$
37	$\mathbb{G}_{3,2}(E_{1g})$					2	$-\frac{\sqrt{6}y(x^2+y^2-4z^2)}{4}$
38	$\mathbb{Q}_{4,1}(E_{1g})$	$E_{1g}$	4	$Q, T$	-	1	$-\frac{\sqrt{10}yz(3x^2+3y^2-4z^2)}{4}$
39	$\mathbb{Q}_{4,2}(E_{1g})$					2	$\frac{\sqrt{10}xz(3x^2+3y^2-4z^2)}{4}$
40	$\mathbb{G}_{5,1}(E_{1g}, 1)$	$E_{1g}$	5	$G, M$	1	1	$\frac{3\sqrt{14}x(x^4-10x^2y^2+5y^4)}{16}$
41	$\mathbb{G}_{5,2}(E_{1g}, 1)$					2	$-\frac{3\sqrt{14}y(5x^4-10x^2y^2+y^4)}{16}$
42	$\mathbb{Q}_{6,1}(E_{1g}, 1)$	$E_{1g}$	6	$Q, T$	1	1	$\frac{3\sqrt{154}yz(5x^4-10x^2y^2+y^4)}{16}$
43	$\mathbb{Q}_{6,2}(E_{1g}, 1)$					2	$\frac{3\sqrt{154}xz(x^4-10x^2y^2+5y^4)}{16}$
44	$\mathbb{Q}_{6,1}(E_{1g}, 2)$	$E_{1g}$	6	$Q, T$	2	1	$\frac{\sqrt{21}yz(5x^4+10x^2y^2-20x^2z^2+5y^4-20y^2z^2+8z^4)}{8}$
45	$\mathbb{Q}_{6,2}(E_{1g}, 2)$					2	$-\frac{\sqrt{21}xz(5x^4+10x^2y^2-20x^2z^2+5y^4-20y^2z^2+8z^4)}{8}$
46	$\mathbb{Q}_{8,1}(E_{1g}, 1)$	$E_{1g}$	8	$Q, T$	1	1	$\frac{3\sqrt{715}yz(7x^6-35x^4y^2+21x^2y^4-y^6)}{32}$
47	$\mathbb{Q}_{8,2}(E_{1g}, 1)$					2	$-\frac{3\sqrt{715}xz(x^6-21x^4y^2+35x^2y^4-7y^6)}{32}$
48	$\mathbb{Q}_{1,1}(E_{1u})$	$E_{1u}$	1	$Q, T$	-	1	$x$

continued ...

Table 2

#	symbol	irrep.	rank	X	multiplicity	component	symmetry
49	$\mathbb{Q}_{1,2}(E_{1u})$					2	$y$
50	$\mathbb{G}_{2,1}(E_{1u})$	$E_{1u}$	2	$G, M$	-	1	$\sqrt{3}yz$
51	$\mathbb{G}_{2,2}(E_{1u})$					2	$-\sqrt{3}xz$
52	$\mathbb{Q}_{3,1}(E_{1u})$	$E_{1u}$	3	$Q, T$	-	1	$-\frac{\sqrt{6}x(x^2+y^2-4z^2)}{4}$
53	$\mathbb{Q}_{3,2}(E_{1u})$					2	$-\frac{\sqrt{6}y(x^2+y^2-4z^2)}{4}$
54	$\mathbb{G}_{4,1}(E_{1u})$	$E_{1u}$	4	$G, M$	-	1	$-\frac{\sqrt{10}yz(3x^2+3y^2-4z^2)}{4}$
55	$\mathbb{G}_{4,2}(E_{1u})$					2	$\frac{\sqrt{10}xz(3x^2+3y^2-4z^2)}{4}$
56	$\mathbb{Q}_{5,1}(E_{1u}, 1)$	$E_{1u}$	5	$Q, T$	1	1	$\frac{3\sqrt{14}x(x^4-10x^2y^2+5y^4)}{16}$
57	$\mathbb{Q}_{5,2}(E_{1u}, 1)$					2	$-\frac{3\sqrt{14}y(5x^4-10x^2y^2+y^4)}{16}$
58	$\mathbb{Q}_{5,1}(E_{1u}, 2)$	$E_{1u}$	5	$Q, T$	2	1	$\frac{\sqrt{15}x(x^4+2x^2y^2-12x^2z^2+y^4-12y^2z^2+8z^4)}{8}$
59	$\mathbb{Q}_{5,2}(E_{1u}, 2)$					2	$\frac{\sqrt{15}y(x^4+2x^2y^2-12x^2z^2+y^4-12y^2z^2+8z^4)}{8}$
60	$\mathbb{Q}_{7,1}(E_{1u}, 1)$	$E_{1u}$	7	$Q, T$	1	1	$\frac{\sqrt{429}x(x^6-21x^4y^2+35x^2y^4-7y^6)}{32}$
61	$\mathbb{Q}_{7,2}(E_{1u}, 1)$					2	$\frac{\sqrt{429}y(7x^6-35x^4y^2+21x^2y^4-y^6)}{32}$
62	$\mathbb{Q}_{2,1}(E_{2g})$	$E_{2g}$	2	$Q, T$	-	1	$\frac{\sqrt{3}(x-y)(x+y)}{2}$
63	$\mathbb{Q}_{2,2}(E_{2g})$					2	$-\sqrt{3}xy$
64	$\mathbb{G}_{3,1}(E_{2g})$	$E_{2g}$	3	$G, M$	-	1	$\sqrt{15}xyz$
65	$\mathbb{G}_{3,2}(E_{2g})$					2	$\frac{\sqrt{15}z(x-y)(x+y)}{2}$
66	$\mathbb{Q}_{4,1}(E_{2g}, 1)$	$E_{2g}$	4	$Q, T$	1	1	$\frac{\sqrt{35}(x^2-2xy-y^2)(x^2+2xy-y^2)}{8}$
67	$\mathbb{Q}_{4,2}(E_{2g}, 1)$					2	$\frac{\sqrt{35}xy(x-y)(x+y)}{2}$
68	$\mathbb{Q}_{4,1}(E_{2g}, 2)$	$E_{2g}$	4	$Q, T$	2	1	$-\frac{\sqrt{5}(x-y)(x+y)(x^2+y^2-6z^2)}{4}$
69	$\mathbb{Q}_{4,2}(E_{2g}, 2)$					2	$\frac{\sqrt{5}xy(x^2+y^2-6z^2)}{2}$

continued ...

Table 2

#	symbol	irrep.	rank	X	multiplicity	component	symmetry
70	$\mathbb{Q}_{6,1}(E_{2g}, 1)$	$E_{2g}$	6	$Q, T$	1	1	$-\frac{3\sqrt{7}(x^2+y^2-10z^2)(x^2-2xy-y^2)(x^2+2xy-y^2)}{16}$
71	$\mathbb{Q}_{6,2}(E_{2g}, 1)$					2	$-\frac{3\sqrt{7}xy(x-y)(x+y)(x^2+y^2-10z^2)}{4}$
72	$\mathbb{Q}_{6,1}(E_{2g}, 2)$	$E_{2g}$	6	$Q, T$	2	1	$\frac{\sqrt{210}(x-y)(x+y)(x^4+2x^2y^2-16x^2z^2+y^4-16y^2z^2+16z^4)}{32}$
73	$\mathbb{Q}_{6,2}(E_{2g}, 2)$					2	$-\frac{\sqrt{210}xy(x^4+2x^2y^2-16x^2z^2+y^4-16y^2z^2+16z^4)}{16}$
74	$\mathbb{Q}_{8,1}(E_{2g}, 1)$	$E_{2g}$	8	$Q, T$	1	1	$\frac{3\sqrt{715}(x^4-4x^3y-6x^2y^2+4xy^3+y^4)(x^4+4x^3y-6x^2y^2-4xy^3+y^4)}{128}$
75	$\mathbb{Q}_{8,2}(E_{2g}, 1)$					2	$-\frac{3\sqrt{715}xy(x-y)(x+y)(x^2-2xy-y^2)(x^2+2xy-y^2)}{16}$
76	$\mathbb{G}_{2,1}(E_{2u})$	$E_{2u}$	2	$G, M$	-	1	$\frac{\sqrt{3}(x-y)(x+y)}{2}$
77	$\mathbb{G}_{2,2}(E_{2u})$					2	$-\sqrt{3}xy$
78	$\mathbb{Q}_{3,1}(E_{2u})$	$E_{2u}$	3	$Q, T$	-	1	$\sqrt{15}xyz$
79	$\mathbb{Q}_{3,2}(E_{2u})$					2	$\frac{\sqrt{15}z(x-y)(x+y)}{2}$
80	$\mathbb{G}_{4,1}(E_{2u}, 1)$	$E_{2u}$	4	$G, M$	1	1	$\frac{\sqrt{35}(x^2-2xy-y^2)(x^2+2xy-y^2)}{8}$
81	$\mathbb{G}_{4,2}(E_{2u}, 1)$					2	$\frac{\sqrt{35}xy(x-y)(x+y)}{2}$
82	$\mathbb{G}_{4,1}(E_{2u}, 2)$	$E_{2u}$	4	$G, M$	2	1	$-\frac{\sqrt{5}(x-y)(x+y)(x^2+y^2-6z^2)}{4}$
83	$\mathbb{G}_{4,2}(E_{2u}, 2)$					2	$\frac{\sqrt{5}xy(x^2+y^2-6z^2)}{2}$
84	$\mathbb{Q}_{5,1}(E_{2u}, 1)$	$E_{2u}$	5	$Q, T$	1	1	$-\frac{3\sqrt{35}xyz(x-y)(x+y)}{2}$
85	$\mathbb{Q}_{5,2}(E_{2u}, 1)$					2	$\frac{3\sqrt{35}z(x^2-2xy-y^2)(x^2+2xy-y^2)}{8}$
86	$\mathbb{Q}_{5,1}(E_{2u}, 2)$	$E_{2u}$	5	$Q, T$	2	1	$-\frac{\sqrt{105}xyz(x^2+y^2-2z^2)}{2}$
87	$\mathbb{Q}_{5,2}(E_{2u}, 2)$					2	$-\frac{\sqrt{105}z(x-y)(x+y)(x^2+y^2-2z^2)}{4}$
88	$\mathbb{Q}_{9,1}(E_{2u}, 1)$	$E_{2u}$	9	$Q, T$	1	1	$\frac{3\sqrt{12155}xyz(x-y)(x+y)(x^2-2xy-y^2)(x^2+2xy-y^2)}{16}$
89	$\mathbb{Q}_{9,2}(E_{2u}, 1)$					2	$\frac{3\sqrt{12155}z(x^4-4x^3y-6x^2y^2+4xy^3+y^4)(x^4+4x^3y-6x^2y^2-4xy^3+y^4)}{128}$

Table 3: dimension = 40

#	orbital@atom(SL)	#	orbital@atom(SL)	#	orbital@atom(SL)	#	orbital@atom(SL)	#	orbital@atom(SL)
0	$ d_v\rangle @\text{Mn}(1)$	1	$ d_{xy}\rangle @\text{Mn}(1)$	2	$ d_{xz}\rangle @\text{Mn}(1)$	3	$ d_{yz}\rangle @\text{Mn}(1)$	4	$ d_u\rangle @\text{Mn}(1)$
5	$ d_v\rangle @\text{Mn}(2)$	6	$ d_{xy}\rangle @\text{Mn}(2)$	7	$ d_{xz}\rangle @\text{Mn}(2)$	8	$ d_{yz}\rangle @\text{Mn}(2)$	9	$ d_u\rangle @\text{Mn}(2)$
10	$ d_v\rangle @\text{Mn}(3)$	11	$ d_{xy}\rangle @\text{Mn}(3)$	12	$ d_{xz}\rangle @\text{Mn}(3)$	13	$ d_{yz}\rangle @\text{Mn}(3)$	14	$ d_u\rangle @\text{Mn}(3)$
15	$ d_v\rangle @\text{Mn}(4)$	16	$ d_{xy}\rangle @\text{Mn}(4)$	17	$ d_{xz}\rangle @\text{Mn}(4)$	18	$ d_{yz}\rangle @\text{Mn}(4)$	19	$ d_u\rangle @\text{Mn}(4)$
20	$ d_v\rangle @\text{Mn}(5)$	21	$ d_{xy}\rangle @\text{Mn}(5)$	22	$ d_{xz}\rangle @\text{Mn}(5)$	23	$ d_{yz}\rangle @\text{Mn}(5)$	24	$ d_u\rangle @\text{Mn}(5)$
25	$ d_v\rangle @\text{Mn}(6)$	26	$ d_{xy}\rangle @\text{Mn}(6)$	27	$ d_{xz}\rangle @\text{Mn}(6)$	28	$ d_{yz}\rangle @\text{Mn}(6)$	29	$ d_u\rangle @\text{Mn}(6)$
30	$ d_v\rangle @\text{Sn}(1)$	31	$ d_{xy}\rangle @\text{Sn}(1)$	32	$ d_{xz}\rangle @\text{Sn}(1)$	33	$ d_{yz}\rangle @\text{Sn}(1)$	34	$ d_u\rangle @\text{Sn}(1)$
35	$ d_v\rangle @\text{Sn}(2)$	36	$ d_{xy}\rangle @\text{Sn}(2)$	37	$ d_{xz}\rangle @\text{Sn}(2)$	38	$ d_{yz}\rangle @\text{Sn}(2)$	39	$ d_u\rangle @\text{Sn}(2)$

Table 4: Atomic basis (orbital part only)

orbital	definition
$ d_v\rangle$	$\frac{\sqrt{3}(x^2-y^2)}{2}$
$ d_{xy}\rangle$	$\sqrt{3}xy$
$ d_{xz}\rangle$	$\sqrt{3}xz$
$ d_{yz}\rangle$	$\sqrt{3}yz$
$ d_u\rangle$	$-\frac{x^2}{2} - \frac{y^2}{2} + z^2$

• Mn : 'Mn' site-cluster

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

\* ket:  $|d_v\rangle, |d_{xy}\rangle, |d_{xz}\rangle, |d_{yz}\rangle, |d_u\rangle$

\* wyckoff: 6h

$$\boxed{\text{z1}} \quad \mathbb{Q}_0^{(c)}(A_{1g}, a) = \mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_0^{(s)}(A_{1g})$$

$$\boxed{\text{z2}} \quad \mathbb{Q}_0^{(c)}(A_{1g}, b) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_{2,1}^{(s)}(E_{2g})}{2} + \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_{2,2}^{(s)}(E_{2g})}{2}$$

$$\boxed{\text{z3}} \quad \mathbb{Q}_2^{(c)}(A_{1g}, a) = \mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_0^{(s)}(A_{1g})$$

$$\boxed{\text{z4}} \quad \mathbb{Q}_2^{(c)}(A_{1g}, b) = \frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,1}^{(s)}(E_{2g})}{2} + \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,2}^{(s)}(E_{2g})}{2}$$

$$\boxed{\text{z5}} \quad \mathbb{Q}_4^{(c)}(A_{1g}) = \mathbb{Q}_4^{(a)}(A_{1g})\mathbb{Q}_0^{(s)}(A_{1g})$$

$$\boxed{\text{z6}} \quad \mathbb{Q}_6^{(c)}(A_{1g}, 2) = \frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,1}^{(s)}(E_{2g})}{2} + \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,2}^{(s)}(E_{2g})}{2}$$

$$\boxed{\text{z41}} \quad \mathbb{Q}_7^{(c)}(A_{1u}) = \mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_3^{(s)}(B_{1u})$$

$$\boxed{\text{z42}} \quad \mathbb{G}_2^{(c)}(A_{1u}) = -\frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_{1,1}^{(s)}(E_{1u})}{2} - \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_{1,2}^{(s)}(E_{1u})}{2}$$

$$\boxed{\text{z43}} \quad \mathbb{G}_4^{(c)}(A_{1u}) = -\frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{1,1}^{(s)}(E_{1u})}{2} - \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{1,2}^{(s)}(E_{1u})}{2}$$

$$\boxed{\text{z67}} \quad \mathbb{Q}_6^{(c)}(A_{2g}) = -\frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,2}^{(s)}(E_{2g})}{2} + \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,1}^{(s)}(E_{2g})}{2}$$

$$\boxed{\text{z68}} \quad \mathbb{G}_1^{(c)}(A_{2g}) = -\frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_{2,2}^{(s)}(E_{2g})}{2} + \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_{2,1}^{(s)}(E_{2g})}{2}$$

$$\boxed{\text{z69}} \quad \mathbb{G}_3^{(c)}(A_{2g}) = -\frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,2}^{(s)}(E_{2g})}{2} + \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,1}^{(s)}(E_{2g})}{2}$$



$$\boxed{\text{z95}} \quad \mathbb{Q}_1^{(c)}(A_{2u}, a) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_{1,2}^{(s)}(E_{1u})}{2} - \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_{1,1}^{(s)}(E_{1u})}{2}$$

$$\boxed{\text{z96}} \quad \mathbb{Q}_1^{(c)}(A_{2u}, b) = \mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_3^{(s)}(B_{1u})$$

$$\boxed{\text{z97}} \quad \mathbb{Q}_3^{(c)}(A_{2u}) = \frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{1,2}^{(s)}(E_{1u})}{2} - \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{1,1}^{(s)}(E_{1u})}{2}$$

$$\boxed{\text{z126}} \quad \mathbb{Q}_4^{(c)}(B_{1g}, a) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(s)}(E_{2g})}{2} - \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(s)}(E_{2g})}{2}$$

$$\boxed{\text{z127}} \quad \mathbb{Q}_4^{(c)}(B_{1g}, b) = \mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_0^{(s)}(A_{1g})$$

$$\boxed{\text{z128}} \quad \mathbb{Q}_4^{(c)}(B_{1g}, c) = -\frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(s)}(E_{2g})}{2} + \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(s)}(E_{2g})}{2}$$

$$\boxed{\text{z129}} \quad \mathbb{Q}_3^{(c)}(B_{1u}, a) = \mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_3^{(s)}(B_{1u})$$

$$\boxed{\text{z130}} \quad \mathbb{Q}_3^{(c)}(B_{1u}, b) = -\mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_3^{(s)}(B_{1u})$$

$$\boxed{\text{z131}} \quad \mathbb{Q}_3^{(c)}(B_{1u}, c) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_{1,2}^{(s)}(E_{1u})}{2} - \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_{1,1}^{(s)}(E_{1u})}{2}$$

$$\boxed{\text{z132}} \quad \mathbb{Q}_3^{(c)}(B_{1u}, d) = \mathbb{Q}_4^{(a)}(A_{1g})\mathbb{Q}_3^{(s)}(B_{1u})$$

$$\boxed{\text{z133}} \quad \mathbb{Q}_3^{(c)}(B_{1u}, e) = -\frac{\sqrt{406}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{1,2}^{(s)}(E_{1u})}{29} - \frac{\sqrt{58}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{1,2}^{(s)}(E_{1u})}{58} + \frac{\sqrt{406}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{1,1}^{(s)}(E_{1u})}{29} + \frac{\sqrt{58}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{1,1}^{(s)}(E_{1u})}{58}$$

$$\boxed{\text{z134}} \quad \mathbb{Q}_5^{(c)}(B_{1u}) = -\frac{\sqrt{58}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{1,2}^{(s)}(E_{1u})}{58} + \frac{\sqrt{406}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{1,2}^{(s)}(E_{1u})}{29} + \frac{\sqrt{58}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{1,1}^{(s)}(E_{1u})}{58} - \frac{\sqrt{406}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{1,1}^{(s)}(E_{1u})}{29}$$

$$\boxed{\text{z135}} \quad \mathbb{Q}_4^{(c)}(B_{2g}, a) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(s)}(E_{2g})}{2} + \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(s)}(E_{2g})}{2}$$

$$\boxed{\text{z136}} \quad \mathbb{Q}_4^{(c)}(B_{2g}, b) = \mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_0^{(s)}(A_{1g})$$

$$\boxed{\text{z137}} \quad \mathbb{Q}_4^{(c)}(B_{2g}, c) = -\frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(s)}(E_{2g})}{2} - \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(s)}(E_{2g})}{2}$$

$$\begin{aligned}
\text{z244} \quad \mathbb{Q}_3^{(c)}(B_{2u}, a) &= \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_{1,1}^{(s)}(E_{1u})}{2} + \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_{1,2}^{(s)}(E_{1u})}{2} \\
\text{z245} \quad \mathbb{Q}_3^{(c)}(B_{2u}, b) &= \frac{\sqrt{406}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{1,1}^{(s)}(E_{1u})}{29} - \frac{\sqrt{58}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{1,1}^{(s)}(E_{1u})}{58} + \frac{\sqrt{406}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{1,2}^{(s)}(E_{1u})}{29} - \frac{\sqrt{58}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{1,2}^{(s)}(E_{1u})}{58} \\
\text{z246} \quad \mathbb{Q}_5^{(c)}(B_{2u}) &= \frac{\sqrt{58}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{1,1}^{(s)}(E_{1u})}{58} + \frac{\sqrt{406}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{1,1}^{(s)}(E_{1u})}{29} + \frac{\sqrt{58}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{1,2}^{(s)}(E_{1u})}{58} + \frac{\sqrt{406}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{1,2}^{(s)}(E_{1u})}{29} \\
\text{z247} \quad \mathbb{Q}_{2,1}^{(c)}(E_{1g}, a) &= \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_0^{(s)}(A_{1g})}{2} \\
\text{z248} \quad \mathbb{Q}_{2,2}^{(c)}(E_{1g}, a) &= \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_0^{(s)}(A_{1g})}{2} \\
\text{z249} \quad \mathbb{Q}_{2,1}^{(c)}(E_{1g}, b) &= -\frac{\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(s)}(E_{2g})}{2} + \frac{\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(s)}(E_{2g})}{2} \\
\text{z250} \quad \mathbb{Q}_{2,2}^{(c)}(E_{1g}, b) &= \frac{\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(s)}(E_{2g})}{2} + \frac{\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(s)}(E_{2g})}{2} \\
\text{z251} \quad \mathbb{Q}_{2,1}^{(c)}(E_{1g}, c) &= \frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(s)}(E_{2g})}{8} - \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(s)}(E_{2g})}{8} + \frac{\sqrt{14}\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{2,2}^{(s)}(E_{2g})}{8} + \frac{\sqrt{14}\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{2,1}^{(s)}(E_{2g})}{8} \\
\text{z252} \quad \mathbb{Q}_{2,2}^{(c)}(E_{1g}, c) &= -\frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(s)}(E_{2g})}{8} - \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(s)}(E_{2g})}{8} - \frac{\sqrt{14}\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{2,1}^{(s)}(E_{2g})}{8} + \frac{\sqrt{14}\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{2,2}^{(s)}(E_{2g})}{8} \\
\text{z253} \quad \mathbb{Q}_{4,1}^{(c)}(E_{1g}, a) &= \frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_0^{(s)}(A_{1g})}{2} \\
\text{z254} \quad \mathbb{Q}_{4,2}^{(c)}(E_{1g}, a) &= \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_0^{(s)}(A_{1g})}{2} \\
\text{z255} \quad \mathbb{Q}_{4,1}^{(c)}(E_{1g}, b) &= -\frac{\sqrt{14}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(s)}(E_{2g})}{8} + \frac{\sqrt{14}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(s)}(E_{2g})}{8} + \frac{\sqrt{2}\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{2,2}^{(s)}(E_{2g})}{8} + \frac{\sqrt{2}\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{2,1}^{(s)}(E_{2g})}{8} \\
\text{z256} \quad \mathbb{Q}_{4,2}^{(c)}(E_{1g}, b) &= \frac{\sqrt{14}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(s)}(E_{2g})}{8} + \frac{\sqrt{14}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(s)}(E_{2g})}{8} - \frac{\sqrt{2}\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{2,1}^{(s)}(E_{2g})}{8} + \frac{\sqrt{2}\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{2,2}^{(s)}(E_{2g})}{8} \\
\text{z257} \quad \mathbb{Q}_{6,1}^{(c)}(E_{1g}, 1) &= -\frac{\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{2,2}^{(s)}(E_{2g})}{2} + \frac{\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{2,1}^{(s)}(E_{2g})}{2}
\end{aligned}$$

$$\begin{aligned}
\boxed{\text{z258}} \quad \mathbb{Q}_{6,2}^{(c)}(E_{1g}, 1) &= \frac{\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{2,1}^{(s)}(E_{2g})}{2} + \frac{\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{2,2}^{(s)}(E_{2g})}{2} \\
\boxed{\text{z259}} \quad \mathbb{Q}_{1,1}^{(c)}(E_{1u}, a) &= \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{1,1}^{(s)}(E_{1u})}{2} \\
\boxed{\text{z260}} \quad \mathbb{Q}_{1,2}^{(c)}(E_{1u}, a) &= \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{1,2}^{(s)}(E_{1u})}{2} \\
\boxed{\text{z261}} \quad \mathbb{Q}_{1,1}^{(c)}(E_{1u}, b) &= -\frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_3^{(s)}(B_{1u})}{2} \\
\boxed{\text{z376}} \quad \mathbb{Q}_{1,2}^{(c)}(E_{1u}, b) &= \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_3^{(s)}(B_{1u})}{2} \\
\boxed{\text{z377}} \quad \mathbb{Q}_{1,1}^{(c)}(E_{1u}, c) &= \frac{\sqrt{42}\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_{1,1}^{(s)}(E_{1u})}{14} - \frac{\sqrt{42}\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_{1,2}^{(s)}(E_{1u})}{14} - \frac{\sqrt{14}\mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_{1,1}^{(s)}(E_{1u})}{14} \\
\boxed{\text{z378}} \quad \mathbb{Q}_{1,2}^{(c)}(E_{1u}, c) &= -\frac{\sqrt{42}\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_{1,2}^{(s)}(E_{1u})}{14} - \frac{\sqrt{42}\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_{1,1}^{(s)}(E_{1u})}{14} - \frac{\sqrt{14}\mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_{1,2}^{(s)}(E_{1u})}{14} \\
\boxed{\text{z404}} \quad \mathbb{Q}_{1,1}^{(c)}(E_{1u}, d) &= \frac{\sqrt{406}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_3^{(s)}(B_{1u})}{29} + \frac{\sqrt{58}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_3^{(s)}(B_{1u})}{58} \\
\boxed{\text{z405}} \quad \mathbb{Q}_{1,2}^{(c)}(E_{1u}, d) &= -\frac{\sqrt{406}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_3^{(s)}(B_{1u})}{29} - \frac{\sqrt{58}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_3^{(s)}(B_{1u})}{58} \\
\boxed{\text{z406}} \quad \mathbb{Q}_{3,1}^{(c)}(E_{1u}, a) &= \frac{\sqrt{7}\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_{1,1}^{(s)}(E_{1u})}{14} - \frac{\sqrt{7}\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_{1,2}^{(s)}(E_{1u})}{14} + \frac{\sqrt{21}\mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_{1,1}^{(s)}(E_{1u})}{7} \\
\boxed{\text{z430}} \quad \mathbb{Q}_{3,2}^{(c)}(E_{1u}, a) &= -\frac{\sqrt{7}\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_{1,2}^{(s)}(E_{1u})}{14} - \frac{\sqrt{7}\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_{1,1}^{(s)}(E_{1u})}{14} + \frac{\sqrt{21}\mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_{1,2}^{(s)}(E_{1u})}{7} \\
\boxed{\text{z431}} \quad \mathbb{Q}_{3,1}^{(c)}(E_{1u}, b) &= \frac{\sqrt{58}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_3^{(s)}(B_{1u})}{58} - \frac{\sqrt{406}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_3^{(s)}(B_{1u})}{29} \\
\boxed{\text{z432}} \quad \mathbb{Q}_{3,2}^{(c)}(E_{1u}, b) &= -\frac{\sqrt{58}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_3^{(s)}(B_{1u})}{58} + \frac{\sqrt{406}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_3^{(s)}(B_{1u})}{29} \\
\boxed{\text{z433}} \quad \mathbb{Q}_{3,1}^{(c)}(E_{1u}, c) &= \frac{\sqrt{35}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{1,1}^{(s)}(E_{1u})}{14} - \frac{\sqrt{35}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{1,2}^{(s)}(E_{1u})}{14} - \frac{\sqrt{7}\mathbb{Q}_4^{(a)}(A_{1g})\mathbb{Q}_{1,1}^{(s)}(E_{1u})}{7}
\end{aligned}$$

$$\boxed{\text{z434}} \quad \mathbb{Q}_{3,2}^{(c)}(E_{1u}, c) = -\frac{\sqrt{35}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{1,2}^{(s)}(E_{1u})}{14} - \frac{\sqrt{35}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{1,1}^{(s)}(E_{1u})}{14} - \frac{\sqrt{7}\mathbb{Q}_4^{(a)}(A_{1g})\mathbb{Q}_{1,2}^{(s)}(E_{1u})}{7}$$

$$\boxed{\text{z435}} \quad \mathbb{Q}_{5,1}^{(c)}(E_{1u}, 1) = \frac{\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{1,1}^{(s)}(E_{1u})}{2} - \frac{\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{1,2}^{(s)}(E_{1u})}{2}$$

$$\boxed{\text{z465}} \quad \mathbb{Q}_{5,2}^{(c)}(E_{1u}, 1) = -\frac{\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{1,2}^{(s)}(E_{1u})}{2} - \frac{\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{1,1}^{(s)}(E_{1u})}{2}$$

$$\boxed{\text{z466}} \quad \mathbb{Q}_{5,1}^{(c)}(E_{1u}, 2) = \frac{\sqrt{14}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{1,1}^{(s)}(E_{1u})}{14} - \frac{\sqrt{14}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{1,2}^{(s)}(E_{1u})}{14} + \frac{\sqrt{70}\mathbb{Q}_4^{(a)}(A_{1g})\mathbb{Q}_{1,1}^{(s)}(E_{1u})}{14}$$

$$\boxed{\text{z467}} \quad \mathbb{Q}_{5,2}^{(c)}(E_{1u}, 2) = -\frac{\sqrt{14}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{1,2}^{(s)}(E_{1u})}{14} - \frac{\sqrt{14}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{1,1}^{(s)}(E_{1u})}{14} + \frac{\sqrt{70}\mathbb{Q}_4^{(a)}(A_{1g})\mathbb{Q}_{1,2}^{(s)}(E_{1u})}{14}$$

$$\boxed{\text{z491}} \quad \mathbb{Q}_{2,1}^{(c)}(E_{2g}, a) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{2,1}^{(s)}(E_{2g})}{2}$$

$$\boxed{\text{z492}} \quad \mathbb{Q}_{2,2}^{(c)}(E_{2g}, a) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{2,2}^{(s)}(E_{2g})}{2}$$

$$\boxed{\text{z493}} \quad \mathbb{Q}_{2,1}^{(c)}(E_{2g}, b) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

$$\boxed{\text{z494}} \quad \mathbb{Q}_{2,2}^{(c)}(E_{2g}, b) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

$$\boxed{\text{z495}} \quad \mathbb{Q}_{2,1}^{(c)}(E_{2g}, c) = -\frac{\sqrt{2}\mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_{2,1}^{(s)}(E_{2g})}{2}$$

$$\boxed{\text{z496}} \quad \mathbb{Q}_{2,2}^{(c)}(E_{2g}, c) = -\frac{\sqrt{2}\mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_{2,2}^{(s)}(E_{2g})}{2}$$

$$\boxed{\text{z497}} \quad \mathbb{Q}_{2,1}^{(c)}(E_{2g}, d) = \frac{\sqrt{4970}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,1}^{(s)}(E_{2g})}{142} - \frac{\sqrt{4970}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,2}^{(s)}(E_{2g})}{142} + \frac{\sqrt{142}\mathbb{Q}_4^{(a)}(A_{1g})\mathbb{Q}_{2,1}^{(s)}(E_{2g})}{142}$$

$$\boxed{\text{z498}} \quad \mathbb{Q}_{2,2}^{(c)}(E_{2g}, d) = -\frac{\sqrt{4970}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,2}^{(s)}(E_{2g})}{142} - \frac{\sqrt{4970}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,1}^{(s)}(E_{2g})}{142} + \frac{\sqrt{142}\mathbb{Q}_4^{(a)}(A_{1g})\mathbb{Q}_{2,2}^{(s)}(E_{2g})}{142}$$

$$\boxed{\text{z499}} \quad \mathbb{Q}_{4,1}^{(c)}(E_{2g}, 1a) = \frac{\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_{2,1}^{(s)}(E_{2g})}{2} - \frac{\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_{2,2}^{(s)}(E_{2g})}{2}$$

$$\boxed{\text{z500}} \quad \mathbb{Q}_{4,2}^{(c)}(E_{2g}, 1a) = -\frac{\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_{2,2}^{(s)}(E_{2g})}{2} - \frac{\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_{2,1}^{(s)}(E_{2g})}{2}$$

$$\boxed{\text{z501}} \quad \mathbb{Q}_{4,1}^{(c)}(E_{2g}, 1b) = \frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

$$\boxed{\text{z502}} \quad \mathbb{Q}_{4,2}^{(c)}(E_{2g}, 1b) = \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

$$\boxed{\text{z503}} \quad \mathbb{Q}_{4,1}^{(c)}(E_{2g}, 1c) = -\frac{\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,1}^{(s)}(E_{2g})}{2} + \frac{\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,2}^{(s)}(E_{2g})}{2}$$

$$\boxed{\text{z504}} \quad \mathbb{Q}_{4,2}^{(c)}(E_{2g}, 1c) = \frac{\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,2}^{(s)}(E_{2g})}{2} + \frac{\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,1}^{(s)}(E_{2g})}{2}$$

$$\boxed{\text{z505}} \quad \mathbb{Q}_{4,1}^{(c)}(E_{2g}, 2a) = \frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

$$\boxed{\text{z506}} \quad \mathbb{Q}_{4,2}^{(c)}(E_{2g}, 2a) = \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

$$\boxed{\text{z507}} \quad \mathbb{Q}_{4,1}^{(c)}(E_{2g}, 2b) = \frac{\sqrt{71}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,1}^{(s)}(E_{2g})}{142} - \frac{\sqrt{71}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,2}^{(s)}(E_{2g})}{142} - \frac{\sqrt{2485}\mathbb{Q}_4^{(a)}(A_{1g})\mathbb{Q}_{2,1}^{(s)}(E_{2g})}{71}$$

$$\boxed{\text{z508}} \quad \mathbb{Q}_{4,2}^{(c)}(E_{2g}, 2b) = -\frac{\sqrt{71}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,2}^{(s)}(E_{2g})}{142} - \frac{\sqrt{71}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,1}^{(s)}(E_{2g})}{142} - \frac{\sqrt{2485}\mathbb{Q}_4^{(a)}(A_{1g})\mathbb{Q}_{2,2}^{(s)}(E_{2g})}{71}$$

$$\boxed{\text{z613}} \quad \mathbb{Q}_{3,1}^{(c)}(E_{2u}, a) = -\frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_3^{(s)}(B_{1u})}{2}$$

$$\boxed{\text{z614}} \quad \mathbb{Q}_{3,2}^{(c)}(E_{2u}, a) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_3^{(s)}(B_{1u})}{2}$$

$$\boxed{\text{z615}} \quad \mathbb{Q}_{3,1}^{(c)}(E_{2u}, b) = \frac{\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_{1,1}^{(s)}(E_{1u})}{2} - \frac{\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_{1,2}^{(s)}(E_{1u})}{2}$$

$$\boxed{\text{z616}} \quad \mathbb{Q}_{3,2}^{(c)}(E_{2u}, b) = -\frac{\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_{1,2}^{(s)}(E_{1u})}{2} - \frac{\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_{1,1}^{(s)}(E_{1u})}{2}$$

$$\boxed{\text{z617}} \quad \mathbb{Q}_{3,1}^{(c)}(E_{2u}, c) = \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_3^{(s)}(B_{1u})}{2}$$

$$\begin{aligned}
\boxed{\text{z618}} \quad \mathbb{Q}_{3,2}^{(c)}(E_{2u}, c) &= -\frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_3^{(s)}(B_{1u})}{2} \\
\boxed{\text{z619}} \quad \mathbb{Q}_{3,1}^{(c)}(E_{2u}, d) &= -\frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{1,1}^{(s)}(E_{1u})}{8} + \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{1,2}^{(s)}(E_{1u})}{8} - \frac{\sqrt{14}\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{1,2}^{(s)}(E_{1u})}{8} + \frac{\sqrt{14}\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{1,1}^{(s)}(E_{1u})}{8} \\
\boxed{\text{z620}} \quad \mathbb{Q}_{3,2}^{(c)}(E_{2u}, d) &= \frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{1,2}^{(s)}(E_{1u})}{8} + \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{1,1}^{(s)}(E_{1u})}{8} + \frac{\sqrt{14}\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{1,1}^{(s)}(E_{1u})}{8} + \frac{\sqrt{14}\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{1,2}^{(s)}(E_{1u})}{8} \\
\boxed{\text{z621}} \quad \mathbb{Q}_{5,1}^{(c)}(E_{2u}, 1) &= -\frac{\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{1,2}^{(s)}(E_{1u})}{2} - \frac{\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{1,1}^{(s)}(E_{1u})}{2} \\
\boxed{\text{z622}} \quad \mathbb{Q}_{5,2}^{(c)}(E_{2u}, 1) &= \frac{\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{1,1}^{(s)}(E_{1u})}{2} - \frac{\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{1,2}^{(s)}(E_{1u})}{2} \\
\boxed{\text{z623}} \quad \mathbb{Q}_{5,1}^{(c)}(E_{2u}, 2) &= \frac{\sqrt{14}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{1,1}^{(s)}(E_{1u})}{8} - \frac{\sqrt{14}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{1,2}^{(s)}(E_{1u})}{8} - \frac{\sqrt{2}\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{1,2}^{(s)}(E_{1u})}{8} + \frac{\sqrt{2}\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{1,1}^{(s)}(E_{1u})}{8} \\
\boxed{\text{z624}} \quad \mathbb{Q}_{5,2}^{(c)}(E_{2u}, 2) &= -\frac{\sqrt{14}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{1,2}^{(s)}(E_{1u})}{8} - \frac{\sqrt{14}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{1,1}^{(s)}(E_{1u})}{8} + \frac{\sqrt{2}\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{1,1}^{(s)}(E_{1u})}{8} + \frac{\sqrt{2}\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{1,2}^{(s)}(E_{1u})}{8}
\end{aligned}$$

• Sn : 'Sn' site-cluster

- \* bra:  $\langle d_v |, \langle d_{xy} |, \langle d_{xz} |, \langle d_{yz} |, \langle d_u |$
- \* ket:  $|d_v\rangle, |d_{xy}\rangle, |d_{xz}\rangle, |d_{yz}\rangle, |d_u\rangle$
- \* wyckoff: 2c

$$\begin{aligned}
\boxed{\text{z7}} \quad \mathbb{Q}_0^{(c)}(A_{1g}) &= \mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_0^{(s)}(A_{1g}) \\
\boxed{\text{z8}} \quad \mathbb{Q}_2^{(c)}(A_{1g}) &= \mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_0^{(s)}(A_{1g}) \\
\boxed{\text{z9}} \quad \mathbb{Q}_4^{(c)}(A_{1g}) &= \mathbb{Q}_4^{(a)}(A_{1g})\mathbb{Q}_0^{(s)}(A_{1g}) \\
\boxed{\text{z70}} \quad \mathbb{Q}_7^{(c)}(A_{1u}) &= \mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_3^{(s)}(B_{1u}) \\
\boxed{\text{z98}} \quad \mathbb{Q}_1^{(c)}(A_{2u}) &= \mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_3^{(s)}(B_{1u}) \\
\boxed{\text{z138}} \quad \mathbb{Q}_4^{(c)}(B_{1g}) &= \mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_0^{(s)}(A_{1g}) \\
\boxed{\text{z139}} \quad \mathbb{Q}_3^{(c)}(B_{1u}, a) &= \mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_3^{(s)}(B_{1u})
\end{aligned}$$

$$\begin{aligned}
\boxed{\text{z140}} \quad \mathbb{Q}_3^{(c)}(B_{1u}, b) &= -\mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_3^{(s)}(B_{1u}) \\
\boxed{\text{z141}} \quad \mathbb{Q}_3^{(c)}(B_{1u}, c) &= \mathbb{Q}_4^{(a)}(A_{1g})\mathbb{Q}_3^{(s)}(B_{1u}) \\
\boxed{\text{z262}} \quad \mathbb{Q}_4^{(c)}(B_{2g}) &= \mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_0^{(s)}(A_{1g}) \\
\boxed{\text{z263}} \quad \mathbb{Q}_{2,1}^{(c)}(E_{1g}) &= \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_0^{(s)}(A_{1g})}{2} \\
\boxed{\text{z264}} \quad \mathbb{Q}_{2,2}^{(c)}(E_{1g}) &= \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_0^{(s)}(A_{1g})}{2} \\
\boxed{\text{z265}} \quad \mathbb{Q}_{4,1}^{(c)}(E_{1g}) &= \frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_0^{(s)}(A_{1g})}{2} \\
\boxed{\text{z266}} \quad \mathbb{Q}_{4,2}^{(c)}(E_{1g}) &= \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_0^{(s)}(A_{1g})}{2} \\
\boxed{\text{z267}} \quad \mathbb{Q}_{1,1}^{(c)}(E_{1u}, a) &= -\frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_3^{(s)}(B_{1u})}{2} \\
\boxed{\text{z379}} \quad \mathbb{Q}_{1,2}^{(c)}(E_{1u}, a) &= \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_3^{(s)}(B_{1u})}{2} \\
\boxed{\text{z407}} \quad \mathbb{Q}_{1,1}^{(c)}(E_{1u}, b) &= \frac{\sqrt{406}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_3^{(s)}(B_{1u})}{29} + \frac{\sqrt{58}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_3^{(s)}(B_{1u})}{58} \\
\boxed{\text{z436}} \quad \mathbb{Q}_{1,2}^{(c)}(E_{1u}, b) &= -\frac{\sqrt{406}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_3^{(s)}(B_{1u})}{29} - \frac{\sqrt{58}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_3^{(s)}(B_{1u})}{58} \\
\boxed{\text{z437}} \quad \mathbb{Q}_{3,1}^{(c)}(E_{1u}) &= \frac{\sqrt{58}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_3^{(s)}(B_{1u})}{58} - \frac{\sqrt{406}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_3^{(s)}(B_{1u})}{29} \\
\boxed{\text{z438}} \quad \mathbb{Q}_{3,2}^{(c)}(E_{1u}) &= -\frac{\sqrt{58}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_3^{(s)}(B_{1u})}{58} + \frac{\sqrt{406}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_3^{(s)}(B_{1u})}{29} \\
\boxed{\text{z509}} \quad \mathbb{Q}_{2,1}^{(c)}(E_{2g}) &= \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_0^{(s)}(A_{1g})}{2}
\end{aligned}$$

$$\boxed{\text{z510}} \quad \mathbb{Q}_{2,2}^{(c)}(E_{2g}) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

$$\boxed{\text{z511}} \quad \mathbb{Q}_{4,1}^{(c)}(E_{2g}, 1) = \frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

$$\boxed{\text{z512}} \quad \mathbb{Q}_{4,2}^{(c)}(E_{2g}, 1) = \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

$$\boxed{\text{z513}} \quad \mathbb{Q}_{4,1}^{(c)}(E_{2g}, 2) = \frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

$$\boxed{\text{z514}} \quad \mathbb{Q}_{4,2}^{(c)}(E_{2g}, 2) = \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

$$\boxed{\text{z625}} \quad \mathbb{Q}_{3,1}^{(c)}(E_{2u}, a) = -\frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_3^{(s)}(B_{1u})}{2}$$

$$\boxed{\text{z626}} \quad \mathbb{Q}_{3,2}^{(c)}(E_{2u}, a) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_3^{(s)}(B_{1u})}{2}$$

$$\boxed{\text{z627}} \quad \mathbb{Q}_{3,1}^{(c)}(E_{2u}, b) = \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_3^{(s)}(B_{1u})}{2}$$

$$\boxed{\text{z628}} \quad \mathbb{Q}_{3,2}^{(c)}(E_{2u}, b) = -\frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_3^{(s)}(B_{1u})}{2}$$

• **Mn;Mn\_001\_1** : 'Mn'-'Mn' bond-cluster

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

\* ket:  $|d_v\rangle$ ,  $|d_{xy}\rangle$ ,  $|d_{xz}\rangle$ ,  $|d_{yz}\rangle$ ,  $|d_u\rangle$

\* wyckoff: **6b06h**

$$\boxed{\text{z10}} \quad \mathbb{Q}_0^{(c)}(A_{1g}, a) = \mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z11}} \quad \mathbb{Q}_0^{(c)}(A_{1g}, b) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2} + \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2}$$

$$\boxed{\text{z12}} \quad \mathbb{Q}_0^{(c)}(A_{1g}, c) = \mathbb{M}_1^{(a)}(A_{2g})\mathbb{M}_1^{(b)}(A_{2g})$$



$$\begin{aligned}
\boxed{\text{z13}} \quad \mathbb{Q}_2^{(c)}(A_{1g}, a) &= \mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_0^{(b)}(A_{1g}) \\
\boxed{\text{z14}} \quad \mathbb{Q}_2^{(c)}(A_{1g}, b) &= \frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2} + \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2} \\
\boxed{\text{z15}} \quad \mathbb{Q}_2^{(c)}(A_{1g}, c) &= \mathbb{M}_3^{(a)}(A_{2g})\mathbb{M}_1^{(b)}(A_{2g}) \\
\boxed{\text{z16}} \quad \mathbb{Q}_2^{(c)}(A_{1g}, d) &= -\frac{\sqrt{2}\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{T}_{2,1}^{(b)}(E_{2g})}{2} - \frac{\sqrt{2}\mathbb{M}_{3,2}^{(a)}(E_{2g})\mathbb{T}_{2,2}^{(b)}(E_{2g})}{2} \\
\boxed{\text{z17}} \quad \mathbb{Q}_4^{(c)}(A_{1g}) &= \mathbb{Q}_4^{(a)}(A_{1g})\mathbb{Q}_0^{(b)}(A_{1g}) \\
\boxed{\text{z18}} \quad \mathbb{Q}_6^{(c)}(A_{1g}, 2) &= \frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2} + \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2} \\
\boxed{\text{z44}} \quad \mathbb{Q}_7^{(c)}(A_{1u}) &= \mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_3^{(b)}(B_{1u}) \\
\boxed{\text{z45}} \quad \mathbb{G}_0^{(c)}(A_{1u}, a) &= \frac{\sqrt{2}\mathbb{M}_{1,1}^{(a)}(E_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{2} + \frac{\sqrt{2}\mathbb{M}_{1,2}^{(a)}(E_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{2} \\
\boxed{\text{z46}} \quad \mathbb{G}_0^{(c)}(A_{1u}, b) &= \mathbb{M}_3^{(a)}(B_{2g})\mathbb{T}_3^{(b)}(B_{2u}) \\
\boxed{\text{z47}} \quad \mathbb{G}_2^{(c)}(A_{1u}, a) &= -\frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{2} - \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{2} \\
\boxed{\text{z71}} \quad \mathbb{G}_2^{(c)}(A_{1u}, b) &= \frac{\sqrt{2}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{2} + \frac{\sqrt{2}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{2} \\
\boxed{\text{z72}} \quad \mathbb{G}_4^{(c)}(A_{1u}) &= -\frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{2} - \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{2} \\
\boxed{\text{z73}} \quad \mathbb{Q}_6^{(c)}(A_{2g}) &= -\frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2} + \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2} \\
\boxed{\text{z74}} \quad \mathbb{G}_1^{(c)}(A_{2g}, a) &= -\frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2} + \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2} \\
\boxed{\text{z75}} \quad \mathbb{G}_1^{(c)}(A_{2g}, b) &= -\frac{\sqrt{2}\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{T}_{2,2}^{(b)}(E_{2g})}{2} + \frac{\sqrt{2}\mathbb{M}_{3,2}^{(a)}(E_{2g})\mathbb{T}_{2,1}^{(b)}(E_{2g})}{2}
\end{aligned}$$

$$\boxed{\text{z76}} \quad \mathbb{G}_3^{(c)}(A_{2g}) = -\frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2} + \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2}$$

$$\boxed{\text{z99}} \quad \mathbb{Q}_1^{(c)}(A_{2u}, a) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{2} - \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{2}$$

$$\boxed{\text{z100}} \quad \mathbb{Q}_1^{(c)}(A_{2u}, b) = \mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_3^{(b)}(B_{1u})$$

$$\boxed{\text{z101}} \quad \mathbb{Q}_1^{(c)}(A_{2u}, c) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(a)}(E_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{2} - \frac{\sqrt{2}\mathbb{M}_{1,2}^{(a)}(E_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{2}$$

$$\boxed{\text{z102}} \quad \mathbb{Q}_1^{(c)}(A_{2u}, d) = -\mathbb{M}_3^{(a)}(B_{1g})\mathbb{T}_3^{(b)}(B_{2u})$$

$$\boxed{\text{z103}} \quad \mathbb{Q}_3^{(c)}(A_{2u}, a) = \frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{2} - \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{2}$$

$$\boxed{\text{z104}} \quad \mathbb{Q}_3^{(c)}(A_{2u}, b) = \frac{\sqrt{2}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{2} - \frac{\sqrt{2}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{2}$$

$$\boxed{\text{z142}} \quad \mathbb{Q}_4^{(c)}(B_{1g}, a) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2} - \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2}$$

$$\boxed{\text{z143}} \quad \mathbb{Q}_4^{(c)}(B_{1g}, b) = \mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z144}} \quad \mathbb{Q}_4^{(c)}(B_{1g}, c) = -\frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2} + \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2}$$

$$\boxed{\text{z145}} \quad \mathbb{Q}_4^{(c)}(B_{1g}, d) = \mathbb{M}_3^{(a)}(B_{2g})\mathbb{M}_1^{(b)}(A_{2g})$$

$$\boxed{\text{z146}} \quad \mathbb{Q}_4^{(c)}(B_{1g}, e) = \frac{\sqrt{2}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{T}_{2,2}^{(b)}(E_{2g})}{2} - \frac{\sqrt{2}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{T}_{2,1}^{(b)}(E_{2g})}{2}$$

$$\boxed{\text{z147}} \quad \mathbb{G}_3^{(c)}(B_{1g}) = -\frac{\sqrt{2}\mathbb{M}_{1,1}^{(a)}(E_{1g})\mathbb{T}_{2,2}^{(b)}(E_{2g})}{2} + \frac{\sqrt{2}\mathbb{M}_{1,2}^{(a)}(E_{1g})\mathbb{T}_{2,1}^{(b)}(E_{2g})}{2}$$

$$\boxed{\text{z148}} \quad \mathbb{Q}_3^{(c)}(B_{1u}, a) = \mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_3^{(b)}(B_{1u})$$

$$\boxed{\text{z149}} \quad \mathbb{Q}_3^{(c)}(B_{1u}, b) = -\mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_3^{(b)}(B_{1u})$$

$$\boxed{\text{z150}} \quad \mathbb{Q}_3^{(c)}(B_{1u}, c) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{2} - \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{2}$$

$$\boxed{\text{z151}} \quad \mathbb{Q}_3^{(c)}(B_{1u}, d) = \mathbb{Q}_4^{(a)}(A_{1g})\mathbb{Q}_3^{(b)}(B_{1u})$$

$$\boxed{\text{z152}} \quad \mathbb{Q}_3^{(c)}(B_{1u}, e) = -\frac{\sqrt{406}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{29} - \frac{\sqrt{58}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{58} + \frac{\sqrt{406}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{29} + \frac{\sqrt{58}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{58}$$

$$\boxed{\text{z153}} \quad \mathbb{Q}_3^{(c)}(B_{1u}, f) = \mathbb{M}_1^{(a)}(A_{2g})\mathbb{T}_3^{(b)}(B_{2u})$$

$$\boxed{\text{z154}} \quad \mathbb{Q}_3^{(c)}(B_{1u}, g) = -\mathbb{M}_3^{(a)}(A_{2g})\mathbb{T}_3^{(b)}(B_{2u})$$

$$\boxed{\text{z155}} \quad \mathbb{Q}_3^{(c)}(B_{1u}, h) = -\frac{\sqrt{2}\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{2} + \frac{\sqrt{2}\mathbb{M}_{3,2}^{(a)}(E_{2g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{2}$$

$$\boxed{\text{z156}} \quad \mathbb{Q}_5^{(c)}(B_{1u}) = -\frac{\sqrt{58}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{58} + \frac{\sqrt{406}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{29} + \frac{\sqrt{58}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{58} - \frac{\sqrt{406}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{29}$$

$$\boxed{\text{z157}} \quad \mathbb{Q}_4^{(c)}(B_{2g}, a) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2} + \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2}$$

$$\boxed{\text{z158}} \quad \mathbb{Q}_4^{(c)}(B_{2g}, b) = \mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z159}} \quad \mathbb{Q}_4^{(c)}(B_{2g}, c) = -\frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2} - \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2}$$

$$\boxed{\text{z160}} \quad \mathbb{Q}_4^{(c)}(B_{2g}, d) = \mathbb{M}_3^{(a)}(B_{1g})\mathbb{M}_1^{(b)}(A_{2g})$$

$$\boxed{\text{z161}} \quad \mathbb{Q}_4^{(c)}(B_{2g}, e) = \frac{\sqrt{2}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{T}_{2,1}^{(b)}(E_{2g})}{2} + \frac{\sqrt{2}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{T}_{2,2}^{(b)}(E_{2g})}{2}$$

$$\boxed{\text{z162}} \quad \mathbb{G}_3^{(c)}(B_{2g}) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(a)}(E_{1g})\mathbb{T}_{2,1}^{(b)}(E_{2g})}{2} + \frac{\sqrt{2}\mathbb{M}_{1,2}^{(a)}(E_{1g})\mathbb{T}_{2,2}^{(b)}(E_{2g})}{2}$$

$$\boxed{\text{z163}} \quad \mathbb{Q}_3^{(c)}(B_{2u}, a) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{2} + \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{2}$$

$$\boxed{\text{z164}} \quad \mathbb{Q}_3^{(c)}(B_{2u}, b) = \frac{\sqrt{406}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{29} - \frac{\sqrt{58}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{58} + \frac{\sqrt{406}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{29} - \frac{\sqrt{58}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{58}$$

$$\begin{aligned}
\text{z165} \quad \mathbb{Q}_3^{(c)}(B_{2u}, c) &= -\frac{\sqrt{2}\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{2} - \frac{\sqrt{2}\mathbb{M}_{3,2}^{(a)}(E_{2g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{2} \\
\text{z268} \quad \mathbb{Q}_5^{(c)}(B_{2u}) &= \frac{\sqrt{58}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{58} + \frac{\sqrt{406}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{29} + \frac{\sqrt{58}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{58} + \frac{\sqrt{406}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{29} \\
\text{z269} \quad \mathbb{Q}_{2,1}^{(c)}(E_{1g}, a) &= \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_0^{(b)}(A_{1g})}{2} \\
\text{z270} \quad \mathbb{Q}_{2,2}^{(c)}(E_{1g}, a) &= \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_0^{(b)}(A_{1g})}{2} \\
\text{z271} \quad \mathbb{Q}_{2,1}^{(c)}(E_{1g}, b) &= -\frac{\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2} + \frac{\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2} \\
\text{z272} \quad \mathbb{Q}_{2,2}^{(c)}(E_{1g}, b) &= \frac{\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2} + \frac{\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2} \\
\text{z273} \quad \mathbb{Q}_{2,1}^{(c)}(E_{1g}, c) &= \frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{8} - \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{8} + \frac{\sqrt{14}\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{8} + \frac{\sqrt{14}\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{8} \\
\text{z274} \quad \mathbb{Q}_{2,2}^{(c)}(E_{1g}, c) &= -\frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{8} - \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{8} - \frac{\sqrt{14}\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{8} + \frac{\sqrt{14}\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{8} \\
\text{z275} \quad \mathbb{Q}_{2,1}^{(c)}(E_{1g}, d) &= \frac{\sqrt{2}\mathbb{M}_{1,2}^{(a)}(E_{1g})\mathbb{M}_1^{(b)}(A_{2g})}{2} \\
\text{z276} \quad \mathbb{Q}_{2,2}^{(c)}(E_{1g}, d) &= -\frac{\sqrt{2}\mathbb{M}_{1,1}^{(a)}(E_{1g})\mathbb{M}_1^{(b)}(A_{2g})}{2} \\
\text{z277} \quad \mathbb{Q}_{2,1}^{(c)}(E_{1g}, e) &= -\frac{\mathbb{M}_{1,1}^{(a)}(E_{1g})\mathbb{T}_{2,1}^{(b)}(E_{2g})}{2} + \frac{\mathbb{M}_{1,2}^{(a)}(E_{1g})\mathbb{T}_{2,2}^{(b)}(E_{2g})}{2} \\
\text{z278} \quad \mathbb{Q}_{2,2}^{(c)}(E_{1g}, e) &= \frac{\mathbb{M}_{1,1}^{(a)}(E_{1g})\mathbb{T}_{2,2}^{(b)}(E_{2g})}{2} + \frac{\mathbb{M}_{1,2}^{(a)}(E_{1g})\mathbb{T}_{2,1}^{(b)}(E_{2g})}{2} \\
\text{z279} \quad \mathbb{Q}_{2,1}^{(c)}(E_{1g}, f) &= \frac{\sqrt{2}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{M}_1^{(b)}(A_{2g})}{2} \\
\text{z280} \quad \mathbb{Q}_{2,2}^{(c)}(E_{1g}, f) &= -\frac{\sqrt{2}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{M}_1^{(b)}(A_{2g})}{2}
\end{aligned}$$

$$\begin{aligned}
\text{z281} \quad \mathbb{Q}_{2,1}^{(c)}(E_{1g}, g) &= \frac{\sqrt{6}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{T}_{2,1}^{(b)}(E_{2g})}{8} - \frac{\sqrt{6}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{T}_{2,2}^{(b)}(E_{2g})}{8} - \frac{\sqrt{10}\mathbb{M}_3^{(a)}(B_{1g})\mathbb{T}_{2,2}^{(b)}(E_{2g})}{8} + \frac{\sqrt{10}\mathbb{M}_3^{(a)}(B_{2g})\mathbb{T}_{2,1}^{(b)}(E_{2g})}{8} \\
\text{z282} \quad \mathbb{Q}_{2,2}^{(c)}(E_{1g}, g) &= -\frac{\sqrt{6}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{T}_{2,2}^{(b)}(E_{2g})}{8} - \frac{\sqrt{6}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{T}_{2,1}^{(b)}(E_{2g})}{8} + \frac{\sqrt{10}\mathbb{M}_3^{(a)}(B_{1g})\mathbb{T}_{2,1}^{(b)}(E_{2g})}{8} + \frac{\sqrt{10}\mathbb{M}_3^{(a)}(B_{2g})\mathbb{T}_{2,2}^{(b)}(E_{2g})}{8} \\
\text{z283} \quad \mathbb{Q}_{4,1}^{(c)}(E_{1g}, a) &= \frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_0^{(b)}(A_{1g})}{2} \\
\text{z284} \quad \mathbb{Q}_{4,2}^{(c)}(E_{1g}, a) &= \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_0^{(b)}(A_{1g})}{2} \\
\text{z285} \quad \mathbb{Q}_{4,1}^{(c)}(E_{1g}, b) &= -\frac{\sqrt{14}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{8} + \frac{\sqrt{14}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{8} + \frac{\sqrt{2}\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{8} + \frac{\sqrt{2}\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{8} \\
\text{z286} \quad \mathbb{Q}_{4,2}^{(c)}(E_{1g}, b) &= \frac{\sqrt{14}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{8} + \frac{\sqrt{14}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{8} - \frac{\sqrt{2}\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{8} + \frac{\sqrt{2}\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{8} \\
\text{z287} \quad \mathbb{Q}_{4,1}^{(c)}(E_{1g}, c) &= -\frac{\sqrt{10}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{T}_{2,1}^{(b)}(E_{2g})}{8} + \frac{\sqrt{10}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{T}_{2,2}^{(b)}(E_{2g})}{8} - \frac{\sqrt{6}\mathbb{M}_3^{(a)}(B_{1g})\mathbb{T}_{2,2}^{(b)}(E_{2g})}{8} + \frac{\sqrt{6}\mathbb{M}_3^{(a)}(B_{2g})\mathbb{T}_{2,1}^{(b)}(E_{2g})}{8} \\
\text{z288} \quad \mathbb{Q}_{4,2}^{(c)}(E_{1g}, c) &= \frac{\sqrt{10}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{T}_{2,2}^{(b)}(E_{2g})}{8} + \frac{\sqrt{10}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{T}_{2,1}^{(b)}(E_{2g})}{8} + \frac{\sqrt{6}\mathbb{M}_3^{(a)}(B_{1g})\mathbb{T}_{2,1}^{(b)}(E_{2g})}{8} + \frac{\sqrt{6}\mathbb{M}_3^{(a)}(B_{2g})\mathbb{T}_{2,2}^{(b)}(E_{2g})}{8} \\
\text{z289} \quad \mathbb{Q}_{6,1}^{(c)}(E_{1g}, 1) &= -\frac{\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2} + \frac{\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2} \\
\text{z290} \quad \mathbb{Q}_{6,2}^{(c)}(E_{1g}, 1) &= \frac{\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2} + \frac{\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2} \\
\text{z291} \quad \mathbb{G}_{5,1}^{(c)}(E_{1g}, 1) &= \frac{\mathbb{M}_3^{(a)}(B_{1g})\mathbb{T}_{2,2}^{(b)}(E_{2g})}{2} + \frac{\mathbb{M}_3^{(a)}(B_{2g})\mathbb{T}_{2,1}^{(b)}(E_{2g})}{2} \\
\text{z292} \quad \mathbb{G}_{5,2}^{(c)}(E_{1g}, 1) &= -\frac{\mathbb{M}_3^{(a)}(B_{1g})\mathbb{T}_{2,1}^{(b)}(E_{2g})}{2} + \frac{\mathbb{M}_3^{(a)}(B_{2g})\mathbb{T}_{2,2}^{(b)}(E_{2g})}{2} \\
\text{z293} \quad \mathbb{Q}_{1,1}^{(c)}(E_{1u}, a) &= \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{2} \\
\text{z380} \quad \mathbb{Q}_{1,2}^{(c)}(E_{1u}, a) &= \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{2}
\end{aligned}$$

$$\begin{aligned}
\boxed{\text{z381}} \quad \mathbb{Q}_{1,1}^{(c)}(E_{1u}, b) &= -\frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_3^{(b)}(B_{1u})}{2} \\
\boxed{\text{z382}} \quad \mathbb{Q}_{1,2}^{(c)}(E_{1u}, b) &= \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_3^{(b)}(B_{1u})}{2} \\
\boxed{\text{z383}} \quad \mathbb{Q}_{1,1}^{(c)}(E_{1u}, c) &= \frac{\sqrt{42}\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{14} - \frac{\sqrt{42}\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{14} - \frac{\sqrt{14}\mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{14} \\
\boxed{\text{z384}} \quad \mathbb{Q}_{1,2}^{(c)}(E_{1u}, c) &= -\frac{\sqrt{42}\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{14} - \frac{\sqrt{42}\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{14} - \frac{\sqrt{14}\mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{14} \\
\boxed{\text{z385}} \quad \mathbb{Q}_{1,1}^{(c)}(E_{1u}, d) &= \frac{\sqrt{406}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_3^{(b)}(B_{1u})}{29} + \frac{\sqrt{58}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_3^{(b)}(B_{1u})}{58} \\
\boxed{\text{z408}} \quad \mathbb{Q}_{1,2}^{(c)}(E_{1u}, d) &= -\frac{\sqrt{406}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_3^{(b)}(B_{1u})}{29} - \frac{\sqrt{58}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_3^{(b)}(B_{1u})}{58} \\
\boxed{\text{z409}} \quad \mathbb{Q}_{1,1}^{(c)}(E_{1u}, e) &= -\frac{\sqrt{2}\mathbb{M}_1^{(a)}(A_{2g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{2} \\
\boxed{\text{z410}} \quad \mathbb{Q}_{1,2}^{(c)}(E_{1u}, e) &= \frac{\sqrt{2}\mathbb{M}_1^{(a)}(A_{2g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{2} \\
\boxed{\text{z411}} \quad \mathbb{Q}_{1,1}^{(c)}(E_{1u}, f) &= \frac{\sqrt{2}\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{T}_3^{(b)}(B_{2u})}{2} \\
\boxed{\text{z412}} \quad \mathbb{Q}_{1,2}^{(c)}(E_{1u}, f) &= \frac{\sqrt{2}\mathbb{M}_{3,2}^{(a)}(E_{2g})\mathbb{T}_3^{(b)}(B_{2u})}{2} \\
\boxed{\text{z413}} \quad \mathbb{Q}_{3,1}^{(c)}(E_{1u}, a) &= \frac{\sqrt{7}\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{14} - \frac{\sqrt{7}\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{14} + \frac{\sqrt{21}\mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{7} \\
\boxed{\text{z439}} \quad \mathbb{Q}_{3,2}^{(c)}(E_{1u}, a) &= -\frac{\sqrt{7}\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{14} - \frac{\sqrt{7}\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{14} + \frac{\sqrt{21}\mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{7} \\
\boxed{\text{z440}} \quad \mathbb{Q}_{3,1}^{(c)}(E_{1u}, b) &= \frac{\sqrt{58}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_3^{(b)}(B_{1u})}{58} - \frac{\sqrt{406}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_3^{(b)}(B_{1u})}{29} \\
\boxed{\text{z441}} \quad \mathbb{Q}_{3,2}^{(c)}(E_{1u}, b) &= -\frac{\sqrt{58}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_3^{(b)}(B_{1u})}{58} + \frac{\sqrt{406}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_3^{(b)}(B_{1u})}{29}
\end{aligned}$$

$$\begin{aligned}
\boxed{\text{z442}} \quad \mathbb{Q}_{3,1}^{(c)}(E_{1u}, c) &= \frac{\sqrt{35}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{14} - \frac{\sqrt{35}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{14} - \frac{\sqrt{7}\mathbb{Q}_4^{(a)}(A_{1g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{7} \\
\boxed{\text{z443}} \quad \mathbb{Q}_{3,2}^{(c)}(E_{1u}, c) &= -\frac{\sqrt{35}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{14} - \frac{\sqrt{35}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{14} - \frac{\sqrt{7}\mathbb{Q}_4^{(a)}(A_{1g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{7} \\
\boxed{\text{z444}} \quad \mathbb{Q}_{3,1}^{(c)}(E_{1u}, d) &= -\frac{\sqrt{55}\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{22} + \frac{\sqrt{55}\mathbb{M}_{3,2}^{(a)}(E_{2g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{22} - \frac{\sqrt{33}\mathbb{M}_3^{(a)}(A_{2g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{11} \\
\boxed{\text{z445}} \quad \mathbb{Q}_{3,2}^{(c)}(E_{1u}, d) &= \frac{\sqrt{55}\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{22} + \frac{\sqrt{55}\mathbb{M}_{3,2}^{(a)}(E_{2g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{22} + \frac{\sqrt{33}\mathbb{M}_3^{(a)}(A_{2g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{11} \\
\boxed{\text{z446}} \quad \mathbb{Q}_{5,1}^{(c)}(E_{1u}, 1) &= \frac{\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{2} - \frac{\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{2} \\
\boxed{\text{z447}} \quad \mathbb{Q}_{5,2}^{(c)}(E_{1u}, 1) &= -\frac{\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{2} - \frac{\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{2} \\
\boxed{\text{z468}} \quad \mathbb{Q}_{5,1}^{(c)}(E_{1u}, 2) &= \frac{\sqrt{14}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{14} - \frac{\sqrt{14}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{14} + \frac{\sqrt{70}\mathbb{Q}_4^{(a)}(A_{1g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{14} \\
\boxed{\text{z469}} \quad \mathbb{Q}_{5,2}^{(c)}(E_{1u}, 2) &= -\frac{\sqrt{14}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{14} - \frac{\sqrt{14}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{14} + \frac{\sqrt{70}\mathbb{Q}_4^{(a)}(A_{1g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{14} \\
\boxed{\text{z470}} \quad \mathbb{G}_{2,1}^{(c)}(E_{1u}) &= \frac{\sqrt{66}\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{22} - \frac{\sqrt{66}\mathbb{M}_{3,2}^{(a)}(E_{2g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{22} - \frac{\sqrt{110}\mathbb{M}_3^{(a)}(A_{2g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{22} \\
\boxed{\text{z471}} \quad \mathbb{G}_{2,2}^{(c)}(E_{1u}) &= -\frac{\sqrt{66}\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{22} - \frac{\sqrt{66}\mathbb{M}_{3,2}^{(a)}(E_{2g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{22} + \frac{\sqrt{110}\mathbb{M}_3^{(a)}(A_{2g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{22} \\
\boxed{\text{z515}} \quad \mathbb{Q}_{2,1}^{(c)}(E_{2g}, a) &= \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2} \\
\boxed{\text{z516}} \quad \mathbb{Q}_{2,2}^{(c)}(E_{2g}, a) &= \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2} \\
\boxed{\text{z517}} \quad \mathbb{Q}_{2,1}^{(c)}(E_{2g}, b) &= \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_0^{(b)}(A_{1g})}{2} \\
\boxed{\text{z518}} \quad \mathbb{Q}_{2,2}^{(c)}(E_{2g}, b) &= \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_0^{(b)}(A_{1g})}{2}
\end{aligned}$$

$$\boxed{\text{z519}} \quad \mathbb{Q}_{2,1}^{(c)}(E_{2g}, c) = -\frac{\sqrt{2}\mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2}$$

$$\boxed{\text{z520}} \quad \mathbb{Q}_{2,2}^{(c)}(E_{2g}, c) = -\frac{\sqrt{2}\mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2}$$

$$\boxed{\text{z521}} \quad \mathbb{Q}_{2,1}^{(c)}(E_{2g}, d) = \frac{\sqrt{4970}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{142} - \frac{\sqrt{4970}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{142} + \frac{\sqrt{142}\mathbb{Q}_4^{(a)}(A_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{142}$$

$$\boxed{\text{z522}} \quad \mathbb{Q}_{2,2}^{(c)}(E_{2g}, d) = -\frac{\sqrt{4970}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{142} - \frac{\sqrt{4970}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{142} + \frac{\sqrt{142}\mathbb{Q}_4^{(a)}(A_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{142}$$

$$\boxed{\text{z523}} \quad \mathbb{Q}_{2,1}^{(c)}(E_{2g}, e) = \frac{\sqrt{2}\mathbb{M}_1^{(a)}(A_{2g})\mathbb{T}_{2,2}^{(b)}(E_{2g})}{2}$$

$$\boxed{\text{z524}} \quad \mathbb{Q}_{2,2}^{(c)}(E_{2g}, e) = -\frac{\sqrt{2}\mathbb{M}_1^{(a)}(A_{2g})\mathbb{T}_{2,1}^{(b)}(E_{2g})}{2}$$

$$\boxed{\text{z525}} \quad \mathbb{Q}_{2,1}^{(c)}(E_{2g}, f) = \frac{\sqrt{2}\mathbb{M}_{3,2}^{(a)}(E_{2g})\mathbb{M}_1^{(b)}(A_{2g})}{2}$$

$$\boxed{\text{z526}} \quad \mathbb{Q}_{2,2}^{(c)}(E_{2g}, f) = -\frac{\sqrt{2}\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{M}_1^{(b)}(A_{2g})}{2}$$

$$\boxed{\text{z527}} \quad \mathbb{Q}_{2,1}^{(c)}(E_{2g}, g) = -\frac{\sqrt{2}\mathbb{M}_3^{(a)}(A_{2g})\mathbb{T}_{2,2}^{(b)}(E_{2g})}{2}$$

$$\boxed{\text{z528}} \quad \mathbb{Q}_{2,2}^{(c)}(E_{2g}, g) = \frac{\sqrt{2}\mathbb{M}_3^{(a)}(A_{2g})\mathbb{T}_{2,1}^{(b)}(E_{2g})}{2}$$

$$\boxed{\text{z529}} \quad \mathbb{Q}_{4,1}^{(c)}(E_{2g}, 1a) = \frac{\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2} - \frac{\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2}$$

$$\boxed{\text{z530}} \quad \mathbb{Q}_{4,2}^{(c)}(E_{2g}, 1a) = -\frac{\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2} - \frac{\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2}$$

$$\boxed{\text{z531}} \quad \mathbb{Q}_{4,1}^{(c)}(E_{2g}, 1b) = \frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z532}} \quad \mathbb{Q}_{4,2}^{(c)}(E_{2g}, 1b) = \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$



$$\boxed{\text{z533}} \quad \mathbb{Q}_{4,1}^{(c)}(E_{2g}, 1c) = -\frac{\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2} + \frac{\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2}$$

$$\boxed{\text{z534}} \quad \mathbb{Q}_{4,2}^{(c)}(E_{2g}, 1c) = \frac{\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2} + \frac{\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2}$$

$$\boxed{\text{z535}} \quad \mathbb{Q}_{4,1}^{(c)}(E_{2g}, 1d) = -\frac{\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{T}_{2,1}^{(b)}(E_{2g})}{2} + \frac{\mathbb{M}_{3,2}^{(a)}(E_{2g})\mathbb{T}_{2,2}^{(b)}(E_{2g})}{2}$$

$$\boxed{\text{z536}} \quad \mathbb{Q}_{4,2}^{(c)}(E_{2g}, 1d) = \frac{\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{T}_{2,2}^{(b)}(E_{2g})}{2} + \frac{\mathbb{M}_{3,2}^{(a)}(E_{2g})\mathbb{T}_{2,1}^{(b)}(E_{2g})}{2}$$

$$\boxed{\text{z537}} \quad \mathbb{Q}_{4,1}^{(c)}(E_{2g}, 2a) = \frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z538}} \quad \mathbb{Q}_{4,2}^{(c)}(E_{2g}, 2a) = \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z539}} \quad \mathbb{Q}_{4,1}^{(c)}(E_{2g}, 2b) = \frac{\sqrt{71}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{142} - \frac{\sqrt{71}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{142} - \frac{\sqrt{2485}\mathbb{Q}_4^{(a)}(A_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{71}$$

$$\boxed{\text{z540}} \quad \mathbb{Q}_{4,2}^{(c)}(E_{2g}, 2b) = -\frac{\sqrt{71}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{142} - \frac{\sqrt{71}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{142} - \frac{\sqrt{2485}\mathbb{Q}_4^{(a)}(A_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{71}$$

$$\boxed{\text{z629}} \quad \mathbb{Q}_{3,1}^{(c)}(E_{2u}, a) = -\frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_3^{(b)}(B_{1u})}{2}$$

$$\boxed{\text{z630}} \quad \mathbb{Q}_{3,2}^{(c)}(E_{2u}, a) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_3^{(b)}(B_{1u})}{2}$$

$$\boxed{\text{z631}} \quad \mathbb{Q}_{3,1}^{(c)}(E_{2u}, b) = \frac{\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{2} - \frac{\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{2}$$

$$\boxed{\text{z632}} \quad \mathbb{Q}_{3,2}^{(c)}(E_{2u}, b) = -\frac{\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{2} - \frac{\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{2}$$

$$\boxed{\text{z633}} \quad \mathbb{Q}_{3,1}^{(c)}(E_{2u}, c) = \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_3^{(b)}(B_{1u})}{2}$$

$$\boxed{\text{z634}} \quad \mathbb{Q}_{3,2}^{(c)}(E_{2u}, c) = -\frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_3^{(b)}(B_{1u})}{2}$$

$$\begin{aligned}
\boxed{\text{z635}} \quad \mathbb{Q}_{3,1}^{(c)}(E_{2u}, d) &= -\frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{8} + \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{8} - \frac{\sqrt{14}\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{8} + \frac{\sqrt{14}\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{8} \\
\boxed{\text{z636}} \quad \mathbb{Q}_{3,2}^{(c)}(E_{2u}, d) &= \frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{8} + \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{8} + \frac{\sqrt{14}\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{8} + \frac{\sqrt{14}\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{8} \\
\boxed{\text{z637}} \quad \mathbb{Q}_{3,1}^{(c)}(E_{2u}, e) &= -\frac{\sqrt{2}\mathbb{M}_{1,1}^{(a)}(E_{1g})\mathbb{T}_3^{(b)}(B_{2u})}{2} \\
\boxed{\text{z638}} \quad \mathbb{Q}_{3,2}^{(c)}(E_{2u}, e) &= -\frac{\sqrt{2}\mathbb{M}_{1,2}^{(a)}(E_{1g})\mathbb{T}_3^{(b)}(B_{2u})}{2} \\
\boxed{\text{z639}} \quad \mathbb{Q}_{3,1}^{(c)}(E_{2u}, f) &= \frac{\sqrt{2}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{T}_3^{(b)}(B_{2u})}{2} \\
\boxed{\text{z640}} \quad \mathbb{Q}_{3,2}^{(c)}(E_{2u}, f) &= \frac{\sqrt{2}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{T}_3^{(b)}(B_{2u})}{2} \\
\boxed{\text{z641}} \quad \mathbb{Q}_{3,1}^{(c)}(E_{2u}, g) &= \frac{\sqrt{10}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{8} - \frac{\sqrt{10}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{8} + \frac{\sqrt{6}\mathbb{M}_3^{(a)}(B_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{8} + \frac{\sqrt{6}\mathbb{M}_3^{(a)}(B_{2g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{8} \\
\boxed{\text{z642}} \quad \mathbb{Q}_{3,2}^{(c)}(E_{2u}, g) &= -\frac{\sqrt{10}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{8} - \frac{\sqrt{10}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{8} - \frac{\sqrt{6}\mathbb{M}_3^{(a)}(B_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{8} + \frac{\sqrt{6}\mathbb{M}_3^{(a)}(B_{2g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{8} \\
\boxed{\text{z643}} \quad \mathbb{Q}_{5,1}^{(c)}(E_{2u}, 1) &= -\frac{\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{2} - \frac{\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{2} \\
\boxed{\text{z644}} \quad \mathbb{Q}_{5,2}^{(c)}(E_{2u}, 1) &= \frac{\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{2} - \frac{\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{2} \\
\boxed{\text{z645}} \quad \mathbb{Q}_{5,1}^{(c)}(E_{2u}, 2) &= \frac{\sqrt{14}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{8} - \frac{\sqrt{14}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{8} - \frac{\sqrt{2}\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{8} + \frac{\sqrt{2}\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{8} \\
\boxed{\text{z646}} \quad \mathbb{Q}_{5,2}^{(c)}(E_{2u}, 2) &= -\frac{\sqrt{14}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{8} - \frac{\sqrt{14}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{8} + \frac{\sqrt{2}\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{8} + \frac{\sqrt{2}\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{8} \\
\boxed{\text{z647}} \quad \mathbb{G}_{2,1}^{(c)}(E_{2u}, a) &= \frac{\mathbb{M}_{1,1}^{(a)}(E_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{2} - \frac{\mathbb{M}_{1,2}^{(a)}(E_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{2} \\
\boxed{\text{z648}} \quad \mathbb{G}_{2,2}^{(c)}(E_{2u}, a) &= -\frac{\mathbb{M}_{1,1}^{(a)}(E_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{2} - \frac{\mathbb{M}_{1,2}^{(a)}(E_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{2}
\end{aligned}$$

$$\boxed{\text{z649}} \quad \mathbb{G}_{2,1}^{(c)}(E_{2u}, b) = -\frac{\sqrt{6}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{8} + \frac{\sqrt{6}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{8} + \frac{\sqrt{10}\mathbb{M}_3^{(a)}(B_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{8} + \frac{\sqrt{10}\mathbb{M}_3^{(a)}(B_{2g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{8}$$

$$\boxed{\text{z650}} \quad \mathbb{G}_{2,2}^{(c)}(E_{2u}, b) = \frac{\sqrt{6}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{8} + \frac{\sqrt{6}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{8} - \frac{\sqrt{10}\mathbb{M}_3^{(a)}(B_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{8} + \frac{\sqrt{10}\mathbb{M}_3^{(a)}(B_{2g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{8}$$

$$\boxed{\text{z651}} \quad \mathbb{G}_{4,1}^{(c)}(E_{2u}, 1) = -\frac{\mathbb{M}_3^{(a)}(B_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{2} + \frac{\mathbb{M}_3^{(a)}(B_{2g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{2}$$

$$\boxed{\text{z652}} \quad \mathbb{G}_{4,2}^{(c)}(E_{2u}, 1) = \frac{\mathbb{M}_3^{(a)}(B_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{2} + \frac{\mathbb{M}_3^{(a)}(B_{2g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{2}$$

• **Sn;Mn\_001\_1** : 'Mn'-'Sn' bond-cluster

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

\* ket:  $|d_v\rangle$ ,  $|d_{xy}\rangle$ ,  $|d_{xz}\rangle$ ,  $|d_{yz}\rangle$ ,  $|d_u\rangle$

\* wyckoff: **12a@12j**

$$\boxed{\text{z19}} \quad \mathbb{Q}_0^{(c)}(A_{1g}, a) = \mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z20}} \quad \mathbb{Q}_0^{(c)}(A_{1g}, b) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2} + \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2}$$

$$\boxed{\text{z21}} \quad \mathbb{Q}_0^{(c)}(A_{1g}, c) = \frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{4,1}^{(b)}(E_{2g}, 1)}{2} + \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{4,2}^{(b)}(E_{2g}, 1)}{2}$$

$$\boxed{\text{z22}} \quad \mathbb{Q}_0^{(c)}(A_{1g}, d) = \mathbb{M}_1^{(a)}(A_{2g})\mathbb{M}_1^{(b)}(A_{2g})$$

$$\boxed{\text{z23}} \quad \mathbb{Q}_2^{(c)}(A_{1g}, a) = \mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z24}} \quad \mathbb{Q}_2^{(c)}(A_{1g}, b) = \frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2} + \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2}$$

$$\boxed{\text{z25}} \quad \mathbb{Q}_2^{(c)}(A_{1g}, c) = \mathbb{M}_3^{(a)}(A_{2g})\mathbb{M}_1^{(b)}(A_{2g})$$

$$\boxed{\text{z26}} \quad \mathbb{Q}_2^{(c)}(A_{1g}, d) = -\frac{\sqrt{2}\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{T}_{2,1}^{(b)}(E_{2g}, a)}{2} - \frac{\sqrt{2}\mathbb{M}_{3,2}^{(a)}(E_{2g})\mathbb{T}_{2,2}^{(b)}(E_{2g}, a)}{2}$$

$$\boxed{\text{z27}} \quad \mathbb{Q}_2^{(c)}(A_{1g}, e) = -\frac{\sqrt{2}\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{T}_{2,1}^{(b)}(E_{2g}, b)}{2} - \frac{\sqrt{2}\mathbb{M}_{3,2}^{(a)}(E_{2g})\mathbb{T}_{2,2}^{(b)}(E_{2g}, b)}{2}$$

$$\boxed{\text{z28}} \quad \mathbb{Q}_4^{(c)}(A_{1g}) = \mathbb{Q}_4^{(a)}(A_{1g})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z29}} \quad \mathbb{Q}_6^{(c)}(A_{1g}, 2a) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_{4,1}^{(b)}(E_{2g}, 1)}{2} + \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_{4,2}^{(b)}(E_{2g}, 1)}{2}$$

$$\boxed{\text{z30}} \quad \mathbb{Q}_6^{(c)}(A_{1g}, 2b) = \frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2} + \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2}$$

$$\boxed{\text{z31}} \quad \mathbb{Q}_6^{(c)}(A_{1g}, 2c) = -\frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{4,1}^{(b)}(E_{2g}, 1)}{2} - \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{4,2}^{(b)}(E_{2g}, 1)}{2}$$

$$\boxed{\text{z48}} \quad \mathbb{Q}_7^{(c)}(A_{1u}, a) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_{5,1}^{(b)}(E_{1u}, 1)}{2} + \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_{5,2}^{(b)}(E_{1u}, 1)}{2}$$

$$\boxed{\text{z49}} \quad \mathbb{Q}_7^{(c)}(A_{1u}, b) = \frac{\sqrt{2}\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_3^{(b)}(B_{1u})}{2} + \frac{\sqrt{2}\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_3^{(b)}(B_{2u})}{2}$$

$$\boxed{\text{z50}} \quad \mathbb{Q}_7^{(c)}(A_{1u}, c) = -\frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{5,1}^{(b)}(E_{1u}, 1)}{2} - \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{5,2}^{(b)}(E_{1u}, 1)}{2}$$

$$\boxed{\text{z51}} \quad \mathbb{G}_0^{(c)}(A_{1u}, a) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(a)}(E_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u}, a)}{2} + \frac{\sqrt{2}\mathbb{M}_{1,2}^{(a)}(E_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u}, a)}{2}$$

$$\boxed{\text{z52}} \quad \mathbb{G}_0^{(c)}(A_{1u}, b) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(a)}(E_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u}, b)}{2} + \frac{\sqrt{2}\mathbb{M}_{1,2}^{(a)}(E_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u}, b)}{2}$$

$$\boxed{\text{z53}} \quad \mathbb{G}_0^{(c)}(A_{1u}, c) = \frac{\sqrt{2}\mathbb{M}_3^{(a)}(B_{1g})\mathbb{T}_3^{(b)}(B_{1u})}{2} + \frac{\sqrt{2}\mathbb{M}_3^{(a)}(B_{2g})\mathbb{T}_3^{(b)}(B_{2u})}{2}$$

$$\boxed{\text{z54}} \quad \mathbb{G}_2^{(c)}(A_{1u}, a) = -\frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{2} - \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{2}$$

$$\boxed{\text{z55}} \quad \mathbb{G}_2^{(c)}(A_{1u}, b) = \frac{\sqrt{2}\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_3^{(b)}(B_{1u})}{2} - \frac{\sqrt{2}\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_3^{(b)}(B_{2u})}{2}$$

$$\boxed{\text{z56}} \quad \mathbb{G}_2^{(c)}(A_{1u}, c) = \frac{\sqrt{2}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u}, a)}{2} + \frac{\sqrt{2}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u}, a)}{2}$$

$$\boxed{\text{z57}} \quad \mathbb{G}_2^{(c)}(A_{1u}, d) = \frac{\sqrt{2}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u}, b)}{2} + \frac{\sqrt{2}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u}, b)}{2}$$

$$\begin{aligned}
\boxed{\text{z58}} \quad \mathbb{G}_4^{(c)}(A_{1u}) &= -\frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{2} - \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{2} \\
\boxed{\text{z59}} \quad \mathbb{G}_6^{(c)}(A_{1u}, 2) &= -\frac{\sqrt{2}\mathbb{M}_3^{(a)}(B_{1g})\mathbb{T}_3^{(b)}(B_{1u})}{2} + \frac{\sqrt{2}\mathbb{M}_3^{(a)}(B_{2g})\mathbb{T}_3^{(b)}(B_{2u})}{2} \\
\boxed{\text{z60}} \quad \mathbb{Q}_6^{(c)}(A_{2g}, a) &= \mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_6^{(b)}(A_{2g}) \\
\boxed{\text{z77}} \quad \mathbb{Q}_6^{(c)}(A_{2g}, b) &= -\mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_6^{(b)}(A_{2g}) \\
\boxed{\text{z78}} \quad \mathbb{Q}_6^{(c)}(A_{2g}, c) &= \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_{4,2}^{(b)}(E_{2g}, 1)}{2} - \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_{4,1}^{(b)}(E_{2g}, 1)}{2} \\
\boxed{\text{z79}} \quad \mathbb{Q}_6^{(c)}(A_{2g}, d) &= \mathbb{Q}_4^{(a)}(A_{1g})\mathbb{Q}_6^{(b)}(A_{2g}) \\
\boxed{\text{z80}} \quad \mathbb{Q}_6^{(c)}(A_{2g}, e) &= -\frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2} + \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2} \\
\boxed{\text{z81}} \quad \mathbb{Q}_6^{(c)}(A_{2g}, f) &= -\frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{4,2}^{(b)}(E_{2g}, 1)}{2} + \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{4,1}^{(b)}(E_{2g}, 1)}{2} \\
\boxed{\text{z82}} \quad \mathbb{G}_1^{(c)}(A_{2g}, a) &= -\frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2} + \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2} \\
\boxed{\text{z83}} \quad \mathbb{G}_1^{(c)}(A_{2g}, b) &= \frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{4,2}^{(b)}(E_{2g}, 1)}{2} - \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{4,1}^{(b)}(E_{2g}, 1)}{2} \\
\boxed{\text{z84}} \quad \mathbb{G}_1^{(c)}(A_{2g}, c) &= \mathbb{M}_1^{(a)}(A_{2g})\mathbb{T}_0^{(b)}(A_{1g}) \\
\boxed{\text{z85}} \quad \mathbb{G}_1^{(c)}(A_{2g}, d) &= -\frac{\sqrt{2}\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{T}_{2,2}^{(b)}(E_{2g}, a)}{2} + \frac{\sqrt{2}\mathbb{M}_{3,2}^{(a)}(E_{2g})\mathbb{T}_{2,1}^{(b)}(E_{2g}, a)}{2} \\
\boxed{\text{z86}} \quad \mathbb{G}_1^{(c)}(A_{2g}, e) &= -\frac{\sqrt{2}\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{T}_{2,2}^{(b)}(E_{2g}, b)}{2} + \frac{\sqrt{2}\mathbb{M}_{3,2}^{(a)}(E_{2g})\mathbb{T}_{2,1}^{(b)}(E_{2g}, b)}{2} \\
\boxed{\text{z87}} \quad \mathbb{G}_3^{(c)}(A_{2g}, a) &= -\frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2} + \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2} \\
\boxed{\text{z88}} \quad \mathbb{G}_3^{(c)}(A_{2g}, b) &= \mathbb{M}_3^{(a)}(A_{2g})\mathbb{T}_0^{(b)}(A_{1g})
\end{aligned}$$

$$\begin{aligned}
\text{z105} \quad \mathbb{Q}_1^{(c)}(A_{2u}, a) &= \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{2} - \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{2} \\
\text{z106} \quad \mathbb{Q}_1^{(c)}(A_{2u}, b) &= \frac{\sqrt{2}\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_3^{(b)}(B_{2u})}{2} + \frac{\sqrt{2}\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_3^{(b)}(B_{1u})}{2} \\
\text{z107} \quad \mathbb{Q}_1^{(c)}(A_{2u}, c) &= \frac{\sqrt{2}\mathbb{M}_{1,1}^{(a)}(E_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u}, a)}{2} - \frac{\sqrt{2}\mathbb{M}_{1,2}^{(a)}(E_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u}, a)}{2} \\
\text{z108} \quad \mathbb{Q}_1^{(c)}(A_{2u}, d) &= \frac{\sqrt{2}\mathbb{M}_{1,1}^{(a)}(E_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u}, b)}{2} - \frac{\sqrt{2}\mathbb{M}_{1,2}^{(a)}(E_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u}, b)}{2} \\
\text{z109} \quad \mathbb{Q}_1^{(c)}(A_{2u}, e) &= -\frac{\sqrt{2}\mathbb{M}_3^{(a)}(B_{1g})\mathbb{T}_3^{(b)}(B_{2u})}{2} + \frac{\sqrt{2}\mathbb{M}_3^{(a)}(B_{2g})\mathbb{T}_3^{(b)}(B_{1u})}{2} \\
\text{z110} \quad \mathbb{Q}_3^{(c)}(A_{2u}, a) &= \frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{2} - \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{2} \\
\text{z111} \quad \mathbb{Q}_3^{(c)}(A_{2u}, b) &= \frac{\sqrt{2}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u}, a)}{2} - \frac{\sqrt{2}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u}, a)}{2} \\
\text{z112} \quad \mathbb{Q}_3^{(c)}(A_{2u}, c) &= \frac{\sqrt{2}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u}, b)}{2} - \frac{\sqrt{2}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u}, b)}{2} \\
\text{z113} \quad \mathbb{Q}_7^{(c)}(A_{2u}, 2a) &= \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_{5,2}^{(b)}(E_{1u}, 1)}{2} - \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_{5,1}^{(b)}(E_{1u}, 1)}{2} \\
\text{z114} \quad \mathbb{Q}_7^{(c)}(A_{2u}, 2b) &= \frac{\sqrt{2}\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_3^{(b)}(B_{2u})}{2} - \frac{\sqrt{2}\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_3^{(b)}(B_{1u})}{2} \\
\text{z115} \quad \mathbb{Q}_7^{(c)}(A_{2u}, 2c) &= -\frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{5,2}^{(b)}(E_{1u}, 1)}{2} + \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{5,1}^{(b)}(E_{1u}, 1)}{2} \\
\text{z116} \quad \mathbb{G}_6^{(c)}(A_{2u}) &= \frac{\sqrt{2}\mathbb{M}_3^{(a)}(B_{1g})\mathbb{T}_3^{(b)}(B_{2u})}{2} + \frac{\sqrt{2}\mathbb{M}_3^{(a)}(B_{2g})\mathbb{T}_3^{(b)}(B_{1u})}{2} \\
\text{z166} \quad \mathbb{Q}_4^{(c)}(B_{1g}, a) &= \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2} - \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2} \\
\text{z167} \quad \mathbb{Q}_4^{(c)}(B_{1g}, b) &= \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_{4,2}^{(b)}(E_{2g}, 1)}{2} - \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_{4,1}^{(b)}(E_{2g}, 1)}{2}
\end{aligned}$$

$$\boxed{\text{z168}} \quad \mathbb{Q}_4^{(c)}(B_{1g}, c) = \mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z169}} \quad \mathbb{Q}_4^{(c)}(B_{1g}, d) = \mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_6^{(b)}(A_{2g})$$

$$\boxed{\text{z170}} \quad \mathbb{Q}_4^{(c)}(B_{1g}, e) = -\frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2} + \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2}$$

$$\boxed{\text{z171}} \quad \mathbb{Q}_4^{(c)}(B_{1g}, f) = -\frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{4,2}^{(b)}(E_{2g}, 1)}{2} + \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{4,1}^{(b)}(E_{2g}, 1)}{2}$$

$$\boxed{\text{z172}} \quad \mathbb{Q}_4^{(c)}(B_{1g}, g) = \mathbb{M}_3^{(a)}(B_{2g})\mathbb{M}_1^{(b)}(A_{2g})$$

$$\boxed{\text{z173}} \quad \mathbb{Q}_4^{(c)}(B_{1g}, h) = \frac{\sqrt{2}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{T}_{2,2}^{(b)}(E_{2g}, a)}{2} - \frac{\sqrt{2}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{T}_{2,1}^{(b)}(E_{2g}, a)}{2}$$

$$\boxed{\text{z174}} \quad \mathbb{Q}_4^{(c)}(B_{1g}, i) = \frac{\sqrt{2}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{T}_{2,2}^{(b)}(E_{2g}, b)}{2} - \frac{\sqrt{2}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{T}_{2,1}^{(b)}(E_{2g}, b)}{2}$$

$$\boxed{\text{z175}} \quad \mathbb{G}_3^{(c)}(B_{1g}, a) = -\frac{\sqrt{2}\mathbb{M}_{1,1}^{(a)}(E_{1g})\mathbb{T}_{2,2}^{(b)}(E_{2g}, a)}{2} + \frac{\sqrt{2}\mathbb{M}_{1,2}^{(a)}(E_{1g})\mathbb{T}_{2,1}^{(b)}(E_{2g}, a)}{2}$$

$$\boxed{\text{z176}} \quad \mathbb{G}_3^{(c)}(B_{1g}, b) = -\frac{\sqrt{2}\mathbb{M}_{1,1}^{(a)}(E_{1g})\mathbb{T}_{2,2}^{(b)}(E_{2g}, b)}{2} + \frac{\sqrt{2}\mathbb{M}_{1,2}^{(a)}(E_{1g})\mathbb{T}_{2,1}^{(b)}(E_{2g}, b)}{2}$$

$$\boxed{\text{z177}} \quad \mathbb{G}_3^{(c)}(B_{1g}, c) = \mathbb{M}_3^{(a)}(B_{1g})\mathbb{T}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z178}} \quad \mathbb{Q}_3^{(c)}(B_{1u}, a) = \mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_3^{(b)}(B_{1u})$$

$$\boxed{\text{z179}} \quad \mathbb{Q}_3^{(c)}(B_{1u}, b) = -\mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_3^{(b)}(B_{1u})$$

$$\boxed{\text{z180}} \quad \mathbb{Q}_3^{(c)}(B_{1u}, c) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{2} - \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{2}$$

$$\boxed{\text{z181}} \quad \mathbb{Q}_3^{(c)}(B_{1u}, d) = -\frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_{5,2}^{(b)}(E_{1u}, 1)}{2} + \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_{5,1}^{(b)}(E_{1u}, 1)}{2}$$

$$\boxed{\text{z182}} \quad \mathbb{Q}_3^{(c)}(B_{1u}, e) = \mathbb{Q}_4^{(a)}(A_{1g})\mathbb{Q}_3^{(b)}(B_{1u})$$

$$\begin{aligned}
\text{z183} \quad \mathbb{Q}_3^{(c)}(B_{1u}, f) &= -\frac{\sqrt{406}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{29} - \frac{\sqrt{58}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{58} + \frac{\sqrt{406}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{29} + \frac{\sqrt{58}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{58} \\
\text{z184} \quad \mathbb{Q}_3^{(c)}(B_{1u}, g) &= \frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{5,2}^{(b)}(E_{1u}, 1)}{2} - \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{5,1}^{(b)}(E_{1u}, 1)}{2} \\
\text{z185} \quad \mathbb{Q}_3^{(c)}(B_{1u}, h) &= \mathbb{M}_1^{(a)}(A_{2g})\mathbb{T}_3^{(b)}(B_{2u}) \\
\text{z186} \quad \mathbb{Q}_3^{(c)}(B_{1u}, i) &= -\mathbb{M}_3^{(a)}(A_{2g})\mathbb{T}_3^{(b)}(B_{2u}) \\
\text{z187} \quad \mathbb{Q}_3^{(c)}(B_{1u}, j) &= -\frac{\sqrt{2}\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{T}_{1,2}^{(b)}(E_{1u}, a)}{2} + \frac{\sqrt{2}\mathbb{M}_{3,2}^{(a)}(E_{2g})\mathbb{T}_{1,1}^{(b)}(E_{1u}, a)}{2} \\
\text{z188} \quad \mathbb{Q}_3^{(c)}(B_{1u}, k) &= -\frac{\sqrt{2}\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{T}_{1,2}^{(b)}(E_{1u}, b)}{2} + \frac{\sqrt{2}\mathbb{M}_{3,2}^{(a)}(E_{2g})\mathbb{T}_{1,1}^{(b)}(E_{1u}, b)}{2} \\
\text{z189} \quad \mathbb{Q}_5^{(c)}(B_{1u}) &= -\frac{\sqrt{58}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{58} + \frac{\sqrt{406}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{29} + \frac{\sqrt{58}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{58} - \frac{\sqrt{406}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{29} \\
\text{z190} \quad \mathbb{Q}_9^{(c)}(B_{1u}, 1) &= -\frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{5,2}^{(b)}(E_{1u}, 1)}{2} + \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{5,1}^{(b)}(E_{1u}, 1)}{2} \\
\text{z191} \quad \mathbb{Q}_4^{(c)}(B_{2g}, a) &= \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2} + \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2} \\
\text{z192} \quad \mathbb{Q}_4^{(c)}(B_{2g}, b) &= -\frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_{4,1}^{(b)}(E_{2g}, 1)}{2} - \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_{4,2}^{(b)}(E_{2g}, 1)}{2} \\
\text{z193} \quad \mathbb{Q}_4^{(c)}(B_{2g}, c) &= \mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_0^{(b)}(A_{1g}) \\
\text{z194} \quad \mathbb{Q}_4^{(c)}(B_{2g}, d) &= \mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_6^{(b)}(A_{2g}) \\
\text{z195} \quad \mathbb{Q}_4^{(c)}(B_{2g}, e) &= -\frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2} - \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2} \\
\text{z196} \quad \mathbb{Q}_4^{(c)}(B_{2g}, f) &= \frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{4,1}^{(b)}(E_{2g}, 1)}{2} + \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{4,2}^{(b)}(E_{2g}, 1)}{2} \\
\text{z197} \quad \mathbb{Q}_4^{(c)}(B_{2g}, g) &= \mathbb{M}_3^{(a)}(B_{1g})\mathbb{M}_1^{(b)}(A_{2g})
\end{aligned}$$



$$\begin{aligned}
\boxed{\text{z198}} \quad \mathbb{Q}_4^{(c)}(B_{2g}, h) &= \frac{\sqrt{2}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{T}_{2,1}^{(b)}(E_{2g}, a)}{2} + \frac{\sqrt{2}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{T}_{2,2}^{(b)}(E_{2g}, a)}{2} \\
\boxed{\text{z199}} \quad \mathbb{Q}_4^{(c)}(B_{2g}, i) &= \frac{\sqrt{2}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{T}_{2,1}^{(b)}(E_{2g}, b)}{2} + \frac{\sqrt{2}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{T}_{2,2}^{(b)}(E_{2g}, b)}{2} \\
\boxed{\text{z200}} \quad \mathbb{G}_3^{(c)}(B_{2g}, a) &= \frac{\sqrt{2}\mathbb{M}_{1,1}^{(a)}(E_{1g})\mathbb{T}_{2,1}^{(b)}(E_{2g}, a)}{2} + \frac{\sqrt{2}\mathbb{M}_{1,2}^{(a)}(E_{1g})\mathbb{T}_{2,2}^{(b)}(E_{2g}, a)}{2} \\
\boxed{\text{z201}} \quad \mathbb{G}_3^{(c)}(B_{2g}, b) &= \frac{\sqrt{2}\mathbb{M}_{1,1}^{(a)}(E_{1g})\mathbb{T}_{2,1}^{(b)}(E_{2g}, b)}{2} + \frac{\sqrt{2}\mathbb{M}_{1,2}^{(a)}(E_{1g})\mathbb{T}_{2,2}^{(b)}(E_{2g}, b)}{2} \\
\boxed{\text{z202}} \quad \mathbb{G}_3^{(c)}(B_{2g}, c) &= \mathbb{M}_3^{(a)}(B_{2g})\mathbb{T}_0^{(b)}(A_{1g}) \\
\boxed{\text{z203}} \quad \mathbb{Q}_3^{(c)}(B_{2u}, a) &= \mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_3^{(b)}(B_{2u}) \\
\boxed{\text{z204}} \quad \mathbb{Q}_3^{(c)}(B_{2u}, b) &= -\mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_3^{(b)}(B_{2u}) \\
\boxed{\text{z205}} \quad \mathbb{Q}_3^{(c)}(B_{2u}, c) &= \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{2} + \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{2} \\
\boxed{\text{z206}} \quad \mathbb{Q}_3^{(c)}(B_{2u}, d) &= \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_{5,1}^{(b)}(E_{1u}, 1)}{2} + \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_{5,2}^{(b)}(E_{1u}, 1)}{2} \\
\boxed{\text{z207}} \quad \mathbb{Q}_3^{(c)}(B_{2u}, e) &= \mathbb{Q}_4^{(a)}(A_{1g})\mathbb{Q}_3^{(b)}(B_{2u}) \\
\boxed{\text{z208}} \quad \mathbb{Q}_3^{(c)}(B_{2u}, f) &= \frac{\sqrt{406}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{29} - \frac{\sqrt{58}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{58} + \frac{\sqrt{406}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{29} - \frac{\sqrt{58}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{58} \\
\boxed{\text{z209}} \quad \mathbb{Q}_3^{(c)}(B_{2u}, g) &= -\frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{5,1}^{(b)}(E_{1u}, 1)}{2} - \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{5,2}^{(b)}(E_{1u}, 1)}{2} \\
\boxed{\text{z210}} \quad \mathbb{Q}_3^{(c)}(B_{2u}, h) &= -\mathbb{M}_1^{(a)}(A_{2g})\mathbb{T}_3^{(b)}(B_{1u}) \\
\boxed{\text{z211}} \quad \mathbb{Q}_3^{(c)}(B_{2u}, i) &= \mathbb{M}_3^{(a)}(A_{2g})\mathbb{T}_3^{(b)}(B_{1u}) \\
\boxed{\text{z212}} \quad \mathbb{Q}_3^{(c)}(B_{2u}, j) &= -\frac{\sqrt{2}\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{T}_{1,1}^{(b)}(E_{1u}, a)}{2} - \frac{\sqrt{2}\mathbb{M}_{3,2}^{(a)}(E_{2g})\mathbb{T}_{1,2}^{(b)}(E_{1u}, a)}{2}
\end{aligned}$$

$$\begin{aligned}
\text{z213} \quad \mathbb{Q}_3^{(c)}(B_{2u}, k) &= -\frac{\sqrt{2}\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{T}_{1,1}^{(b)}(E_{1u}, b)}{2} - \frac{\sqrt{2}\mathbb{M}_{3,2}^{(a)}(E_{2g})\mathbb{T}_{1,2}^{(b)}(E_{1u}, b)}{2} \\
\text{z294} \quad \mathbb{Q}_5^{(c)}(B_{2u}) &= \frac{\sqrt{58}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{58} + \frac{\sqrt{406}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{29} + \frac{\sqrt{58}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{58} + \frac{\sqrt{406}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{29} \\
\text{z295} \quad \mathbb{Q}_9^{(c)}(B_{2u}, 1) &= \frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{5,1}^{(b)}(E_{1u}, 1)}{2} + \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{5,2}^{(b)}(E_{1u}, 1)}{2} \\
\text{z296} \quad \mathbb{Q}_{2,1}^{(c)}(E_{1g}, a) &= \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_0^{(b)}(A_{1g})}{2} \\
\text{z297} \quad \mathbb{Q}_{2,2}^{(c)}(E_{1g}, a) &= \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_0^{(b)}(A_{1g})}{2} \\
\text{z298} \quad \mathbb{Q}_{2,1}^{(c)}(E_{1g}, b) &= -\frac{\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2} + \frac{\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2} \\
\text{z299} \quad \mathbb{Q}_{2,2}^{(c)}(E_{1g}, b) &= \frac{\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2} + \frac{\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2} \\
\text{z300} \quad \mathbb{Q}_{2,1}^{(c)}(E_{1g}, c) &= \frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{8} - \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{8} + \frac{\sqrt{14}\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{8} + \frac{\sqrt{14}\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{8} \\
\text{z301} \quad \mathbb{Q}_{2,2}^{(c)}(E_{1g}, c) &= -\frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{8} - \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{8} - \frac{\sqrt{14}\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{8} + \frac{\sqrt{14}\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{8} \\
\text{z302} \quad \mathbb{Q}_{2,1}^{(c)}(E_{1g}, d) &= \frac{\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{4,2}^{(b)}(E_{2g}, 1)}{2} - \frac{\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{4,1}^{(b)}(E_{2g}, 1)}{2} \\
\text{z303} \quad \mathbb{Q}_{2,2}^{(c)}(E_{1g}, d) &= -\frac{\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{4,1}^{(b)}(E_{2g}, 1)}{2} - \frac{\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{4,2}^{(b)}(E_{2g}, 1)}{2} \\
\text{z304} \quad \mathbb{Q}_{2,1}^{(c)}(E_{1g}, e) &= \frac{\sqrt{2}\mathbb{M}_{1,2}^{(a)}(E_{1g})\mathbb{M}_1^{(b)}(A_{2g})}{2} \\
\text{z305} \quad \mathbb{Q}_{2,2}^{(c)}(E_{1g}, e) &= -\frac{\sqrt{2}\mathbb{M}_{1,1}^{(a)}(E_{1g})\mathbb{M}_1^{(b)}(A_{2g})}{2} \\
\text{z306} \quad \mathbb{Q}_{2,1}^{(c)}(E_{1g}, f) &= -\frac{\mathbb{M}_{1,1}^{(a)}(E_{1g})\mathbb{T}_{2,1}^{(b)}(E_{2g}, a)}{2} + \frac{\mathbb{M}_{1,2}^{(a)}(E_{1g})\mathbb{T}_{2,2}^{(b)}(E_{2g}, a)}{2}
\end{aligned}$$

$$\begin{aligned}
\text{z307} \quad \mathbb{Q}_{2,2}^{(c)}(E_{1g}, f) &= \frac{\mathbb{M}_{1,1}^{(a)}(E_{1g})\mathbb{T}_{2,2}^{(b)}(E_{2g}, a)}{2} + \frac{\mathbb{M}_{1,2}^{(a)}(E_{1g})\mathbb{T}_{2,1}^{(b)}(E_{2g}, a)}{2} \\
\text{z308} \quad \mathbb{Q}_{2,1}^{(c)}(E_{1g}, g) &= -\frac{\mathbb{M}_{1,1}^{(a)}(E_{1g})\mathbb{T}_{2,1}^{(b)}(E_{2g}, b)}{2} + \frac{\mathbb{M}_{1,2}^{(a)}(E_{1g})\mathbb{T}_{2,2}^{(b)}(E_{2g}, b)}{2} \\
\text{z309} \quad \mathbb{Q}_{2,2}^{(c)}(E_{1g}, g) &= \frac{\mathbb{M}_{1,1}^{(a)}(E_{1g})\mathbb{T}_{2,2}^{(b)}(E_{2g}, b)}{2} + \frac{\mathbb{M}_{1,2}^{(a)}(E_{1g})\mathbb{T}_{2,1}^{(b)}(E_{2g}, b)}{2} \\
\text{z310} \quad \mathbb{Q}_{2,1}^{(c)}(E_{1g}, h) &= \frac{\sqrt{2}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{M}_1^{(b)}(A_{2g})}{2} \\
\text{z311} \quad \mathbb{Q}_{2,2}^{(c)}(E_{1g}, h) &= -\frac{\sqrt{2}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{M}_1^{(b)}(A_{2g})}{2} \\
\text{z312} \quad \mathbb{Q}_{2,1}^{(c)}(E_{1g}, i) &= \frac{\sqrt{6}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{T}_{2,1}^{(b)}(E_{2g}, a)}{8} - \frac{\sqrt{6}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{T}_{2,2}^{(b)}(E_{2g}, a)}{8} - \frac{\sqrt{10}\mathbb{M}_3^{(a)}(B_{1g})\mathbb{T}_{2,2}^{(b)}(E_{2g}, a)}{8} + \frac{\sqrt{10}\mathbb{M}_3^{(a)}(B_{2g})\mathbb{T}_{2,1}^{(b)}(E_{2g}, a)}{8} \\
\text{z313} \quad \mathbb{Q}_{2,2}^{(c)}(E_{1g}, i) &= -\frac{\sqrt{6}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{T}_{2,2}^{(b)}(E_{2g}, a)}{8} - \frac{\sqrt{6}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{T}_{2,1}^{(b)}(E_{2g}, a)}{8} + \frac{\sqrt{10}\mathbb{M}_3^{(a)}(B_{1g})\mathbb{T}_{2,1}^{(b)}(E_{2g}, a)}{8} + \frac{\sqrt{10}\mathbb{M}_3^{(a)}(B_{2g})\mathbb{T}_{2,2}^{(b)}(E_{2g}, a)}{8} \\
\text{z314} \quad \mathbb{Q}_{2,1}^{(c)}(E_{1g}, j) &= \frac{\sqrt{6}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{T}_{2,1}^{(b)}(E_{2g}, b)}{8} - \frac{\sqrt{6}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{T}_{2,2}^{(b)}(E_{2g}, b)}{8} - \frac{\sqrt{10}\mathbb{M}_3^{(a)}(B_{1g})\mathbb{T}_{2,2}^{(b)}(E_{2g}, b)}{8} + \frac{\sqrt{10}\mathbb{M}_3^{(a)}(B_{2g})\mathbb{T}_{2,1}^{(b)}(E_{2g}, b)}{8} \\
\text{z315} \quad \mathbb{Q}_{2,2}^{(c)}(E_{1g}, j) &= -\frac{\sqrt{6}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{T}_{2,2}^{(b)}(E_{2g}, b)}{8} - \frac{\sqrt{6}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{T}_{2,1}^{(b)}(E_{2g}, b)}{8} + \frac{\sqrt{10}\mathbb{M}_3^{(a)}(B_{1g})\mathbb{T}_{2,1}^{(b)}(E_{2g}, b)}{8} + \frac{\sqrt{10}\mathbb{M}_3^{(a)}(B_{2g})\mathbb{T}_{2,2}^{(b)}(E_{2g}, b)}{8} \\
\text{z316} \quad \mathbb{Q}_{4,1}^{(c)}(E_{1g}, a) &= \frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_0^{(b)}(A_{1g})}{2} \\
\text{z317} \quad \mathbb{Q}_{4,2}^{(c)}(E_{1g}, a) &= \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_0^{(b)}(A_{1g})}{2} \\
\text{z318} \quad \mathbb{Q}_{4,1}^{(c)}(E_{1g}, b) &= -\frac{\sqrt{14}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{8} + \frac{\sqrt{14}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{8} + \frac{\sqrt{2}\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{8} + \frac{\sqrt{2}\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{8} \\
\text{z319} \quad \mathbb{Q}_{4,2}^{(c)}(E_{1g}, b) &= \frac{\sqrt{14}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{8} + \frac{\sqrt{14}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{8} - \frac{\sqrt{2}\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{8} + \frac{\sqrt{2}\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{8} \\
\text{z320} \quad \mathbb{Q}_{4,1}^{(c)}(E_{1g}, c) &= -\frac{\sqrt{10}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{T}_{2,1}^{(b)}(E_{2g}, a)}{8} + \frac{\sqrt{10}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{T}_{2,2}^{(b)}(E_{2g}, a)}{8} - \frac{\sqrt{6}\mathbb{M}_3^{(a)}(B_{1g})\mathbb{T}_{2,2}^{(b)}(E_{2g}, a)}{8} + \frac{\sqrt{6}\mathbb{M}_3^{(a)}(B_{2g})\mathbb{T}_{2,1}^{(b)}(E_{2g}, a)}{8}
\end{aligned}$$

$$\begin{aligned}
\text{z321} \quad \mathbb{Q}_{4,2}^{(c)}(E_{1g}, c) &= \frac{\sqrt{10}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{T}_{2,2}^{(b)}(E_{2g}, a)}{8} + \frac{\sqrt{10}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{T}_{2,1}^{(b)}(E_{2g}, a)}{8} + \frac{\sqrt{6}\mathbb{M}_3^{(a)}(B_{1g})\mathbb{T}_{2,1}^{(b)}(E_{2g}, a)}{8} + \frac{\sqrt{6}\mathbb{M}_3^{(a)}(B_{2g})\mathbb{T}_{2,2}^{(b)}(E_{2g}, a)}{8} \\
\text{z322} \quad \mathbb{Q}_{4,1}^{(c)}(E_{1g}, d) &= -\frac{\sqrt{10}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{T}_{2,1}^{(b)}(E_{2g}, b)}{8} + \frac{\sqrt{10}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{T}_{2,2}^{(b)}(E_{2g}, b)}{8} - \frac{\sqrt{6}\mathbb{M}_3^{(a)}(B_{1g})\mathbb{T}_{2,2}^{(b)}(E_{2g}, b)}{8} + \frac{\sqrt{6}\mathbb{M}_3^{(a)}(B_{2g})\mathbb{T}_{2,1}^{(b)}(E_{2g}, b)}{8} \\
\text{z323} \quad \mathbb{Q}_{4,2}^{(c)}(E_{1g}, d) &= \frac{\sqrt{10}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{T}_{2,2}^{(b)}(E_{2g}, b)}{8} + \frac{\sqrt{10}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{T}_{2,1}^{(b)}(E_{2g}, b)}{8} + \frac{\sqrt{6}\mathbb{M}_3^{(a)}(B_{1g})\mathbb{T}_{2,1}^{(b)}(E_{2g}, b)}{8} + \frac{\sqrt{6}\mathbb{M}_3^{(a)}(B_{2g})\mathbb{T}_{2,2}^{(b)}(E_{2g}, b)}{8} \\
\text{z324} \quad \mathbb{Q}_{6,1}^{(c)}(E_{1g}, 1a) &= -\frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_6^{(b)}(A_{2g})}{2} \\
\text{z325} \quad \mathbb{Q}_{6,2}^{(c)}(E_{1g}, 1a) &= \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_6^{(b)}(A_{2g})}{2} \\
\text{z326} \quad \mathbb{Q}_{6,1}^{(c)}(E_{1g}, 1b) &= \frac{\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_{4,1}^{(b)}(E_{2g}, 1)}{2} - \frac{\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_{4,2}^{(b)}(E_{2g}, 1)}{2} \\
\text{z327} \quad \mathbb{Q}_{6,2}^{(c)}(E_{1g}, 1b) &= -\frac{\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_{4,2}^{(b)}(E_{2g}, 1)}{2} - \frac{\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_{4,1}^{(b)}(E_{2g}, 1)}{2} \\
\text{z328} \quad \mathbb{Q}_{6,1}^{(c)}(E_{1g}, 1c) &= \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_6^{(b)}(A_{2g})}{2} \\
\text{z329} \quad \mathbb{Q}_{6,2}^{(c)}(E_{1g}, 1c) &= -\frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_6^{(b)}(A_{2g})}{2} \\
\text{z330} \quad \mathbb{Q}_{6,1}^{(c)}(E_{1g}, 1d) &= -\frac{\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2} + \frac{\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2} \\
\text{z331} \quad \mathbb{Q}_{6,2}^{(c)}(E_{1g}, 1d) &= \frac{\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2} + \frac{\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2} \\
\text{z332} \quad \mathbb{Q}_{6,1}^{(c)}(E_{1g}, 1e) &= -\frac{\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{4,1}^{(b)}(E_{2g}, 1)}{2} + \frac{\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{4,2}^{(b)}(E_{2g}, 1)}{2} \\
\text{z333} \quad \mathbb{Q}_{6,2}^{(c)}(E_{1g}, 1e) &= \frac{\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{4,2}^{(b)}(E_{2g}, 1)}{2} + \frac{\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{4,1}^{(b)}(E_{2g}, 1)}{2} \\
\text{z334} \quad \mathbb{Q}_{8,1}^{(c)}(E_{1g}, 1) &= \frac{\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{4,2}^{(b)}(E_{2g}, 1)}{2} + \frac{\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{4,1}^{(b)}(E_{2g}, 1)}{2}
\end{aligned}$$

$$\boxed{\text{z335}} \quad \mathbb{Q}_{8,2}^{(c)}(E_{1g}, 1) = -\frac{\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{4,1}^{(b)}(E_{2g}, 1)}{2} + \frac{\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{4,2}^{(b)}(E_{2g}, 1)}{2}$$

$$\boxed{\text{z336}} \quad \mathbb{G}_{1,1}^{(c)}(E_{1g}) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(a)}(E_{1g})\mathbb{T}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z337}} \quad \mathbb{G}_{1,2}^{(c)}(E_{1g}) = \frac{\sqrt{2}\mathbb{M}_{1,2}^{(a)}(E_{1g})\mathbb{T}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z338}} \quad \mathbb{G}_{3,1}^{(c)}(E_{1g}) = \frac{\sqrt{2}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{T}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z339}} \quad \mathbb{G}_{3,2}^{(c)}(E_{1g}) = \frac{\sqrt{2}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{T}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z340}} \quad \mathbb{G}_{5,1}^{(c)}(E_{1g}, 1a) = \frac{\mathbb{M}_3^{(a)}(B_{1g})\mathbb{T}_{2,2}^{(b)}(E_{2g}, a)}{2} + \frac{\mathbb{M}_3^{(a)}(B_{2g})\mathbb{T}_{2,1}^{(b)}(E_{2g}, a)}{2}$$

$$\boxed{\text{z341}} \quad \mathbb{G}_{5,2}^{(c)}(E_{1g}, 1a) = -\frac{\mathbb{M}_3^{(a)}(B_{1g})\mathbb{T}_{2,1}^{(b)}(E_{2g}, a)}{2} + \frac{\mathbb{M}_3^{(a)}(B_{2g})\mathbb{T}_{2,2}^{(b)}(E_{2g}, a)}{2}$$

$$\boxed{\text{z342}} \quad \mathbb{G}_{5,1}^{(c)}(E_{1g}, 1b) = \frac{\mathbb{M}_3^{(a)}(B_{1g})\mathbb{T}_{2,2}^{(b)}(E_{2g}, b)}{2} + \frac{\mathbb{M}_3^{(a)}(B_{2g})\mathbb{T}_{2,1}^{(b)}(E_{2g}, b)}{2}$$

$$\boxed{\text{z343}} \quad \mathbb{G}_{5,2}^{(c)}(E_{1g}, 1b) = -\frac{\mathbb{M}_3^{(a)}(B_{1g})\mathbb{T}_{2,1}^{(b)}(E_{2g}, b)}{2} + \frac{\mathbb{M}_3^{(a)}(B_{2g})\mathbb{T}_{2,2}^{(b)}(E_{2g}, b)}{2}$$

$$\boxed{\text{z344}} \quad \mathbb{Q}_{1,1}^{(c)}(E_{1u}, a) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{2}$$

$$\boxed{\text{z345}} \quad \mathbb{Q}_{1,2}^{(c)}(E_{1u}, a) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{2}$$

$$\boxed{\text{z386}} \quad \mathbb{Q}_{1,1}^{(c)}(E_{1u}, b) = \frac{\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_3^{(b)}(B_{2u})}{2} - \frac{\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_3^{(b)}(B_{1u})}{2}$$

$$\boxed{\text{z387}} \quad \mathbb{Q}_{1,2}^{(c)}(E_{1u}, b) = \frac{\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_3^{(b)}(B_{1u})}{2} + \frac{\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_3^{(b)}(B_{2u})}{2}$$

$$\boxed{\text{z388}} \quad \mathbb{Q}_{1,1}^{(c)}(E_{1u}, c) = \frac{\sqrt{42}\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{14} - \frac{\sqrt{42}\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{14} - \frac{\sqrt{14}\mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{14}$$

$$\begin{aligned}
\text{z389} \quad \mathbb{Q}_{1,2}^{(c)}(E_{1u}, c) &= -\frac{\sqrt{42}\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{14} - \frac{\sqrt{42}\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{14} - \frac{\sqrt{14}\mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{14} \\
\text{z390} \quad \mathbb{Q}_{1,1}^{(c)}(E_{1u}, d) &= \frac{\sqrt{203}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_3^{(b)}(B_{2u})}{29} - \frac{\sqrt{29}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_3^{(b)}(B_{2u})}{58} + \frac{\sqrt{203}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_3^{(b)}(B_{1u})}{29} + \frac{\sqrt{29}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_3^{(b)}(B_{1u})}{58} \\
\text{z391} \quad \mathbb{Q}_{1,2}^{(c)}(E_{1u}, d) &= -\frac{\sqrt{203}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_3^{(b)}(B_{1u})}{29} - \frac{\sqrt{29}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_3^{(b)}(B_{1u})}{58} + \frac{\sqrt{203}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_3^{(b)}(B_{2u})}{29} - \frac{\sqrt{29}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_3^{(b)}(B_{2u})}{58} \\
\text{z392} \quad \mathbb{Q}_{1,1}^{(c)}(E_{1u}, e) &= \frac{\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{5,1}^{(b)}(E_{1u}, 1)}{2} - \frac{\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{5,2}^{(b)}(E_{1u}, 1)}{2} \\
\text{z393} \quad \mathbb{Q}_{1,2}^{(c)}(E_{1u}, e) &= -\frac{\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{5,2}^{(b)}(E_{1u}, 1)}{2} - \frac{\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{5,1}^{(b)}(E_{1u}, 1)}{2} \\
\text{z394} \quad \mathbb{Q}_{1,1}^{(c)}(E_{1u}, f) &= -\frac{\sqrt{2}\mathbb{M}_1^{(a)}(A_{2g})\mathbb{T}_{1,2}^{(b)}(E_{1u}, a)}{2} \\
\text{z395} \quad \mathbb{Q}_{1,2}^{(c)}(E_{1u}, f) &= \frac{\sqrt{2}\mathbb{M}_1^{(a)}(A_{2g})\mathbb{T}_{1,1}^{(b)}(E_{1u}, a)}{2} \\
\text{z396} \quad \mathbb{Q}_{1,1}^{(c)}(E_{1u}, g) &= -\frac{\sqrt{2}\mathbb{M}_1^{(a)}(A_{2g})\mathbb{T}_{1,2}^{(b)}(E_{1u}, b)}{2} \\
\text{z397} \quad \mathbb{Q}_{1,2}^{(c)}(E_{1u}, g) &= \frac{\sqrt{2}\mathbb{M}_1^{(a)}(A_{2g})\mathbb{T}_{1,1}^{(b)}(E_{1u}, b)}{2} \\
\text{z414} \quad \mathbb{Q}_{1,1}^{(c)}(E_{1u}, h) &= \frac{\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{T}_3^{(b)}(B_{2u})}{2} - \frac{\mathbb{M}_{3,2}^{(a)}(E_{2g})\mathbb{T}_3^{(b)}(B_{1u})}{2} \\
\text{z415} \quad \mathbb{Q}_{1,2}^{(c)}(E_{1u}, h) &= \frac{\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{T}_3^{(b)}(B_{1u})}{2} + \frac{\mathbb{M}_{3,2}^{(a)}(E_{2g})\mathbb{T}_3^{(b)}(B_{2u})}{2} \\
\text{z416} \quad \mathbb{Q}_{3,1}^{(c)}(E_{1u}, a) &= \frac{\sqrt{7}\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{14} - \frac{\sqrt{7}\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{14} + \frac{\sqrt{21}\mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{7} \\
\text{z417} \quad \mathbb{Q}_{3,2}^{(c)}(E_{1u}, a) &= -\frac{\sqrt{7}\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{14} - \frac{\sqrt{7}\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{14} + \frac{\sqrt{21}\mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{7} \\
\text{z418} \quad \mathbb{Q}_{3,1}^{(c)}(E_{1u}, b) &= \frac{\sqrt{29}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_3^{(b)}(B_{2u})}{58} + \frac{\sqrt{203}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_3^{(b)}(B_{2u})}{29} + \frac{\sqrt{29}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_3^{(b)}(B_{1u})}{58} - \frac{\sqrt{203}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_3^{(b)}(B_{1u})}{29}
\end{aligned}$$

$$\begin{aligned}
\text{z419} \quad \mathbb{Q}_{3,2}^{(c)}(E_{1u}, b) &= -\frac{\sqrt{29}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_3^{(b)}(B_{1u})}{58} + \frac{\sqrt{203}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_3^{(b)}(B_{1u})}{29} + \frac{\sqrt{29}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_3^{(b)}(B_{2u})}{58} + \frac{\sqrt{203}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_3^{(b)}(B_{2u})}{29} \\
\text{z420} \quad \mathbb{Q}_{3,1}^{(c)}(E_{1u}, c) &= \frac{\sqrt{35}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{14} - \frac{\sqrt{35}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{14} - \frac{\sqrt{7}\mathbb{Q}_4^{(a)}(A_{1g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{7} \\
\text{z421} \quad \mathbb{Q}_{3,2}^{(c)}(E_{1u}, c) &= -\frac{\sqrt{35}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{14} - \frac{\sqrt{35}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{14} - \frac{\sqrt{7}\mathbb{Q}_4^{(a)}(A_{1g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{7} \\
\text{z422} \quad \mathbb{Q}_{3,1}^{(c)}(E_{1u}, d) &= -\frac{\sqrt{55}\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{T}_{1,1}^{(b)}(E_{1u}, a)}{22} + \frac{\sqrt{55}\mathbb{M}_{3,2}^{(a)}(E_{2g})\mathbb{T}_{1,2}^{(b)}(E_{1u}, a)}{22} - \frac{\sqrt{33}\mathbb{M}_3^{(a)}(A_{2g})\mathbb{T}_{1,2}^{(b)}(E_{1u}, a)}{11} \\
\text{z423} \quad \mathbb{Q}_{3,2}^{(c)}(E_{1u}, d) &= \frac{\sqrt{55}\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{T}_{1,2}^{(b)}(E_{1u}, a)}{22} + \frac{\sqrt{55}\mathbb{M}_{3,2}^{(a)}(E_{2g})\mathbb{T}_{1,1}^{(b)}(E_{1u}, a)}{22} + \frac{\sqrt{33}\mathbb{M}_3^{(a)}(A_{2g})\mathbb{T}_{1,1}^{(b)}(E_{1u}, a)}{11} \\
\text{z424} \quad \mathbb{Q}_{3,1}^{(c)}(E_{1u}, e) &= -\frac{\sqrt{55}\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{T}_{1,1}^{(b)}(E_{1u}, b)}{22} + \frac{\sqrt{55}\mathbb{M}_{3,2}^{(a)}(E_{2g})\mathbb{T}_{1,2}^{(b)}(E_{1u}, b)}{22} - \frac{\sqrt{33}\mathbb{M}_3^{(a)}(A_{2g})\mathbb{T}_{1,2}^{(b)}(E_{1u}, b)}{11} \\
\text{z425} \quad \mathbb{Q}_{3,2}^{(c)}(E_{1u}, e) &= \frac{\sqrt{55}\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{T}_{1,2}^{(b)}(E_{1u}, b)}{22} + \frac{\sqrt{55}\mathbb{M}_{3,2}^{(a)}(E_{2g})\mathbb{T}_{1,1}^{(b)}(E_{1u}, b)}{22} + \frac{\sqrt{33}\mathbb{M}_3^{(a)}(A_{2g})\mathbb{T}_{1,1}^{(b)}(E_{1u}, b)}{11} \\
\text{z448} \quad \mathbb{Q}_{5,1}^{(c)}(E_{1u}, 1a) &= \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{5,1}^{(b)}(E_{1u}, 1)}{2} \\
\text{z449} \quad \mathbb{Q}_{5,2}^{(c)}(E_{1u}, 1a) &= \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{5,2}^{(b)}(E_{1u}, 1)}{2} \\
\text{z450} \quad \mathbb{Q}_{5,1}^{(c)}(E_{1u}, 1b) &= \frac{\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_3^{(b)}(B_{2u})}{2} + \frac{\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_3^{(b)}(B_{1u})}{2} \\
\text{z451} \quad \mathbb{Q}_{5,2}^{(c)}(E_{1u}, 1b) &= -\frac{\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_3^{(b)}(B_{1u})}{2} + \frac{\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_3^{(b)}(B_{2u})}{2} \\
\text{z452} \quad \mathbb{Q}_{5,1}^{(c)}(E_{1u}, 1c) &= -\frac{\sqrt{2}\mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_{5,1}^{(b)}(E_{1u}, 1)}{2} \\
\text{z453} \quad \mathbb{Q}_{5,2}^{(c)}(E_{1u}, 1c) &= -\frac{\sqrt{2}\mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_{5,2}^{(b)}(E_{1u}, 1)}{2} \\
\text{z454} \quad \mathbb{Q}_{5,1}^{(c)}(E_{1u}, 1d) &= -\frac{\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_3^{(b)}(B_{2u})}{2} - \frac{\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_3^{(b)}(B_{1u})}{2}
\end{aligned}$$

$$\begin{aligned}
\text{z455} \quad \mathbb{Q}_{5,2}^{(c)}(E_{1u}, 1d) &= \frac{\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_3^{(b)}(B_{1u})}{2} - \frac{\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_3^{(b)}(B_{2u})}{2} \\
\text{z456} \quad \mathbb{Q}_{5,1}^{(c)}(E_{1u}, 1e) &= \frac{\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{2} - \frac{\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{2} \\
\text{z457} \quad \mathbb{Q}_{5,2}^{(c)}(E_{1u}, 1e) &= -\frac{\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{2} - \frac{\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{2} \\
\text{z458} \quad \mathbb{Q}_{5,1}^{(c)}(E_{1u}, 1f) &= \frac{\sqrt{2}\mathbb{Q}_4^{(a)}(A_{1g})\mathbb{Q}_{5,1}^{(b)}(E_{1u}, 1)}{2} \\
\text{z459} \quad \mathbb{Q}_{5,2}^{(c)}(E_{1u}, 1f) &= \frac{\sqrt{2}\mathbb{Q}_4^{(a)}(A_{1g})\mathbb{Q}_{5,2}^{(b)}(E_{1u}, 1)}{2} \\
\text{z460} \quad \mathbb{Q}_{5,1}^{(c)}(E_{1u}, 1g) &= -\frac{\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{T}_3^{(b)}(B_{2u})}{2} - \frac{\mathbb{M}_{3,2}^{(a)}(E_{2g})\mathbb{T}_3^{(b)}(B_{1u})}{2} \\
\text{z472} \quad \mathbb{Q}_{5,2}^{(c)}(E_{1u}, 1g) &= \frac{\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{T}_3^{(b)}(B_{1u})}{2} - \frac{\mathbb{M}_{3,2}^{(a)}(E_{2g})\mathbb{T}_3^{(b)}(B_{2u})}{2} \\
\text{z473} \quad \mathbb{Q}_{5,1}^{(c)}(E_{1u}, 2) &= \frac{\sqrt{14}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{14} - \frac{\sqrt{14}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{14} + \frac{\sqrt{70}\mathbb{Q}_4^{(a)}(A_{1g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{14} \\
\text{z474} \quad \mathbb{Q}_{5,2}^{(c)}(E_{1u}, 2) &= -\frac{\sqrt{14}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{14} - \frac{\sqrt{14}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{14} + \frac{\sqrt{70}\mathbb{Q}_4^{(a)}(A_{1g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{14} \\
\text{z475} \quad \mathbb{Q}_{7,1}^{(c)}(E_{1u}, 1a) &= \frac{\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_{5,1}^{(b)}(E_{1u}, 1)}{2} - \frac{\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_{5,2}^{(b)}(E_{1u}, 1)}{2} \\
\text{z476} \quad \mathbb{Q}_{7,2}^{(c)}(E_{1u}, 1a) &= -\frac{\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_{5,2}^{(b)}(E_{1u}, 1)}{2} - \frac{\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_{5,1}^{(b)}(E_{1u}, 1)}{2} \\
\text{z477} \quad \mathbb{Q}_{7,1}^{(c)}(E_{1u}, 1b) &= \frac{\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_3^{(b)}(B_{2u})}{2} - \frac{\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_3^{(b)}(B_{1u})}{2} \\
\text{z478} \quad \mathbb{Q}_{7,2}^{(c)}(E_{1u}, 1b) &= \frac{\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_3^{(b)}(B_{1u})}{2} + \frac{\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_3^{(b)}(B_{2u})}{2} \\
\text{z479} \quad \mathbb{Q}_{7,1}^{(c)}(E_{1u}, 1c) &= -\frac{\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{5,1}^{(b)}(E_{1u}, 1)}{2} + \frac{\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{5,2}^{(b)}(E_{1u}, 1)}{2}
\end{aligned}$$



$$\begin{aligned}
\boxed{\text{z480}} \quad \mathbb{Q}_{7,2}^{(c)}(E_{1u}, 1c) &= \frac{\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{5,2}^{(b)}(E_{1u}, 1)}{2} + \frac{\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{5,1}^{(b)}(E_{1u}, 1)}{2} \\
\boxed{\text{z481}} \quad \mathbb{G}_{2,1}^{(c)}(E_{1u}, a) &= \frac{\sqrt{66}\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{T}_{1,1}^{(b)}(E_{1u}, a)}{22} - \frac{\sqrt{66}\mathbb{M}_{3,2}^{(a)}(E_{2g})\mathbb{T}_{1,2}^{(b)}(E_{1u}, a)}{22} - \frac{\sqrt{110}\mathbb{M}_3^{(a)}(A_{2g})\mathbb{T}_{1,2}^{(b)}(E_{1u}, a)}{22} \\
\boxed{\text{z482}} \quad \mathbb{G}_{2,2}^{(c)}(E_{1u}, a) &= -\frac{\sqrt{66}\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{T}_{1,2}^{(b)}(E_{1u}, a)}{22} - \frac{\sqrt{66}\mathbb{M}_{3,2}^{(a)}(E_{2g})\mathbb{T}_{1,1}^{(b)}(E_{1u}, a)}{22} + \frac{\sqrt{110}\mathbb{M}_3^{(a)}(A_{2g})\mathbb{T}_{1,1}^{(b)}(E_{1u}, a)}{22} \\
\boxed{\text{z483}} \quad \mathbb{G}_{2,1}^{(c)}(E_{1u}, b) &= \frac{\sqrt{66}\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{T}_{1,1}^{(b)}(E_{1u}, b)}{22} - \frac{\sqrt{66}\mathbb{M}_{3,2}^{(a)}(E_{2g})\mathbb{T}_{1,2}^{(b)}(E_{1u}, b)}{22} - \frac{\sqrt{110}\mathbb{M}_3^{(a)}(A_{2g})\mathbb{T}_{1,2}^{(b)}(E_{1u}, b)}{22} \\
\boxed{\text{z484}} \quad \mathbb{G}_{2,2}^{(c)}(E_{1u}, b) &= -\frac{\sqrt{66}\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{T}_{1,2}^{(b)}(E_{1u}, b)}{22} - \frac{\sqrt{66}\mathbb{M}_{3,2}^{(a)}(E_{2g})\mathbb{T}_{1,1}^{(b)}(E_{1u}, b)}{22} + \frac{\sqrt{110}\mathbb{M}_3^{(a)}(A_{2g})\mathbb{T}_{1,1}^{(b)}(E_{1u}, b)}{22} \\
\boxed{\text{z541}} \quad \mathbb{Q}_{2,1}^{(c)}(E_{2g}, a) &= \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2} \\
\boxed{\text{z542}} \quad \mathbb{Q}_{2,2}^{(c)}(E_{2g}, a) &= \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2} \\
\boxed{\text{z543}} \quad \mathbb{Q}_{2,1}^{(c)}(E_{2g}, b) &= \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_0^{(b)}(A_{1g})}{2} \\
\boxed{\text{z544}} \quad \mathbb{Q}_{2,2}^{(c)}(E_{2g}, b) &= \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_0^{(b)}(A_{1g})}{2} \\
\boxed{\text{z545}} \quad \mathbb{Q}_{2,1}^{(c)}(E_{2g}, c) &= -\frac{\sqrt{2}\mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2} \\
\boxed{\text{z546}} \quad \mathbb{Q}_{2,2}^{(c)}(E_{2g}, c) &= -\frac{\sqrt{2}\mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2} \\
\boxed{\text{z547}} \quad \mathbb{Q}_{2,1}^{(c)}(E_{2g}, d) &= \frac{\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_{4,1}^{(b)}(E_{2g}, 1)}{2} - \frac{\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_{4,2}^{(b)}(E_{2g}, 1)}{2} \\
\boxed{\text{z548}} \quad \mathbb{Q}_{2,2}^{(c)}(E_{2g}, d) &= -\frac{\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_{4,2}^{(b)}(E_{2g}, 1)}{2} - \frac{\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_{4,1}^{(b)}(E_{2g}, 1)}{2} \\
\boxed{\text{z549}} \quad \mathbb{Q}_{2,1}^{(c)}(E_{2g}, e) &= \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_6^{(b)}(A_{2g})}{2}
\end{aligned}$$

$$\begin{aligned}
\boxed{z550} \quad \mathbb{Q}_{2,2}^{(c)}(E_{2g}, e) &= -\frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_6^{(b)}(A_{2g})}{2} \\
\boxed{z551} \quad \mathbb{Q}_{2,1}^{(c)}(E_{2g}, f) &= \frac{\sqrt{4970}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{142} - \frac{\sqrt{4970}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{142} + \frac{\sqrt{142}\mathbb{Q}_4^{(a)}(A_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{142} \\
\boxed{z552} \quad \mathbb{Q}_{2,2}^{(c)}(E_{2g}, f) &= -\frac{\sqrt{4970}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{142} - \frac{\sqrt{4970}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{142} + \frac{\sqrt{142}\mathbb{Q}_4^{(a)}(A_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{142} \\
\boxed{z553} \quad \mathbb{Q}_{2,1}^{(c)}(E_{2g}, g) &= -\frac{\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{4,1}^{(b)}(E_{2g}, 1)}{2} + \frac{\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{4,2}^{(b)}(E_{2g}, 1)}{2} \\
\boxed{z554} \quad \mathbb{Q}_{2,2}^{(c)}(E_{2g}, g) &= \frac{\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{4,2}^{(b)}(E_{2g}, 1)}{2} + \frac{\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{4,1}^{(b)}(E_{2g}, 1)}{2} \\
\boxed{z555} \quad \mathbb{Q}_{2,1}^{(c)}(E_{2g}, h) &= \frac{\sqrt{2}\mathbb{M}_1^{(a)}(A_{2g})\mathbb{T}_{2,2}^{(b)}(E_{2g}, a)}{2} \\
\boxed{z556} \quad \mathbb{Q}_{2,2}^{(c)}(E_{2g}, h) &= -\frac{\sqrt{2}\mathbb{M}_1^{(a)}(A_{2g})\mathbb{T}_{2,1}^{(b)}(E_{2g}, a)}{2} \\
\boxed{z557} \quad \mathbb{Q}_{2,1}^{(c)}(E_{2g}, i) &= \frac{\sqrt{2}\mathbb{M}_1^{(a)}(A_{2g})\mathbb{T}_{2,2}^{(b)}(E_{2g}, b)}{2} \\
\boxed{z558} \quad \mathbb{Q}_{2,2}^{(c)}(E_{2g}, i) &= -\frac{\sqrt{2}\mathbb{M}_1^{(a)}(A_{2g})\mathbb{T}_{2,1}^{(b)}(E_{2g}, b)}{2} \\
\boxed{z559} \quad \mathbb{Q}_{2,1}^{(c)}(E_{2g}, j) &= \frac{\sqrt{2}\mathbb{M}_{3,2}^{(a)}(E_{2g})\mathbb{M}_1^{(b)}(A_{2g})}{2} \\
\boxed{z560} \quad \mathbb{Q}_{2,2}^{(c)}(E_{2g}, j) &= -\frac{\sqrt{2}\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{M}_1^{(b)}(A_{2g})}{2} \\
\boxed{z561} \quad \mathbb{Q}_{2,1}^{(c)}(E_{2g}, k) &= -\frac{\sqrt{2}\mathbb{M}_3^{(a)}(A_{2g})\mathbb{T}_{2,2}^{(b)}(E_{2g}, a)}{2} \\
\boxed{z562} \quad \mathbb{Q}_{2,2}^{(c)}(E_{2g}, k) &= \frac{\sqrt{2}\mathbb{M}_3^{(a)}(A_{2g})\mathbb{T}_{2,1}^{(b)}(E_{2g}, a)}{2} \\
\boxed{z563} \quad \mathbb{Q}_{2,1}^{(c)}(E_{2g}, l) &= -\frac{\sqrt{2}\mathbb{M}_3^{(a)}(A_{2g})\mathbb{T}_{2,2}^{(b)}(E_{2g}, b)}{2}
\end{aligned}$$

$$\begin{aligned}
\boxed{\text{z564}} \quad \mathbb{Q}_{2,2}^{(c)}(E_{2g}, l) &= \frac{\sqrt{2}\mathbb{M}_3^{(a)}(A_{2g})\mathbb{T}_{2,1}^{(b)}(E_{2g}, b)}{2} \\
\boxed{\text{z565}} \quad \mathbb{Q}_{4,1}^{(c)}(E_{2g}, 1a) &= \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{4,1}^{(b)}(E_{2g}, 1)}{2} \\
\boxed{\text{z566}} \quad \mathbb{Q}_{4,2}^{(c)}(E_{2g}, 1a) &= \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{4,2}^{(b)}(E_{2g}, 1)}{2} \\
\boxed{\text{z567}} \quad \mathbb{Q}_{4,1}^{(c)}(E_{2g}, 1b) &= -\frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_6^{(b)}(A_{2g})}{2} \\
\boxed{\text{z568}} \quad \mathbb{Q}_{4,2}^{(c)}(E_{2g}, 1b) &= \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_6^{(b)}(A_{2g})}{2} \\
\boxed{\text{z569}} \quad \mathbb{Q}_{4,1}^{(c)}(E_{2g}, 1c) &= \frac{\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2} - \frac{\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2} \\
\boxed{\text{z570}} \quad \mathbb{Q}_{4,2}^{(c)}(E_{2g}, 1c) &= -\frac{\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2} - \frac{\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2} \\
\boxed{\text{z571}} \quad \mathbb{Q}_{4,1}^{(c)}(E_{2g}, 1d) &= -\frac{\sqrt{2}\mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_{4,1}^{(b)}(E_{2g}, 1)}{2} \\
\boxed{\text{z572}} \quad \mathbb{Q}_{4,2}^{(c)}(E_{2g}, 1d) &= -\frac{\sqrt{2}\mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_{4,2}^{(b)}(E_{2g}, 1)}{2} \\
\boxed{\text{z573}} \quad \mathbb{Q}_{4,1}^{(c)}(E_{2g}, 1e) &= \frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_0^{(b)}(A_{1g})}{2} \\
\boxed{\text{z574}} \quad \mathbb{Q}_{4,2}^{(c)}(E_{2g}, 1e) &= \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_0^{(b)}(A_{1g})}{2} \\
\boxed{\text{z575}} \quad \mathbb{Q}_{4,1}^{(c)}(E_{2g}, 1f) &= \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_6^{(b)}(A_{2g})}{2} \\
\boxed{\text{z576}} \quad \mathbb{Q}_{4,2}^{(c)}(E_{2g}, 1f) &= -\frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_6^{(b)}(A_{2g})}{2} \\
\boxed{\text{z577}} \quad \mathbb{Q}_{4,1}^{(c)}(E_{2g}, 1g) &= -\frac{\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2} + \frac{\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2}
\end{aligned}$$

$$\boxed{\text{z578}} \quad \mathbb{Q}_{4,2}^{(c)}(E_{2g}, 1g) = \frac{\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2} + \frac{\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2}$$

$$\boxed{\text{z579}} \quad \mathbb{Q}_{4,1}^{(c)}(E_{2g}, 1h) = \frac{\sqrt{2}\mathbb{Q}_4^{(a)}(A_{1g})\mathbb{Q}_{4,1}^{(b)}(E_{2g}, 1)}{2}$$

$$\boxed{\text{z580}} \quad \mathbb{Q}_{4,2}^{(c)}(E_{2g}, 1h) = \frac{\sqrt{2}\mathbb{Q}_4^{(a)}(A_{1g})\mathbb{Q}_{4,2}^{(b)}(E_{2g}, 1)}{2}$$

$$\boxed{\text{z581}} \quad \mathbb{Q}_{4,1}^{(c)}(E_{2g}, 1i) = -\frac{\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{T}_{2,1}^{(b)}(E_{2g}, a)}{2} + \frac{\mathbb{M}_{3,2}^{(a)}(E_{2g})\mathbb{T}_{2,2}^{(b)}(E_{2g}, a)}{2}$$

$$\boxed{\text{z582}} \quad \mathbb{Q}_{4,2}^{(c)}(E_{2g}, 1i) = \frac{\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{T}_{2,2}^{(b)}(E_{2g}, a)}{2} + \frac{\mathbb{M}_{3,2}^{(a)}(E_{2g})\mathbb{T}_{2,1}^{(b)}(E_{2g}, a)}{2}$$

$$\boxed{\text{z583}} \quad \mathbb{Q}_{4,1}^{(c)}(E_{2g}, 1j) = -\frac{\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{T}_{2,1}^{(b)}(E_{2g}, b)}{2} + \frac{\mathbb{M}_{3,2}^{(a)}(E_{2g})\mathbb{T}_{2,2}^{(b)}(E_{2g}, b)}{2}$$

$$\boxed{\text{z584}} \quad \mathbb{Q}_{4,2}^{(c)}(E_{2g}, 1j) = \frac{\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{T}_{2,2}^{(b)}(E_{2g}, b)}{2} + \frac{\mathbb{M}_{3,2}^{(a)}(E_{2g})\mathbb{T}_{2,1}^{(b)}(E_{2g}, b)}{2}$$

$$\boxed{\text{z585}} \quad \mathbb{Q}_{4,1}^{(c)}(E_{2g}, 2a) = \frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z586}} \quad \mathbb{Q}_{4,2}^{(c)}(E_{2g}, 2a) = \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z587}} \quad \mathbb{Q}_{4,1}^{(c)}(E_{2g}, 2b) = \frac{\sqrt{71}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{142} - \frac{\sqrt{71}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{142} - \frac{\sqrt{2485}\mathbb{Q}_4^{(a)}(A_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{71}$$

$$\boxed{\text{z588}} \quad \mathbb{Q}_{4,2}^{(c)}(E_{2g}, 2b) = -\frac{\sqrt{71}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{142} - \frac{\sqrt{71}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{142} - \frac{\sqrt{2485}\mathbb{Q}_4^{(a)}(A_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{71}$$

$$\boxed{\text{z589}} \quad \mathbb{Q}_{8,1}^{(c)}(E_{2g}, 1) = \frac{\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{4,1}^{(b)}(E_{2g}, 1)}{2} - \frac{\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{4,2}^{(b)}(E_{2g}, 1)}{2}$$

$$\boxed{\text{z590}} \quad \mathbb{Q}_{8,2}^{(c)}(E_{2g}, 1) = -\frac{\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{4,2}^{(b)}(E_{2g}, 1)}{2} - \frac{\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{4,1}^{(b)}(E_{2g}, 1)}{2}$$

$$\boxed{\text{z591}} \quad \mathbb{G}_{3,1}^{(c)}(E_{2g}) = \frac{\sqrt{2}\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{T}_0^{(b)}(A_{1g})}{2}$$

$$\begin{aligned}
\boxed{\text{z592}} \quad \mathbb{G}_{3,2}^{(c)}(E_{2g}) &= \frac{\sqrt{2}\mathbb{M}_{3,2}^{(a)}(E_{2g})\mathbb{T}_0^{(b)}(A_{1g})}{2} \\
\boxed{\text{z653}} \quad \mathbb{Q}_{3,1}^{(c)}(E_{2u}, a) &= -\frac{\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_3^{(b)}(B_{2u})}{2} - \frac{\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_3^{(b)}(B_{1u})}{2} \\
\boxed{\text{z654}} \quad \mathbb{Q}_{3,2}^{(c)}(E_{2u}, a) &= \frac{\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_3^{(b)}(B_{1u})}{2} - \frac{\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_3^{(b)}(B_{2u})}{2} \\
\boxed{\text{z655}} \quad \mathbb{Q}_{3,1}^{(c)}(E_{2u}, b) &= \frac{\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{2} - \frac{\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{2} \\
\boxed{\text{z656}} \quad \mathbb{Q}_{3,2}^{(c)}(E_{2u}, b) &= -\frac{\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{2} - \frac{\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{2} \\
\boxed{\text{z657}} \quad \mathbb{Q}_{3,1}^{(c)}(E_{2u}, c) &= \frac{\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_3^{(b)}(B_{2u})}{2} + \frac{\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_3^{(b)}(B_{1u})}{2} \\
\boxed{\text{z658}} \quad \mathbb{Q}_{3,2}^{(c)}(E_{2u}, c) &= -\frac{\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_3^{(b)}(B_{1u})}{2} + \frac{\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_3^{(b)}(B_{2u})}{2} \\
\boxed{\text{z659}} \quad \mathbb{Q}_{3,1}^{(c)}(E_{2u}, d) &= -\frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{8} + \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{8} - \frac{\sqrt{14}\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{8} + \frac{\sqrt{14}\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{8} \\
\boxed{\text{z660}} \quad \mathbb{Q}_{3,2}^{(c)}(E_{2u}, d) &= \frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{8} + \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{8} + \frac{\sqrt{14}\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{8} + \frac{\sqrt{14}\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{8} \\
\boxed{\text{z661}} \quad \mathbb{Q}_{3,1}^{(c)}(E_{2u}, e) &= -\frac{\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{5,2}^{(b)}(E_{1u}, 1)}{2} - \frac{\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{5,1}^{(b)}(E_{1u}, 1)}{2} \\
\boxed{\text{z662}} \quad \mathbb{Q}_{3,2}^{(c)}(E_{2u}, e) &= \frac{\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{5,1}^{(b)}(E_{1u}, 1)}{2} - \frac{\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{5,2}^{(b)}(E_{1u}, 1)}{2} \\
\boxed{\text{z663}} \quad \mathbb{Q}_{3,1}^{(c)}(E_{2u}, f) &= -\frac{\mathbb{M}_{1,1}^{(a)}(E_{1g})\mathbb{T}_3^{(b)}(B_{2u})}{2} - \frac{\mathbb{M}_{1,2}^{(a)}(E_{1g})\mathbb{T}_3^{(b)}(B_{1u})}{2} \\
\boxed{\text{z664}} \quad \mathbb{Q}_{3,2}^{(c)}(E_{2u}, f) &= \frac{\mathbb{M}_{1,1}^{(a)}(E_{1g})\mathbb{T}_3^{(b)}(B_{1u})}{2} - \frac{\mathbb{M}_{1,2}^{(a)}(E_{1g})\mathbb{T}_3^{(b)}(B_{2u})}{2} \\
\boxed{\text{z665}} \quad \mathbb{Q}_{3,1}^{(c)}(E_{2u}, g) &= \frac{\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{T}_3^{(b)}(B_{2u})}{2} + \frac{\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{T}_3^{(b)}(B_{1u})}{2}
\end{aligned}$$

$$\begin{aligned}
\text{z666} \quad \mathbb{Q}_{3,2}^{(c)}(E_{2u}, g) &= -\frac{\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{T}_3^{(b)}(B_{1u})}{2} + \frac{\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{T}_3^{(b)}(B_{2u})}{2} \\
\text{z667} \quad \mathbb{Q}_{3,1}^{(c)}(E_{2u}, h) &= \frac{\sqrt{10}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u}, a)}{8} - \frac{\sqrt{10}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u}, a)}{8} + \frac{\sqrt{6}\mathbb{M}_3^{(a)}(B_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u}, a)}{8} + \frac{\sqrt{6}\mathbb{M}_3^{(a)}(B_{2g})\mathbb{T}_{1,1}^{(b)}(E_{1u}, a)}{8} \\
\text{z668} \quad \mathbb{Q}_{3,2}^{(c)}(E_{2u}, h) &= -\frac{\sqrt{10}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u}, a)}{8} - \frac{\sqrt{10}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u}, a)}{8} - \frac{\sqrt{6}\mathbb{M}_3^{(a)}(B_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u}, a)}{8} + \frac{\sqrt{6}\mathbb{M}_3^{(a)}(B_{2g})\mathbb{T}_{1,2}^{(b)}(E_{1u}, a)}{8} \\
\text{z669} \quad \mathbb{Q}_{3,1}^{(c)}(E_{2u}, i) &= \frac{\sqrt{10}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u}, b)}{8} - \frac{\sqrt{10}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u}, b)}{8} + \frac{\sqrt{6}\mathbb{M}_3^{(a)}(B_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u}, b)}{8} + \frac{\sqrt{6}\mathbb{M}_3^{(a)}(B_{2g})\mathbb{T}_{1,1}^{(b)}(E_{1u}, b)}{8} \\
\text{z670} \quad \mathbb{Q}_{3,2}^{(c)}(E_{2u}, i) &= -\frac{\sqrt{10}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u}, b)}{8} - \frac{\sqrt{10}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u}, b)}{8} - \frac{\sqrt{6}\mathbb{M}_3^{(a)}(B_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u}, b)}{8} + \frac{\sqrt{6}\mathbb{M}_3^{(a)}(B_{2g})\mathbb{T}_{1,2}^{(b)}(E_{1u}, b)}{8} \\
\text{z671} \quad \mathbb{Q}_{5,1}^{(c)}(E_{2u}, 1a) &= -\frac{\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_3^{(b)}(B_{2u})}{2} + \frac{\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_3^{(b)}(B_{1u})}{2} \\
\text{z672} \quad \mathbb{Q}_{5,2}^{(c)}(E_{2u}, 1a) &= -\frac{\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_3^{(b)}(B_{1u})}{2} - \frac{\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_3^{(b)}(B_{2u})}{2} \\
\text{z673} \quad \mathbb{Q}_{5,1}^{(c)}(E_{2u}, 1b) &= \frac{\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_{5,1}^{(b)}(E_{1u}, 1)}{2} - \frac{\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_{5,2}^{(b)}(E_{1u}, 1)}{2} \\
\text{z674} \quad \mathbb{Q}_{5,2}^{(c)}(E_{2u}, 1b) &= -\frac{\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_{5,2}^{(b)}(E_{1u}, 1)}{2} - \frac{\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_{5,1}^{(b)}(E_{1u}, 1)}{2} \\
\text{z675} \quad \mathbb{Q}_{5,1}^{(c)}(E_{2u}, 1c) &= \frac{\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_3^{(b)}(B_{2u})}{2} - \frac{\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_3^{(b)}(B_{1u})}{2} \\
\text{z676} \quad \mathbb{Q}_{5,2}^{(c)}(E_{2u}, 1c) &= \frac{\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_3^{(b)}(B_{1u})}{2} + \frac{\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_3^{(b)}(B_{2u})}{2} \\
\text{z677} \quad \mathbb{Q}_{5,1}^{(c)}(E_{2u}, 1d) &= -\frac{\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{2} - \frac{\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{2} \\
\text{z678} \quad \mathbb{Q}_{5,2}^{(c)}(E_{2u}, 1d) &= \frac{\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{2} - \frac{\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{2} \\
\text{z679} \quad \mathbb{Q}_{5,1}^{(c)}(E_{2u}, 1e) &= -\frac{\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{5,1}^{(b)}(E_{1u}, 1)}{2} + \frac{\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{5,2}^{(b)}(E_{1u}, 1)}{2}
\end{aligned}$$

$$\boxed{\text{z680}} \quad \mathbb{Q}_{5,2}^{(c)}(E_{2u}, 1e) = \frac{\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{5,2}^{(b)}(E_{1u}, 1)}{2} + \frac{\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{5,1}^{(b)}(E_{1u}, 1)}{2}$$

$$\boxed{\text{z681}} \quad \mathbb{Q}_{5,1}^{(c)}(E_{2u}, 1f) = -\frac{\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{T}_3^{(b)}(B_{2u})}{2} + \frac{\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{T}_3^{(b)}(B_{1u})}{2}$$

$$\boxed{\text{z682}} \quad \mathbb{Q}_{5,2}^{(c)}(E_{2u}, 1f) = -\frac{\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{T}_3^{(b)}(B_{1u})}{2} - \frac{\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{T}_3^{(b)}(B_{2u})}{2}$$

$$\boxed{\text{z683}} \quad \mathbb{Q}_{5,1}^{(c)}(E_{2u}, 2) = \frac{\sqrt{14}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{8} - \frac{\sqrt{14}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{8} - \frac{\sqrt{2}\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{8} + \frac{\sqrt{2}\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{8}$$

$$\boxed{\text{z684}} \quad \mathbb{Q}_{5,2}^{(c)}(E_{2u}, 2) = -\frac{\sqrt{14}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{8} - \frac{\sqrt{14}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{8} + \frac{\sqrt{2}\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{8} + \frac{\sqrt{2}\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{8}$$

$$\boxed{\text{z685}} \quad \mathbb{Q}_{9,1}^{(c)}(E_{2u}, 1) = -\frac{\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{5,2}^{(b)}(E_{1u}, 1)}{2} + \frac{\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{5,1}^{(b)}(E_{1u}, 1)}{2}$$

$$\boxed{\text{z686}} \quad \mathbb{Q}_{9,2}^{(c)}(E_{2u}, 1) = \frac{\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{5,1}^{(b)}(E_{1u}, 1)}{2} + \frac{\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{5,2}^{(b)}(E_{1u}, 1)}{2}$$

$$\boxed{\text{z687}} \quad \mathbb{G}_{2,1}^{(c)}(E_{2u}, a) = \frac{\mathbb{M}_{1,1}^{(a)}(E_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u}, a)}{2} - \frac{\mathbb{M}_{1,2}^{(a)}(E_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u}, a)}{2}$$

$$\boxed{\text{z688}} \quad \mathbb{G}_{2,2}^{(c)}(E_{2u}, a) = -\frac{\mathbb{M}_{1,1}^{(a)}(E_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u}, a)}{2} - \frac{\mathbb{M}_{1,2}^{(a)}(E_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u}, a)}{2}$$

$$\boxed{\text{z689}} \quad \mathbb{G}_{2,1}^{(c)}(E_{2u}, b) = \frac{\mathbb{M}_{1,1}^{(a)}(E_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u}, b)}{2} - \frac{\mathbb{M}_{1,2}^{(a)}(E_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u}, b)}{2}$$

$$\boxed{\text{z690}} \quad \mathbb{G}_{2,2}^{(c)}(E_{2u}, b) = -\frac{\mathbb{M}_{1,1}^{(a)}(E_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u}, b)}{2} - \frac{\mathbb{M}_{1,2}^{(a)}(E_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u}, b)}{2}$$

$$\boxed{\text{z691}} \quad \mathbb{G}_{2,1}^{(c)}(E_{2u}, c) = -\frac{\sqrt{6}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u}, a)}{8} + \frac{\sqrt{6}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u}, a)}{8} + \frac{\sqrt{10}\mathbb{M}_3^{(a)}(B_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u}, a)}{8} + \frac{\sqrt{10}\mathbb{M}_3^{(a)}(B_{2g})\mathbb{T}_{1,1}^{(b)}(E_{1u}, a)}{8}$$

$$\boxed{\text{z692}} \quad \mathbb{G}_{2,2}^{(c)}(E_{2u}, c) = \frac{\sqrt{6}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u}, a)}{8} + \frac{\sqrt{6}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u}, a)}{8} - \frac{\sqrt{10}\mathbb{M}_3^{(a)}(B_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u}, a)}{8} + \frac{\sqrt{10}\mathbb{M}_3^{(a)}(B_{2g})\mathbb{T}_{1,2}^{(b)}(E_{1u}, a)}{8}$$

$$\boxed{\text{z693}} \quad \mathbb{G}_{2,1}^{(c)}(E_{2u}, d) = -\frac{\sqrt{6}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u}, b)}{8} + \frac{\sqrt{6}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u}, b)}{8} + \frac{\sqrt{10}\mathbb{M}_3^{(a)}(B_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u}, b)}{8} + \frac{\sqrt{10}\mathbb{M}_3^{(a)}(B_{2g})\mathbb{T}_{1,1}^{(b)}(E_{1u}, b)}{8}$$

$$\boxed{\text{z694}} \quad \mathbb{G}_{2,2}^{(c)}(E_{2u}, d) = \frac{\sqrt{6}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u}, b)}{8} + \frac{\sqrt{6}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u}, b)}{8} - \frac{\sqrt{10}\mathbb{M}_3^{(a)}(B_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u}, b)}{8} + \frac{\sqrt{10}\mathbb{M}_3^{(a)}(B_{2g})\mathbb{T}_{1,2}^{(b)}(E_{1u}, b)}{8}$$

$$\boxed{\text{z695}} \quad \mathbb{G}_{4,1}^{(c)}(E_{2u}, 1a) = \frac{\mathbb{M}_{1,1}^{(a)}(E_{1g})\mathbb{T}_3^{(b)}(B_{2u})}{2} - \frac{\mathbb{M}_{1,2}^{(a)}(E_{1g})\mathbb{T}_3^{(b)}(B_{1u})}{2}$$

$$\boxed{\text{z696}} \quad \mathbb{G}_{4,2}^{(c)}(E_{2u}, 1a) = \frac{\mathbb{M}_{1,1}^{(a)}(E_{1g})\mathbb{T}_3^{(b)}(B_{1u})}{2} + \frac{\mathbb{M}_{1,2}^{(a)}(E_{1g})\mathbb{T}_3^{(b)}(B_{2u})}{2}$$

$$\boxed{\text{z697}} \quad \mathbb{G}_{4,1}^{(c)}(E_{2u}, 1b) = -\frac{\mathbb{M}_3^{(a)}(B_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u}, a)}{2} + \frac{\mathbb{M}_3^{(a)}(B_{2g})\mathbb{T}_{1,1}^{(b)}(E_{1u}, a)}{2}$$

$$\boxed{\text{z698}} \quad \mathbb{G}_{4,2}^{(c)}(E_{2u}, 1b) = \frac{\mathbb{M}_3^{(a)}(B_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u}, a)}{2} + \frac{\mathbb{M}_3^{(a)}(B_{2g})\mathbb{T}_{1,2}^{(b)}(E_{1u}, a)}{2}$$

$$\boxed{\text{z699}} \quad \mathbb{G}_{4,1}^{(c)}(E_{2u}, 1c) = -\frac{\mathbb{M}_3^{(a)}(B_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u}, b)}{2} + \frac{\mathbb{M}_3^{(a)}(B_{2g})\mathbb{T}_{1,1}^{(b)}(E_{1u}, b)}{2}$$

$$\boxed{\text{z700}} \quad \mathbb{G}_{4,2}^{(c)}(E_{2u}, 1c) = \frac{\mathbb{M}_3^{(a)}(B_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u}, b)}{2} + \frac{\mathbb{M}_3^{(a)}(B_{2g})\mathbb{T}_{1,2}^{(b)}(E_{1u}, b)}{2}$$

- **Sn;Sn\_001\_1** : 'Sn'-'Sn' bond-cluster

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

\* ket:  $|d_v\rangle, |d_{xy}\rangle, |d_{xz}\rangle, |d_{yz}\rangle, |d_u\rangle$

\* wyckoff: **6a06g**

$$\boxed{\text{z32}} \quad \mathbb{Q}_0^{(c)}(A_{1g}, a) = \mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z33}} \quad \mathbb{Q}_0^{(c)}(A_{1g}, b) = \frac{\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{2} + \frac{\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2} + \frac{\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{2} + \frac{\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2}$$

$$\boxed{\text{z34}} \quad \mathbb{Q}_0^{(c)}(A_{1g}, c) = \mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_4^{(b)}(B_{2g})$$

$$\boxed{\text{z35}} \quad \mathbb{Q}_2^{(c)}(A_{1g}, a) = \mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z36}} \quad \mathbb{Q}_2^{(c)}(A_{1g}, b) = \frac{\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{2} - \frac{\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2} + \frac{\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{2} - \frac{\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2}$$

$$\boxed{\text{z37}} \quad \mathbb{Q}_2^{(c)}(A_{1g}, c) = \frac{\sqrt{3}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{3} + \frac{\sqrt{6}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{6} + \frac{\sqrt{3}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{3} + \frac{\sqrt{6}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{6}$$



$$\boxed{\text{z38}} \quad \mathbb{Q}_4^{(c)}(A_{1g}, a) = \mathbb{Q}_4^{(a)}(A_{1g})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z39}} \quad \mathbb{Q}_4^{(c)}(A_{1g}, b) = \frac{\sqrt{6}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{6} - \frac{\sqrt{3}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{3} + \frac{\sqrt{6}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{6} - \frac{\sqrt{3}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{3}$$

$$\boxed{\text{z40}} \quad \mathbb{Q}_6^{(c)}(A_{1g}, 2) = \frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2} + \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2}$$

$$\boxed{\text{z61}} \quad \mathbb{G}_0^{(c)}(A_{1u}, a) = \frac{\sqrt{3}\mathbb{M}_{1,1}^{(a)}(E_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{3} + \frac{\sqrt{3}\mathbb{M}_{1,2}^{(a)}(E_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{3} + \frac{\sqrt{3}\mathbb{M}_1^{(a)}(A_{2g})\mathbb{T}_1^{(b)}(A_{2u})}{3}$$

$$\boxed{\text{z62}} \quad \mathbb{G}_0^{(c)}(A_{1u}, b) = \mathbb{M}_3^{(a)}(B_{1g})\mathbb{T}_3^{(b)}(B_{1u})$$

$$\boxed{\text{z63}} \quad \mathbb{G}_2^{(c)}(A_{1u}, a) = -\frac{\sqrt{6}\mathbb{M}_{1,1}^{(a)}(E_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{6} - \frac{\sqrt{6}\mathbb{M}_{1,2}^{(a)}(E_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{6} + \frac{\sqrt{6}\mathbb{M}_1^{(a)}(A_{2g})\mathbb{T}_1^{(b)}(A_{2u})}{3}$$

$$\boxed{\text{z64}} \quad \mathbb{G}_2^{(c)}(A_{1u}, b) = \frac{\sqrt{14}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{7} + \frac{\sqrt{14}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{7} + \frac{\sqrt{21}\mathbb{M}_3^{(a)}(A_{2g})\mathbb{T}_1^{(b)}(A_{2u})}{7}$$

$$\boxed{\text{z65}} \quad \mathbb{G}_2^{(c)}(A_{1u}, c) = -\frac{\sqrt{2}\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{M}_{2,1}^{(b)}(E_{2u})}{2} - \frac{\sqrt{2}\mathbb{M}_{3,2}^{(a)}(E_{2g})\mathbb{M}_{2,2}^{(b)}(E_{2u})}{2}$$

$$\boxed{\text{z66}} \quad \mathbb{G}_4^{(c)}(A_{1u}) = -\frac{\sqrt{42}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{14} - \frac{\sqrt{42}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{14} + \frac{2\sqrt{7}\mathbb{M}_3^{(a)}(A_{2g})\mathbb{T}_1^{(b)}(A_{2u})}{7}$$

$$\boxed{\text{z89}} \quad \mathbb{Q}_6^{(c)}(A_{2g}, a) = \mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_4^{(b)}(B_{2g})$$

$$\boxed{\text{z90}} \quad \mathbb{Q}_6^{(c)}(A_{2g}, b) = -\frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2} + \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2}$$

$$\boxed{\text{z91}} \quad \mathbb{G}_1^{(c)}(A_{2g}) = \frac{\sqrt{10}\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{10} - \frac{\sqrt{10}\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{5} - \frac{\sqrt{10}\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{10} + \frac{\sqrt{10}\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{5}$$

$$\boxed{\text{z92}} \quad \mathbb{G}_3^{(c)}(A_{2g}, a) = \frac{\sqrt{10}\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{5} + \frac{\sqrt{10}\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{10} - \frac{\sqrt{10}\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{5} - \frac{\sqrt{10}\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{10}$$

$$\boxed{\text{z93}} \quad \mathbb{G}_3^{(c)}(A_{2g}, b) = \frac{\sqrt{6}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{6} - \frac{\sqrt{3}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{3} - \frac{\sqrt{6}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{6} + \frac{\sqrt{3}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{3}$$

$$\boxed{\text{z94}} \quad \mathbb{G}_5^{(c)}(A_{2g}) = \frac{\sqrt{3}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{3} + \frac{\sqrt{6}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{6} - \frac{\sqrt{3}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{3} - \frac{\sqrt{6}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{6}$$

$$\boxed{\text{z117}} \quad \mathbb{Q}_1^{(c)}(A_{2u}, a) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(a)}(E_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{2} - \frac{\sqrt{2}\mathbb{M}_{1,2}^{(a)}(E_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{2}$$

$$\boxed{\text{z118}} \quad \mathbb{Q}_1^{(c)}(A_{2u}, b) = \mathbb{M}_3^{(a)}(B_{2g})\mathbb{T}_3^{(b)}(B_{1u})$$

$$\boxed{\text{z119}} \quad \mathbb{Q}_1^{(c)}(A_{2u}, c) = -\frac{\sqrt{2}\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{M}_{2,2}^{(b)}(E_{2u})}{2} + \frac{\sqrt{2}\mathbb{M}_{3,2}^{(a)}(E_{2g})\mathbb{M}_{2,1}^{(b)}(E_{2u})}{2}$$

$$\boxed{\text{z120}} \quad \mathbb{Q}_3^{(c)}(A_{2u}) = \frac{\sqrt{2}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{2} - \frac{\sqrt{2}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{2}$$

$$\boxed{\text{z121}} \quad \mathbb{Q}_4^{(c)}(B_{1g}, a) = \frac{\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2} - \frac{\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{2} - \frac{\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2} + \frac{\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{2}$$

$$\boxed{\text{z122}} \quad \mathbb{Q}_4^{(c)}(B_{1g}, b) = \mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z123}} \quad \mathbb{Q}_4^{(c)}(B_{1g}, c) = -\frac{3\sqrt{71}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{71} - \frac{\sqrt{994}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{71} - \frac{5\sqrt{142}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{142} \\ + \frac{3\sqrt{71}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{71} + \frac{\sqrt{994}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{71} + \frac{5\sqrt{142}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{142}$$

$$\boxed{\text{z124}} \quad \mathbb{Q}_6^{(c)}(B_{1g}) = \frac{7\sqrt{497}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{355} + \frac{9\sqrt{142}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{710} - \frac{6\sqrt{994}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{355} \\ - \frac{7\sqrt{497}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{355} - \frac{9\sqrt{142}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{710} + \frac{6\sqrt{994}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{355}$$

$$\boxed{\text{z125}} \quad \mathbb{G}_3^{(c)}(B_{1g}, a) = \frac{\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2} + \frac{\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{2} - \frac{\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2} - \frac{\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{2}$$

$$\boxed{\text{z214}} \quad \mathbb{G}_3^{(c)}(B_{1g}, b) = -\frac{3\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{10} + \frac{\sqrt{7}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{5} - \frac{\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{5} + \frac{3\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{10} - \frac{\sqrt{7}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{5} + \frac{\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{5}$$

$$\boxed{\text{z215}} \quad \mathbb{Q}_3^{(c)}(B_{1u}, a) = -\frac{\sqrt{2}\mathbb{M}_{1,1}^{(a)}(E_{1g})\mathbb{M}_{2,2}^{(b)}(E_{2u})}{2} + \frac{\sqrt{2}\mathbb{M}_{1,2}^{(a)}(E_{1g})\mathbb{M}_{2,1}^{(b)}(E_{2u})}{2}$$

$$\boxed{\text{z216}} \quad \mathbb{Q}_3^{(c)}(B_{1u}, b) = -\frac{\sqrt{2}\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{4} + \frac{\sqrt{2}\mathbb{M}_{3,2}^{(a)}(E_{2g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{4} - \frac{\sqrt{3}\mathbb{M}_3^{(a)}(B_{2g})\mathbb{T}_1^{(b)}(A_{2u})}{2}$$

$$\text{z217} \quad \mathbb{Q}_3^{(c)}(B_{1u}, c) = \frac{\sqrt{2}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{M}_{2,2}^{(b)}(E_{2u})}{2} - \frac{\sqrt{2}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{M}_{2,1}^{(b)}(E_{2u})}{2}$$

$$\text{z218} \quad \mathbb{G}_4^{(c)}(B_{1u}) = -\frac{\sqrt{6}\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{4} + \frac{\sqrt{6}\mathbb{M}_{3,2}^{(a)}(E_{2g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{4} + \frac{\mathbb{M}_3^{(a)}(B_{2g})\mathbb{T}_1^{(b)}(A_{2u})}{2}$$

$$\text{z219} \quad \mathbb{Q}_4^{(c)}(B_{2g}, a) = \mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_4^{(b)}(B_{2g})$$

$$\text{z220} \quad \mathbb{Q}_4^{(c)}(B_{2g}, b) = -\mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_4^{(b)}(B_{2g})$$

$$\text{z221} \quad \mathbb{Q}_4^{(c)}(B_{2g}, c) = \frac{\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2} + \frac{\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{2} + \frac{\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2} + \frac{\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{2}$$

$$\text{z222} \quad \mathbb{Q}_4^{(c)}(B_{2g}, d) = \mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\text{z223} \quad \mathbb{Q}_4^{(c)}(B_{2g}, e) = -\mathbb{Q}_4^{(a)}(A_{1g})\mathbb{Q}_4^{(b)}(B_{2g})$$

$$\text{z224} \quad \mathbb{Q}_4^{(c)}(B_{2g}, f) = -\frac{3\sqrt{71}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{71} - \frac{\sqrt{994}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{71} + \frac{5\sqrt{142}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{142} \\ - \frac{3\sqrt{71}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{71} - \frac{\sqrt{994}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{71} + \frac{5\sqrt{142}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{142}$$

$$\text{z225} \quad \mathbb{Q}_6^{(c)}(B_{2g}) = \frac{7\sqrt{497}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{355} + \frac{9\sqrt{142}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{710} + \frac{6\sqrt{994}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{355} \\ + \frac{7\sqrt{497}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{355} + \frac{9\sqrt{142}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{710} + \frac{6\sqrt{994}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{355}$$

$$\text{z226} \quad \mathbb{G}_3^{(c)}(B_{2g}, a) = -\frac{\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2} + \frac{\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{2} - \frac{\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2} + \frac{\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{2}$$

$$\text{z227} \quad \mathbb{G}_3^{(c)}(B_{2g}, b) = \frac{3\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{10} - \frac{\sqrt{7}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{5} - \frac{\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{5} + \frac{3\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{10} - \frac{\sqrt{7}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{5} - \frac{\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{5}$$

$$\text{z228} \quad \mathbb{Q}_3^{(c)}(B_{2u}, a) = -\mathbb{M}_1^{(a)}(A_{2g})\mathbb{T}_3^{(b)}(B_{1u})$$

$$\text{z229} \quad \mathbb{Q}_3^{(c)}(B_{2u}, b) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(a)}(E_{1g})\mathbb{M}_{2,1}^{(b)}(E_{2u})}{2} + \frac{\sqrt{2}\mathbb{M}_{1,2}^{(a)}(E_{1g})\mathbb{M}_{2,2}^{(b)}(E_{2u})}{2}$$

$$\text{z230} \quad \mathbb{Q}_3^{(c)}(B_{2u}, c) = -\frac{\sqrt{2}\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{4} - \frac{\sqrt{2}\mathbb{M}_{3,2}^{(a)}(E_{2g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{4} + \frac{\sqrt{3}\mathbb{M}_3^{(a)}(B_{1g})\mathbb{T}_1^{(b)}(A_{2u})}{2}$$

$$\text{z231} \quad \mathbb{Q}_3^{(c)}(B_{2u}, d) = \mathbb{M}_3^{(a)}(A_{2g})\mathbb{T}_3^{(b)}(B_{1u})$$

$$\text{z232} \quad \mathbb{Q}_3^{(c)}(B_{2u}, e) = -\frac{\sqrt{2}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{M}_{2,1}^{(b)}(E_{2u})}{2} - \frac{\sqrt{2}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{M}_{2,2}^{(b)}(E_{2u})}{2}$$

$$\text{z233} \quad \mathbb{G}_4^{(c)}(B_{2u}) = \frac{\sqrt{6}\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{4} + \frac{\sqrt{6}\mathbb{M}_{3,2}^{(a)}(E_{2g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{4} + \frac{\mathbb{M}_3^{(a)}(B_{1g})\mathbb{T}_1^{(b)}(A_{2u})}{2}$$

$$\text{z234} \quad \mathbb{Q}_{2,1}^{(c)}(E_{1g}, a) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{2}$$

$$\text{z235} \quad \mathbb{Q}_{2,2}^{(c)}(E_{1g}, a) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{2}$$

$$\text{z236} \quad \mathbb{Q}_{2,1}^{(c)}(E_{1g}, b) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\text{z237} \quad \mathbb{Q}_{2,2}^{(c)}(E_{1g}, b) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\text{z238} \quad \mathbb{Q}_{2,1}^{(c)}(E_{1g}, c) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_4^{(b)}(B_{2g})}{2}$$

$$\text{z239} \quad \mathbb{Q}_{2,2}^{(c)}(E_{1g}, c) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_4^{(b)}(B_{2g})}{2}$$

$$\text{z240} \quad \mathbb{Q}_{2,1}^{(c)}(E_{1g}, d) = -\frac{\sqrt{78}\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{26} - \frac{\sqrt{78}\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{26} + \frac{\sqrt{78}\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{26} + \frac{\sqrt{78}\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{26} + \frac{\sqrt{26}\mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{26}$$

$$\text{z241} \quad \mathbb{Q}_{2,2}^{(c)}(E_{1g}, d) = \frac{\sqrt{78}\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{26} + \frac{\sqrt{78}\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{26} + \frac{\sqrt{78}\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{26} + \frac{\sqrt{78}\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{26} + \frac{\sqrt{26}\mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{26}$$

$$\text{z242} \quad \mathbb{Q}_{2,1}^{(c)}(E_{1g}, e) = -\frac{\sqrt{742}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_4^{(b)}(B_{2g})}{53} + \frac{5\sqrt{106}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_4^{(b)}(B_{2g})}{106}$$

$$\text{z243} \quad \mathbb{Q}_{2,2}^{(c)}(E_{1g}, e) = -\frac{\sqrt{742}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_4^{(b)}(B_{2g})}{53} + \frac{5\sqrt{106}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_4^{(b)}(B_{2g})}{106}$$

$$\begin{aligned}
\text{z346} \quad \mathbb{Q}_{2,1}^{(c)}(E_{1g}, f) &= \frac{\sqrt{30}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{48} - \frac{\sqrt{15}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{12} - \frac{\sqrt{30}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{48} + \frac{\sqrt{15}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{12} \\
&\quad - \frac{\sqrt{3}\mathbb{Q}_4^{(a)}(A_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{6} + \frac{\sqrt{210}\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{48} + \frac{\sqrt{210}\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{48} \\
\text{z347} \quad \mathbb{Q}_{2,2}^{(c)}(E_{1g}, f) &= -\frac{\sqrt{30}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{48} + \frac{\sqrt{15}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{12} - \frac{\sqrt{30}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{48} \\
&\quad + \frac{\sqrt{15}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{12} - \frac{\sqrt{3}\mathbb{Q}_4^{(a)}(A_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{6} - \frac{\sqrt{210}\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{48} + \frac{\sqrt{210}\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{48} \\
\text{z348} \quad \mathbb{Q}_{4,1}^{(c)}(E_{1g}, a) &= \frac{\sqrt{26}\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{52} + \frac{\sqrt{26}\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{52} - \frac{\sqrt{26}\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{52} - \frac{\sqrt{26}\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{52} + \frac{\sqrt{78}\mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{13} \\
\text{z349} \quad \mathbb{Q}_{4,2}^{(c)}(E_{1g}, a) &= -\frac{\sqrt{26}\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{52} - \frac{\sqrt{26}\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{52} - \frac{\sqrt{26}\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{52} - \frac{\sqrt{26}\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{52} + \frac{\sqrt{78}\mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{13} \\
\text{z350} \quad \mathbb{Q}_{4,1}^{(c)}(E_{1g}, b) &= \frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_0^{(b)}(A_{1g})}{2} \\
\text{z351} \quad \mathbb{Q}_{4,2}^{(c)}(E_{1g}, b) &= \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_0^{(b)}(A_{1g})}{2} \\
\text{z352} \quad \mathbb{Q}_{4,1}^{(c)}(E_{1g}, c) &= \frac{5\sqrt{106}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_4^{(b)}(B_{2g})}{106} + \frac{\sqrt{742}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_4^{(b)}(B_{2g})}{53} \\
\text{z353} \quad \mathbb{Q}_{4,2}^{(c)}(E_{1g}, c) &= \frac{5\sqrt{106}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_4^{(b)}(B_{2g})}{106} + \frac{\sqrt{742}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_4^{(b)}(B_{2g})}{53} \\
\text{z354} \quad \mathbb{Q}_{4,1}^{(c)}(E_{1g}, d) &= -\frac{125\sqrt{2274}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{18192} - \frac{43\sqrt{1137}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{4548} + \frac{125\sqrt{2274}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{18192} \\
&\quad + \frac{43\sqrt{1137}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{4548} + \frac{\sqrt{5685}\mathbb{Q}_4^{(a)}(A_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{2274} - \frac{29\sqrt{15918}\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{18192} - \frac{29\sqrt{15918}\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{18192} \\
\text{z355} \quad \mathbb{Q}_{4,2}^{(c)}(E_{1g}, d) &= \frac{125\sqrt{2274}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{18192} + \frac{43\sqrt{1137}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{4548} + \frac{125\sqrt{2274}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{18192} \\
&\quad + \frac{43\sqrt{1137}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{4548} + \frac{\sqrt{5685}\mathbb{Q}_4^{(a)}(A_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{2274} + \frac{29\sqrt{15918}\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{18192} - \frac{29\sqrt{15918}\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{18192} \\
\text{z356} \quad \mathbb{Q}_{6,1}^{(c)}(E_{1g}, 1) &= \frac{\sqrt{3}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{6} - \frac{\sqrt{3}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{6} - \frac{\sqrt{6}\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{6} + \frac{\sqrt{6}\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{6}
\end{aligned}$$

$$\begin{aligned}
\text{z357} \quad \mathbb{Q}_{6,2}^{(c)}(E_{1g}, 1) &= -\frac{\sqrt{3}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{6} - \frac{\sqrt{3}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{6} + \frac{\sqrt{6}\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{6} + \frac{\sqrt{6}\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{6} \\
\text{z358} \quad \mathbb{Q}_{6,1}^{(c)}(E_{1g}, 2) &= \frac{\sqrt{2653}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{758} - \frac{2\sqrt{5306}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{1137} - \frac{\sqrt{2653}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{758} + \frac{2\sqrt{5306}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{1137} \\
&\quad + \frac{3\sqrt{26530}\mathbb{Q}_4^{(a)}(A_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{758} + \frac{17\sqrt{379}\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2274} + \frac{17\sqrt{379}\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2274} \\
\text{z359} \quad \mathbb{Q}_{6,2}^{(c)}(E_{1g}, 2) &= -\frac{\sqrt{2653}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{758} + \frac{2\sqrt{5306}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{1137} - \frac{\sqrt{2653}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{758} + \frac{2\sqrt{5306}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{1137} \\
&\quad + \frac{3\sqrt{26530}\mathbb{Q}_4^{(a)}(A_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{758} - \frac{17\sqrt{379}\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2274} + \frac{17\sqrt{379}\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2274} \\
\text{z360} \quad \mathbb{G}_{1,1}^{(c)}(E_{1g}) &= \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{4} - \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{4} - \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{4} + \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{4} \\
\text{z361} \quad \mathbb{G}_{1,2}^{(c)}(E_{1g}) &= -\frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{4} + \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{4} - \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{4} + \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{4} \\
\text{z362} \quad \mathbb{G}_{3,1}^{(c)}(E_{1g}) &= \frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{4} - \frac{\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{6} - \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{4} + \frac{\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{6} - \frac{\sqrt{14}\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{12} - \frac{\sqrt{14}\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{12} \\
\text{z363} \quad \mathbb{G}_{3,2}^{(c)}(E_{1g}) &= -\frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{4} + \frac{\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{6} - \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{4} + \frac{\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{6} + \frac{\sqrt{14}\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{12} - \frac{\sqrt{14}\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{12} \\
\text{z364} \quad \mathbb{G}_{5,1}^{(c)}(E_{1g}, 1) &= \frac{\sqrt{6}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{6} - \frac{\sqrt{6}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{6} + \frac{\sqrt{3}\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{6} - \frac{\sqrt{3}\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{6} \\
\text{z365} \quad \mathbb{G}_{5,2}^{(c)}(E_{1g}, 1) &= -\frac{\sqrt{6}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{6} - \frac{\sqrt{6}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{6} - \frac{\sqrt{3}\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{6} - \frac{\sqrt{3}\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{6} \\
\text{z366} \quad \mathbb{Q}_{1,1}^{(c)}(E_{1u}, a) &= \frac{\mathbb{M}_{1,2}^{(a)}(E_{1g})\mathbb{T}_1^{(b)}(A_{2u})}{2} - \frac{\mathbb{M}_1^{(a)}(A_{2g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{2} \\
\text{z367} \quad \mathbb{Q}_{1,2}^{(c)}(E_{1u}, a) &= -\frac{\mathbb{M}_{1,1}^{(a)}(E_{1g})\mathbb{T}_1^{(b)}(A_{2u})}{2} + \frac{\mathbb{M}_1^{(a)}(A_{2g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{2} \\
\text{z368} \quad \mathbb{Q}_{1,1}^{(c)}(E_{1u}, b) &= \frac{\mathbb{M}_{1,1}^{(a)}(E_{1g})\mathbb{M}_{2,1}^{(b)}(E_{2u})}{2} - \frac{\mathbb{M}_{1,2}^{(a)}(E_{1g})\mathbb{M}_{2,2}^{(b)}(E_{2u})}{2}
\end{aligned}$$

$$\text{z369} \quad \mathbb{Q}_{1,2}^{(c)}(E_{1u}, b) = -\frac{\mathbb{M}_{1,1}^{(a)}(E_{1g})\mathbb{M}_{2,2}^{(b)}(E_{2u})}{2} - \frac{\mathbb{M}_{1,2}^{(a)}(E_{1g})\mathbb{M}_{2,1}^{(b)}(E_{2u})}{2}$$

$$\text{z370} \quad \mathbb{Q}_{1,1}^{(c)}(E_{1u}, c) = -\frac{\sqrt{2}\mathbb{M}_{3,2}^{(a)}(E_{2g})\mathbb{T}_3^{(b)}(B_{1u})}{2}$$

$$\text{z371} \quad \mathbb{Q}_{1,2}^{(c)}(E_{1u}, c) = \frac{\sqrt{2}\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{T}_3^{(b)}(B_{1u})}{2}$$

$$\text{z372} \quad \mathbb{Q}_{1,1}^{(c)}(E_{1u}, d) = -\frac{\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{M}_{2,1}^{(b)}(E_{2u})}{8} + \frac{\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{M}_{2,2}^{(b)}(E_{2u})}{8} - \frac{\sqrt{15}\mathbb{M}_3^{(a)}(B_{1g})\mathbb{M}_{2,2}^{(b)}(E_{2u})}{8} + \frac{\sqrt{15}\mathbb{M}_3^{(a)}(B_{2g})\mathbb{M}_{2,1}^{(b)}(E_{2u})}{8}$$

$$\text{z373} \quad \mathbb{Q}_{1,2}^{(c)}(E_{1u}, d) = \frac{\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{M}_{2,2}^{(b)}(E_{2u})}{8} + \frac{\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{M}_{2,1}^{(b)}(E_{2u})}{8} + \frac{\sqrt{15}\mathbb{M}_3^{(a)}(B_{1g})\mathbb{M}_{2,1}^{(b)}(E_{2u})}{8} + \frac{\sqrt{15}\mathbb{M}_3^{(a)}(B_{2g})\mathbb{M}_{2,2}^{(b)}(E_{2u})}{8}$$

$$\text{z374} \quad \mathbb{Q}_{3,1}^{(c)}(E_{1u}, a) = -\frac{\sqrt{15}\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{12} + \frac{\sqrt{6}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{T}_1^{(b)}(A_{2u})}{12} + \frac{\sqrt{15}\mathbb{M}_{3,2}^{(a)}(E_{2g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{12} - \frac{\mathbb{M}_3^{(a)}(A_{2g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{2}$$

$$\text{z375} \quad \mathbb{Q}_{3,2}^{(c)}(E_{1u}, a) = -\frac{\sqrt{6}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{T}_1^{(b)}(A_{2u})}{12} + \frac{\sqrt{15}\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{12} + \frac{\sqrt{15}\mathbb{M}_{3,2}^{(a)}(E_{2g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{12} + \frac{\mathbb{M}_3^{(a)}(A_{2g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{2}$$

$$\text{z398} \quad \mathbb{Q}_{3,1}^{(c)}(E_{1u}, b) = \frac{\sqrt{15}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{M}_{2,1}^{(b)}(E_{2u})}{8} - \frac{\sqrt{15}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{M}_{2,2}^{(b)}(E_{2u})}{8} - \frac{\mathbb{M}_3^{(a)}(B_{1g})\mathbb{M}_{2,2}^{(b)}(E_{2u})}{8} + \frac{\mathbb{M}_3^{(a)}(B_{2g})\mathbb{M}_{2,1}^{(b)}(E_{2u})}{8}$$

$$\text{z399} \quad \mathbb{Q}_{3,2}^{(c)}(E_{1u}, b) = -\frac{\sqrt{15}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{M}_{2,2}^{(b)}(E_{2u})}{8} - \frac{\sqrt{15}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{M}_{2,1}^{(b)}(E_{2u})}{8} + \frac{\mathbb{M}_3^{(a)}(B_{1g})\mathbb{M}_{2,1}^{(b)}(E_{2u})}{8} + \frac{\mathbb{M}_3^{(a)}(B_{2g})\mathbb{M}_{2,2}^{(b)}(E_{2u})}{8}$$

$$\text{z400} \quad \mathbb{Q}_{5,1}^{(c)}(E_{1u}, 1) = \frac{\mathbb{M}_3^{(a)}(B_{1g})\mathbb{M}_{2,2}^{(b)}(E_{2u})}{2} + \frac{\mathbb{M}_3^{(a)}(B_{2g})\mathbb{M}_{2,1}^{(b)}(E_{2u})}{2}$$

$$\text{z401} \quad \mathbb{Q}_{5,2}^{(c)}(E_{1u}, 1) = -\frac{\mathbb{M}_3^{(a)}(B_{1g})\mathbb{M}_{2,1}^{(b)}(E_{2u})}{2} + \frac{\mathbb{M}_3^{(a)}(B_{2g})\mathbb{M}_{2,2}^{(b)}(E_{2u})}{2}$$

$$\text{z402} \quad \mathbb{G}_{2,1}^{(c)}(E_{1u}, a) = \frac{\mathbb{M}_{1,2}^{(a)}(E_{1g})\mathbb{T}_1^{(b)}(A_{2u})}{2} + \frac{\mathbb{M}_1^{(a)}(A_{2g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{2}$$

$$\text{z403} \quad \mathbb{G}_{2,2}^{(c)}(E_{1u}, a) = -\frac{\mathbb{M}_{1,1}^{(a)}(E_{1g})\mathbb{T}_1^{(b)}(A_{2u})}{2} - \frac{\mathbb{M}_1^{(a)}(A_{2g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{2}$$

$$\text{z426} \quad \mathbb{G}_{2,1}^{(c)}(E_{1u}, b) = \frac{\sqrt{210}\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{42} + \frac{2\sqrt{21}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{T}_1^{(b)}(A_{2u})}{21} - \frac{\sqrt{210}\mathbb{M}_3^{(a)}(E_{2g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{42} - \frac{\sqrt{14}\mathbb{M}_3^{(a)}(A_{2g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{14}$$

$$\begin{aligned}
\text{z427} \quad \mathbb{G}_{2,2}^{(c)}(E_{1u}, b) &= -\frac{2\sqrt{21}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{T}_1^{(b)}(A_{2u})}{21} - \frac{\sqrt{210}\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{42} - \frac{\sqrt{210}\mathbb{M}_{3,2}^{(a)}(E_{2g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{42} + \frac{\sqrt{14}\mathbb{M}_3^{(a)}(A_{2g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{14} \\
\text{z428} \quad \mathbb{G}_{4,1}^{(c)}(E_{1u}) &= -\frac{\sqrt{21}\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{28} + \frac{\sqrt{210}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{T}_1^{(b)}(A_{2u})}{28} + \frac{\sqrt{21}\mathbb{M}_{3,2}^{(a)}(E_{2g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{28} + \frac{\sqrt{35}\mathbb{M}_3^{(a)}(A_{2g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{14} \\
\text{z429} \quad \mathbb{G}_{4,2}^{(c)}(E_{1u}) &= -\frac{\sqrt{210}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{T}_1^{(b)}(A_{2u})}{28} + \frac{\sqrt{21}\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{28} + \frac{\sqrt{21}\mathbb{M}_{3,2}^{(a)}(E_{2g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{28} - \frac{\sqrt{35}\mathbb{M}_3^{(a)}(A_{2g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{14} \\
\text{z461} \quad \mathbb{Q}_{2,1}^{(c)}(E_{2g}, a) &= \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2} \\
\text{z462} \quad \mathbb{Q}_{2,2}^{(c)}(E_{2g}, a) &= \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2} \\
\text{z463} \quad \mathbb{Q}_{2,1}^{(c)}(E_{2g}, b) &= \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_0^{(b)}(A_{1g})}{2} \\
\text{z464} \quad \mathbb{Q}_{2,2}^{(c)}(E_{2g}, b) &= \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_0^{(b)}(A_{1g})}{2} \\
\text{z485} \quad \mathbb{Q}_{2,1}^{(c)}(E_{2g}, c) &= \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_4^{(b)}(B_{2g})}{2} \\
\text{z486} \quad \mathbb{Q}_{2,2}^{(c)}(E_{2g}, c) &= \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_4^{(b)}(B_{2g})}{2} \\
\text{z487} \quad \mathbb{Q}_{2,1}^{(c)}(E_{2g}, d) &= -\frac{\sqrt{15}\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{10} + \frac{\sqrt{15}\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{10} - \frac{\sqrt{5}\mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{5} \\
\text{z488} \quad \mathbb{Q}_{2,2}^{(c)}(E_{2g}, d) &= \frac{\sqrt{15}\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{10} + \frac{\sqrt{15}\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{10} - \frac{\sqrt{5}\mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{5} \\
\text{z489} \quad \mathbb{Q}_{2,1}^{(c)}(E_{2g}, e) &= -\frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_4^{(b)}(B_{2g})}{2} \\
\text{z490} \quad \mathbb{Q}_{2,2}^{(c)}(E_{2g}, e) &= -\frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_4^{(b)}(B_{2g})}{2}
\end{aligned}$$



$$\begin{aligned}
\boxed{\text{z593}} \quad \mathbb{Q}_{2,1}^{(c)}(E_{2g}, f) &= \frac{\sqrt{555}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{222} + \frac{\sqrt{7770}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{222} - \frac{\sqrt{555}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{222} - \frac{\sqrt{7770}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{222} \\
&+ \frac{\sqrt{222}\mathbb{Q}_4^{(a)}(A_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{222} - \frac{\sqrt{3885}\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{222} + \frac{\sqrt{3885}\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{222} \\
\boxed{\text{z594}} \quad \mathbb{Q}_{2,2}^{(c)}(E_{2g}, f) &= -\frac{\sqrt{555}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{222} - \frac{\sqrt{7770}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{222} - \frac{\sqrt{555}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{222} \\
&- \frac{\sqrt{7770}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{222} + \frac{\sqrt{222}\mathbb{Q}_4^{(a)}(A_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{222} + \frac{\sqrt{3885}\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{222} + \frac{\sqrt{3885}\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{222} \\
\boxed{\text{z595}} \quad \mathbb{Q}_{4,1}^{(c)}(E_{2g}, 1a) &= \frac{\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2} - \frac{\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2} \\
\boxed{\text{z596}} \quad \mathbb{Q}_{4,2}^{(c)}(E_{2g}, 1a) &= -\frac{\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2} - \frac{\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2} \\
\boxed{\text{z597}} \quad \mathbb{Q}_{4,1}^{(c)}(E_{2g}, 1b) &= \frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_0^{(b)}(A_{1g})}{2} \\
\boxed{\text{z598}} \quad \mathbb{Q}_{4,2}^{(c)}(E_{2g}, 1b) &= \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_0^{(b)}(A_{1g})}{2} \\
\boxed{\text{z599}} \quad \mathbb{Q}_{4,1}^{(c)}(E_{2g}, 1c) &= -\frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{6} + \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{6} - \frac{\sqrt{7}\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{6} - \frac{\sqrt{7}\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{6} \\
\boxed{\text{z600}} \quad \mathbb{Q}_{4,2}^{(c)}(E_{2g}, 1c) &= \frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{6} + \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{6} + \frac{\sqrt{7}\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{6} - \frac{\sqrt{7}\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{6} \\
\boxed{\text{z601}} \quad \mathbb{Q}_{4,1}^{(c)}(E_{2g}, 2a) &= -\frac{\sqrt{10}\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{10} + \frac{\sqrt{10}\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{10} + \frac{\sqrt{30}\mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{10} \\
\boxed{\text{z602}} \quad \mathbb{Q}_{4,2}^{(c)}(E_{2g}, 2a) &= \frac{\sqrt{10}\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{10} + \frac{\sqrt{10}\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{10} + \frac{\sqrt{30}\mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{10} \\
\boxed{\text{z603}} \quad \mathbb{Q}_{4,1}^{(c)}(E_{2g}, 2b) &= \frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_0^{(b)}(A_{1g})}{2} \\
\boxed{\text{z604}} \quad \mathbb{Q}_{4,2}^{(c)}(E_{2g}, 2b) &= \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_0^{(b)}(A_{1g})}{2}
\end{aligned}$$

$$\begin{aligned}
\boxed{\text{z605}} \quad \mathbb{Q}_{4,1}^{(c)}(E_{2g}, 2c) &= -\frac{137\sqrt{30747}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{122988} - \frac{13\sqrt{430458}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{61494} + \frac{137\sqrt{30747}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{122988} \\
&+ \frac{13\sqrt{430458}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{61494} - \frac{47\sqrt{307470}\mathbb{Q}_4^{(a)}(A_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{61494} - \frac{85\sqrt{215229}\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{122988} + \frac{85\sqrt{215229}\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{122988} \\
\boxed{\text{z606}} \quad \mathbb{Q}_{4,2}^{(c)}(E_{2g}, 2c) &= \frac{137\sqrt{30747}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{122988} + \frac{13\sqrt{430458}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{61494} + \frac{137\sqrt{30747}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{122988} + \frac{13\sqrt{430458}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{61494} \\
&- \frac{47\sqrt{307470}\mathbb{Q}_4^{(a)}(A_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{61494} + \frac{85\sqrt{215229}\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{122988} + \frac{85\sqrt{215229}\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{122988} \\
\boxed{\text{z607}} \quad \mathbb{Q}_{6,1}^{(c)}(E_{2g}, 1) &= \frac{\sqrt{7}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{6} - \frac{\sqrt{7}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{6} - \frac{\sqrt{2}\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{6} - \frac{\sqrt{2}\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{6} \\
\boxed{\text{z608}} \quad \mathbb{Q}_{6,2}^{(c)}(E_{2g}, 1) &= -\frac{\sqrt{7}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{6} - \frac{\sqrt{7}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{6} + \frac{\sqrt{2}\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{6} - \frac{\sqrt{2}\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{6} \\
\boxed{\text{z609}} \quad \mathbb{Q}_{6,1}^{(c)}(E_{2g}, 2) &= -\frac{17\sqrt{11634}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{4155} + \frac{11\sqrt{831}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2770} + \frac{17\sqrt{11634}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{4155} \\
&- \frac{11\sqrt{831}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2770} + \frac{7\sqrt{29085}\mathbb{Q}_4^{(a)}(A_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{4155} + \frac{\sqrt{1662}\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{1385} - \frac{\sqrt{1662}\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{1385} \\
\boxed{\text{z610}} \quad \mathbb{Q}_{6,2}^{(c)}(E_{2g}, 2) &= \frac{17\sqrt{11634}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{4155} - \frac{11\sqrt{831}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2770} + \frac{17\sqrt{11634}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{4155} \\
&- \frac{11\sqrt{831}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2770} + \frac{7\sqrt{29085}\mathbb{Q}_4^{(a)}(A_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{4155} - \frac{\sqrt{1662}\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{1385} - \frac{\sqrt{1662}\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{1385} \\
\boxed{\text{z611}} \quad \mathbb{G}_{3,1}^{(c)}(E_{2g}) &= -\frac{\sqrt{21}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{60} + \frac{\sqrt{6}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{10} + \frac{\sqrt{21}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{60} - \frac{\sqrt{6}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{10} \\
&- \frac{\sqrt{210}\mathbb{Q}_4^{(a)}(A_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{30} + \frac{3\sqrt{3}\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{20} - \frac{3\sqrt{3}\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{20} \\
\boxed{\text{z612}} \quad \mathbb{G}_{3,2}^{(c)}(E_{2g}) &= \frac{\sqrt{21}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{60} - \frac{\sqrt{6}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{10} + \frac{\sqrt{21}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{60} - \frac{\sqrt{6}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{10} \\
&- \frac{\sqrt{210}\mathbb{Q}_4^{(a)}(A_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{30} - \frac{3\sqrt{3}\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{20} - \frac{3\sqrt{3}\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{20} \\
\boxed{\text{z701}} \quad \mathbb{Q}_{3,1}^{(c)}(E_{2u}, a) &= -\frac{\sqrt{2}\mathbb{M}_{1,2}^{(a)}(E_{1g})\mathbb{T}_3^{(b)}(B_{1u})}{2}
\end{aligned}$$

$$\begin{aligned}
\boxed{\text{z702}} \quad \mathbb{Q}_{3,2}^{(c)}(E_{2u}, a) &= \frac{\sqrt{2}\mathbb{M}_{1,1}^{(a)}(E_{1g})\mathbb{T}_3^{(b)}(B_{1u})}{2} \\
\boxed{\text{z703}} \quad \mathbb{Q}_{3,1}^{(c)}(E_{2u}, b) &= -\frac{\sqrt{2}\mathbb{M}_1^{(a)}(A_{2g})\mathbb{M}_{2,2}^{(b)}(E_{2u})}{2} \\
\boxed{\text{z704}} \quad \mathbb{Q}_{3,2}^{(c)}(E_{2u}, b) &= \frac{\sqrt{2}\mathbb{M}_1^{(a)}(A_{2g})\mathbb{M}_{2,1}^{(b)}(E_{2u})}{2} \\
\boxed{\text{z705}} \quad \mathbb{Q}_{3,1}^{(c)}(E_{2u}, c) &= \frac{\sqrt{15}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{12} - \frac{\sqrt{15}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{12} - \frac{\sqrt{6}\mathbb{M}_{3,2}^{(a)}(E_{2g})\mathbb{T}_1^{(b)}(A_{2u})}{6} + \frac{\mathbb{M}_3^{(a)}(B_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{4} + \frac{\mathbb{M}_3^{(a)}(B_{2g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{4} \\
\boxed{\text{z706}} \quad \mathbb{Q}_{3,2}^{(c)}(E_{2u}, c) &= -\frac{\sqrt{15}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{12} + \frac{\sqrt{6}\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{T}_1^{(b)}(A_{2u})}{6} - \frac{\sqrt{15}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{12} - \frac{\mathbb{M}_3^{(a)}(B_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{4} + \frac{\mathbb{M}_3^{(a)}(B_{2g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{4} \\
\boxed{\text{z707}} \quad \mathbb{Q}_{3,1}^{(c)}(E_{2u}, d) &= \frac{\sqrt{2}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{T}_3^{(b)}(B_{1u})}{2} \\
\boxed{\text{z708}} \quad \mathbb{Q}_{3,2}^{(c)}(E_{2u}, d) &= -\frac{\sqrt{2}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{T}_3^{(b)}(B_{1u})}{2} \\
\boxed{\text{z709}} \quad \mathbb{Q}_{3,1}^{(c)}(E_{2u}, e) &= \frac{\sqrt{2}\mathbb{M}_3^{(a)}(A_{2g})\mathbb{M}_{2,2}^{(b)}(E_{2u})}{2} \\
\boxed{\text{z710}} \quad \mathbb{Q}_{3,2}^{(c)}(E_{2u}, e) &= -\frac{\sqrt{2}\mathbb{M}_3^{(a)}(A_{2g})\mathbb{M}_{2,1}^{(b)}(E_{2u})}{2} \\
\boxed{\text{z711}} \quad \mathbb{Q}_{5,1}^{(c)}(E_{2u}, 1) &= -\frac{\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{M}_{2,1}^{(b)}(E_{2u})}{2} + \frac{\mathbb{M}_{3,2}^{(a)}(E_{2g})\mathbb{M}_{2,2}^{(b)}(E_{2u})}{2} \\
\boxed{\text{z712}} \quad \mathbb{Q}_{5,2}^{(c)}(E_{2u}, 1) &= \frac{\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{M}_{2,2}^{(b)}(E_{2u})}{2} + \frac{\mathbb{M}_{3,2}^{(a)}(E_{2g})\mathbb{M}_{2,1}^{(b)}(E_{2u})}{2} \\
\boxed{\text{z713}} \quad \mathbb{G}_{2,1}^{(c)}(E_{2u}, a) &= \frac{\mathbb{M}_{1,1}^{(a)}(E_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{2} - \frac{\mathbb{M}_{1,2}^{(a)}(E_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{2} \\
\boxed{\text{z714}} \quad \mathbb{G}_{2,2}^{(c)}(E_{2u}, a) &= -\frac{\mathbb{M}_{1,1}^{(a)}(E_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{2} - \frac{\mathbb{M}_{1,2}^{(a)}(E_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{2} \\
\boxed{\text{z715}} \quad \mathbb{G}_{2,1}^{(c)}(E_{2u}, b) &= -\frac{\sqrt{21}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{42} + \frac{\sqrt{21}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{42} + \frac{\sqrt{210}\mathbb{M}_{3,2}^{(a)}(E_{2g})\mathbb{T}_1^{(b)}(A_{2u})}{42} + \frac{\sqrt{35}\mathbb{M}_3^{(a)}(B_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{14} + \frac{\sqrt{35}\mathbb{M}_3^{(a)}(B_{2g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{14}
\end{aligned}$$

$$\boxed{\text{z716}} \quad \mathbb{G}_{2,2}^{(c)}(E_{2u}, b) = \frac{\sqrt{21}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{42} - \frac{\sqrt{210}\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{T}_1^{(b)}(A_{2u})}{42} + \frac{\sqrt{21}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{42} - \frac{\sqrt{35}\mathbb{M}_3^{(a)}(B_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{14} + \frac{\sqrt{35}\mathbb{M}_3^{(a)}(B_{2g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{14}$$

$$\boxed{\text{z717}} \quad \mathbb{G}_{4,1}^{(c)}(E_{2u}, 1) = -\frac{\mathbb{M}_3^{(a)}(B_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{2} + \frac{\mathbb{M}_3^{(a)}(B_{2g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{2}$$

$$\boxed{\text{z718}} \quad \mathbb{G}_{4,2}^{(c)}(E_{2u}, 1) = \frac{\mathbb{M}_3^{(a)}(B_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{2} + \frac{\mathbb{M}_3^{(a)}(B_{2g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{2}$$

$$\boxed{\text{z719}} \quad \mathbb{G}_{4,1}^{(c)}(E_{2u}, 2) = \frac{\sqrt{105}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{28} - \frac{\sqrt{105}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{28} + \frac{\sqrt{42}\mathbb{M}_{3,2}^{(a)}(E_{2g})\mathbb{T}_1^{(b)}(A_{2u})}{14} - \frac{\sqrt{7}\mathbb{M}_3^{(a)}(B_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{28} - \frac{\sqrt{7}\mathbb{M}_3^{(a)}(B_{2g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{28}$$

$$\boxed{\text{z720}} \quad \mathbb{G}_{4,2}^{(c)}(E_{2u}, 2) = -\frac{\sqrt{105}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{28} - \frac{\sqrt{42}\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{T}_1^{(b)}(A_{2u})}{14} - \frac{\sqrt{105}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{28} + \frac{\sqrt{7}\mathbb{M}_3^{(a)}(B_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{28} - \frac{\sqrt{7}\mathbb{M}_3^{(a)}(B_{2g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{28}$$

---

## Atomic SAMB

---

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

$$\boxed{\text{x1}} \quad \mathbb{Q}_0^{(a)}(A_{1g}) = \begin{bmatrix} \frac{\sqrt{5}}{5} & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{5}}{5} & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{5}}{5} & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{5}}{5} & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{5}}{5} \end{bmatrix}$$

$$\boxed{\text{x2}} \quad \mathbb{Q}_2^{(a)}(A_{1g}) = \begin{bmatrix} -\frac{\sqrt{14}}{7} & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{14}}{7} & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{14}}{14} & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{14}}{14} & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{14}}{7} \end{bmatrix}$$

$$\boxed{\text{x3}} \quad \mathbb{Q}_4^{(a)}(A_{1g}) = \begin{bmatrix} \frac{\sqrt{70}}{70} & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{70}}{70} & 0 & 0 & 0 \\ 0 & 0 & -\frac{2\sqrt{70}}{35} & 0 & 0 \\ 0 & 0 & 0 & -\frac{2\sqrt{70}}{35} & 0 \\ 0 & 0 & 0 & 0 & \frac{3\sqrt{70}}{35} \end{bmatrix}$$

$$\boxed{\text{x4}} \quad \mathbb{Q}_4^{(a)}(B_{1g}) = \begin{bmatrix} 0 & 0 & \frac{1}{2} & 0 & 0 \\ 0 & 0 & 0 & -\frac{1}{2} & 0 \\ \frac{1}{2} & 0 & 0 & 0 & 0 \\ 0 & -\frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x5}} \quad \mathbb{Q}_4^{(a)}(B_{2g}) = \begin{bmatrix} 0 & 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & \frac{1}{2} & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 & 0 \\ \frac{1}{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x6}} \quad \mathbb{Q}_{2,1}^{(a)}(E_{1g}) = \begin{bmatrix} 0 & 0 & 0 & -\frac{\sqrt{42}}{14} & 0 \\ 0 & 0 & \frac{\sqrt{42}}{14} & 0 & 0 \\ 0 & \frac{\sqrt{42}}{14} & 0 & 0 & 0 \\ -\frac{\sqrt{42}}{14} & 0 & 0 & 0 & \frac{\sqrt{14}}{14} \\ 0 & 0 & 0 & \frac{\sqrt{14}}{14} & 0 \end{bmatrix}$$

$$\boxed{\text{x7}} \quad \mathbb{Q}_{2,2}^{(a)}(E_{1g}) = \begin{bmatrix} 0 & 0 & -\frac{\sqrt{42}}{14} & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{42}}{14} & 0 \\ -\frac{\sqrt{42}}{14} & 0 & 0 & 0 & -\frac{\sqrt{14}}{14} \\ 0 & -\frac{\sqrt{42}}{14} & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{14}}{14} & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x8}} \quad \mathbb{Q}_{4,1}^{(a)}(E_{1g}) = \begin{bmatrix} 0 & 0 & 0 & \frac{\sqrt{7}}{14} & 0 \\ 0 & 0 & -\frac{\sqrt{7}}{14} & 0 & 0 \\ 0 & -\frac{\sqrt{7}}{14} & 0 & 0 & 0 \\ \frac{\sqrt{7}}{14} & 0 & 0 & 0 & \frac{\sqrt{21}}{7} \\ 0 & 0 & 0 & \frac{\sqrt{21}}{7} & 0 \end{bmatrix}$$

$$\boxed{\text{x9}} \quad \mathbb{Q}_{4,2}^{(a)}(E_{1g}) = \begin{bmatrix} 0 & 0 & \frac{\sqrt{7}}{14} & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{7}}{14} & 0 \\ \frac{\sqrt{7}}{14} & 0 & 0 & 0 & -\frac{\sqrt{21}}{7} \\ 0 & \frac{\sqrt{7}}{14} & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{21}}{7} & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x10}} \quad \mathbb{Q}_{2,1}^{(a)}(E_{2g}) = \begin{bmatrix} 0 & 0 & 0 & 0 & -\frac{\sqrt{14}}{7} \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{42}}{14} & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{42}}{14} & 0 \\ -\frac{\sqrt{14}}{7} & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x11}} \quad \mathbb{Q}_{2,2}^{(a)}(E_{2g}) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{14}}{7} \\ 0 & 0 & 0 & -\frac{\sqrt{42}}{14} & 0 \\ 0 & 0 & -\frac{\sqrt{42}}{14} & 0 & 0 \\ 0 & \frac{\sqrt{14}}{7} & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x12}} \quad \mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1) = \begin{bmatrix} \frac{\sqrt{2}}{2} & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{2}}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x13}} \quad \mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1) = \begin{bmatrix} 0 & \frac{\sqrt{2}}{2} & 0 & 0 & 0 \\ \frac{\sqrt{2}}{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x14}} \quad \mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2) = \begin{bmatrix} 0 & 0 & 0 & 0 & \frac{\sqrt{42}}{14} \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{14}}{7} & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{14}}{7} & 0 \\ \frac{\sqrt{42}}{14} & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x15}} \quad \mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{42}}{14} \\ 0 & 0 & 0 & -\frac{\sqrt{14}}{7} & 0 \\ 0 & 0 & -\frac{\sqrt{14}}{7} & 0 & 0 \\ 0 & -\frac{\sqrt{42}}{14} & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x16}} \quad \mathbb{M}_1^{(a)}(A_{2g}) = \begin{bmatrix} 0 & -\frac{\sqrt{10}i}{5} & 0 & 0 & 0 \\ \frac{\sqrt{10}i}{5} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{10}i}{10} & 0 \\ 0 & 0 & \frac{\sqrt{10}i}{10} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x17}} \quad \mathbb{M}_3^{(a)}(A_{2g}) = \begin{bmatrix} 0 & \frac{\sqrt{10}i}{10} & 0 & 0 & 0 \\ -\frac{\sqrt{10}i}{10} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{10}i}{5} & 0 \\ 0 & 0 & \frac{\sqrt{10}i}{5} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x18}} \quad \mathbb{M}_3^{(a)}(B_{1g}) = \begin{bmatrix} 0 & 0 & \frac{i}{2} & 0 & 0 \\ 0 & 0 & 0 & -\frac{i}{2} & 0 \\ -\frac{i}{2} & 0 & 0 & 0 & 0 \\ 0 & \frac{i}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x19}} \quad \mathbb{M}_3^{(a)}(B_{2g}) = \begin{bmatrix} 0 & 0 & 0 & -\frac{i}{2} & 0 \\ 0 & 0 & -\frac{i}{2} & 0 & 0 \\ 0 & \frac{i}{2} & 0 & 0 & 0 \\ \frac{i}{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x20}} \quad \mathbb{M}_{1,1}^{(a)}(E_{1g}) = \begin{bmatrix} 0 & 0 & 0 & \frac{\sqrt{10}i}{10} & 0 \\ 0 & 0 & -\frac{\sqrt{10}i}{10} & 0 & 0 \\ 0 & \frac{\sqrt{10}i}{10} & 0 & 0 & 0 \\ -\frac{\sqrt{10}i}{10} & 0 & 0 & 0 & -\frac{\sqrt{30}i}{10} \\ 0 & 0 & 0 & \frac{\sqrt{30}i}{10} & 0 \end{bmatrix}$$

$$\boxed{\text{x21}} \quad \mathbb{M}_{1,2}^{(a)}(E_{1g}) = \begin{bmatrix} 0 & 0 & \frac{\sqrt{10}i}{10} & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{10}i}{10} & 0 \\ -\frac{\sqrt{10}i}{10} & 0 & 0 & 0 & \frac{\sqrt{30}i}{10} \\ 0 & -\frac{\sqrt{10}i}{10} & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{30}i}{10} & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x22}} \quad \mathbb{M}_{3,1}^{(a)}(E_{1g}) = \begin{bmatrix} 0 & 0 & 0 & -\frac{\sqrt{15}i}{10} & 0 \\ 0 & 0 & \frac{\sqrt{15}i}{10} & 0 & 0 \\ 0 & -\frac{\sqrt{15}i}{10} & 0 & 0 & 0 \\ \frac{\sqrt{15}i}{10} & 0 & 0 & 0 & -\frac{\sqrt{5}i}{5} \\ 0 & 0 & 0 & \frac{\sqrt{5}i}{5} & 0 \end{bmatrix}$$



$$\boxed{\text{x23}} \quad \mathbb{M}_{3,2}^{(a)}(E_{1g}) = \begin{bmatrix} 0 & 0 & -\frac{\sqrt{15}i}{10} & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{15}i}{10} & 0 \\ \frac{\sqrt{15}i}{10} & 0 & 0 & 0 & \frac{\sqrt{5}i}{5} \\ 0 & \frac{\sqrt{15}i}{10} & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{5}i}{5} & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x24}} \quad \mathbb{M}_{3,1}^{(a)}(E_{2g}) = \begin{bmatrix} 0 & 0 & 0 & 0 & \frac{\sqrt{2}i}{2} \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ -\frac{\sqrt{2}i}{2} & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x25}} \quad \mathbb{M}_{3,2}^{(a)}(E_{2g}) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{2}i}{2} \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{2}i}{2} & 0 & 0 & 0 \end{bmatrix}$$

---

### Cluster SAMB

---

- Site cluster

\*\* Wyckoff: 2c

$$\boxed{\text{y1}} \quad \mathbb{Q}_0^{(s)}(A_{1g}) = \left[ \frac{\sqrt{2}}{2}, \frac{\sqrt{2}}{2} \right]$$

$$\boxed{\text{y2}} \quad \mathbb{Q}_3^{(s)}(B_{1u}) = \left[ \frac{\sqrt{2}}{2}, -\frac{\sqrt{2}}{2} \right]$$

\*\* Wyckoff: 6h

$$\boxed{\text{y3}} \quad \mathbb{Q}_0^{(s)}(A_{1g}) = \left[ \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6} \right]$$

$$\boxed{\text{y4}} \quad \mathbb{Q}_3^{(s)}(B_{1u}) = \left[ \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, -\frac{\sqrt{6}}{6}, -\frac{\sqrt{6}}{6}, -\frac{\sqrt{6}}{6} \right]$$

$$\boxed{\text{y5}} \quad \mathbb{Q}_{1,1}^{(s)}(E_{1u}) = \left[ 0, -\frac{1}{2}, \frac{1}{2}, 0, \frac{1}{2}, -\frac{1}{2} \right]$$

$$\boxed{\text{y6}} \quad \mathbb{Q}_{1,2}^{(s)}(E_{1u}) = \left[ \frac{\sqrt{3}}{3}, -\frac{\sqrt{3}}{6}, -\frac{\sqrt{3}}{6}, -\frac{\sqrt{3}}{3}, \frac{\sqrt{3}}{6}, \frac{\sqrt{3}}{6} \right]$$

$$\boxed{\text{y7}} \quad \mathbb{Q}_{2,1}^{(s)}(E_{2g}) = \left[ \frac{\sqrt{3}}{3}, -\frac{\sqrt{3}}{6}, -\frac{\sqrt{3}}{6}, \frac{\sqrt{3}}{3}, -\frac{\sqrt{3}}{6}, -\frac{\sqrt{3}}{6} \right]$$

$$\boxed{\text{y8}} \quad \mathbb{Q}_{2,2}^{(s)}(E_{2g}) = \left[ 0, \frac{1}{2}, -\frac{1}{2}, 0, \frac{1}{2}, -\frac{1}{2} \right]$$

• Bond cluster

\*\* Wyckoff: 6a@6g

$$\boxed{\text{y9}} \quad \mathbb{Q}_0^{(s)}(A_{1g}) = \left[ \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6} \right]$$

$$\boxed{\text{y10}} \quad \mathbb{T}_1^{(s)}(A_{2u}) = \left[ \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6} \right]$$

$$\boxed{\text{y11}} \quad \mathbb{T}_3^{(s)}(B_{1u}) = \left[ \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, -\frac{\sqrt{6}i}{6}, -\frac{\sqrt{6}i}{6}, -\frac{\sqrt{6}i}{6} \right]$$

$$\boxed{\text{y12}} \quad \mathbb{Q}_4^{(s)}(B_{2g}) = \left[ \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, -\frac{\sqrt{6}}{6}, -\frac{\sqrt{6}}{6}, -\frac{\sqrt{6}}{6} \right]$$

$$\boxed{\text{y13}} \quad \mathbb{Q}_{2,1}^{(s)}(E_{1g}) = \left[ \frac{\sqrt{3}}{3}, -\frac{\sqrt{3}}{6}, -\frac{\sqrt{3}}{6}, -\frac{\sqrt{3}}{3}, \frac{\sqrt{3}}{6}, \frac{\sqrt{3}}{6} \right]$$

$$\boxed{\text{y14}} \quad \mathbb{Q}_{2,2}^{(s)}(E_{1g}) = \left[ 0, \frac{1}{2}, -\frac{1}{2}, 0, -\frac{1}{2}, \frac{1}{2} \right]$$

$$\boxed{\text{y15}} \quad \mathbb{T}_{1,1}^{(s)}(E_{1u}) = \left[ 0, -\frac{i}{2}, \frac{i}{2}, 0, \frac{i}{2}, -\frac{i}{2} \right]$$

$$\boxed{\text{y16}} \quad \mathbb{T}_{1,2}^{(s)}(E_{1u}) = \left[ \frac{\sqrt{3}i}{3}, -\frac{\sqrt{3}i}{6}, -\frac{\sqrt{3}i}{6}, -\frac{\sqrt{3}i}{3}, \frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{6} \right]$$

$$\boxed{\text{y17}} \quad \mathbb{Q}_{2,1}^{(s)}(E_{2g}) = \left[ \frac{\sqrt{3}}{3}, -\frac{\sqrt{3}}{6}, -\frac{\sqrt{3}}{6}, \frac{\sqrt{3}}{3}, -\frac{\sqrt{3}}{6}, -\frac{\sqrt{3}}{6} \right]$$

$$\boxed{\text{y18}} \quad \mathbb{Q}_{2,2}^{(s)}(E_{2g}) = \left[ 0, \frac{1}{2}, -\frac{1}{2}, 0, \frac{1}{2}, -\frac{1}{2} \right]$$

$$\boxed{\text{y19}} \quad \mathbb{M}_{2,1}^{(s)}(E_{2u}) = \left[ 0, -\frac{i}{2}, \frac{i}{2}, 0, -\frac{i}{2}, \frac{i}{2} \right]$$

$$\boxed{\text{y20}} \quad \mathbb{M}_{2,2}^{(s)}(E_{2u}) = \left[ \frac{\sqrt{3}i}{3}, -\frac{\sqrt{3}i}{6}, -\frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{3}, -\frac{\sqrt{3}i}{6}, -\frac{\sqrt{3}i}{6} \right]$$

\*\* Wyckoff: 6b@6h

$$\boxed{\text{y21}} \quad \mathbb{Q}_0^{(s)}(A_{1g}) = \left[ \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6} \right]$$

$$\boxed{\text{y22}} \quad \mathbb{M}_1^{(s)}(A_{2g}) = \left[ \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6} \right]$$

$$\boxed{\text{y23}} \quad \mathbb{Q}_3^{(s)}(B_{1u}) = \left[ \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, -\frac{\sqrt{6}}{6}, -\frac{\sqrt{6}}{6}, -\frac{\sqrt{6}}{6} \right]$$

$$\boxed{\text{y24}} \quad \mathbb{T}_3^{(s)}(B_{2u}) = \left[ \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, -\frac{\sqrt{6}i}{6}, -\frac{\sqrt{6}i}{6}, -\frac{\sqrt{6}i}{6} \right]$$

$$\boxed{\text{y25}} \quad \mathbb{Q}_{1,1}^{(s)}(E_{1u}) = \left[ 0, -\frac{1}{2}, \frac{1}{2}, 0, \frac{1}{2}, -\frac{1}{2} \right]$$

$$\boxed{\text{y26}} \quad \mathbb{Q}_{1,2}^{(s)}(E_{1u}) = \left[ \frac{\sqrt{3}}{3}, -\frac{\sqrt{3}}{6}, -\frac{\sqrt{3}}{6}, -\frac{\sqrt{3}}{3}, \frac{\sqrt{3}}{6}, \frac{\sqrt{3}}{6} \right]$$

$$\boxed{\text{y27}} \quad \mathbb{T}_{1,1}^{(s)}(E_{1u}) = \left[ \frac{\sqrt{3}i}{3}, -\frac{\sqrt{3}i}{6}, -\frac{\sqrt{3}i}{6}, -\frac{\sqrt{3}i}{3}, \frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{6} \right]$$

$$\boxed{\text{y28}} \quad \mathbb{T}_{1,2}^{(s)}(E_{1u}) = \left[ 0, \frac{i}{2}, -\frac{i}{2}, 0, -\frac{i}{2}, \frac{i}{2} \right]$$

$$\boxed{\text{y29}} \quad \mathbb{Q}_{2,1}^{(s)}(E_{2g}) = \left[ \frac{\sqrt{3}}{3}, -\frac{\sqrt{3}}{6}, -\frac{\sqrt{3}}{6}, \frac{\sqrt{3}}{3}, -\frac{\sqrt{3}}{6}, -\frac{\sqrt{3}}{6} \right]$$

$$\boxed{\text{y30}} \quad \mathbb{Q}_{2,2}^{(s)}(E_{2g}) = \left[ 0, \frac{1}{2}, -\frac{1}{2}, 0, \frac{1}{2}, -\frac{1}{2} \right]$$

$$\boxed{\text{y31}} \quad \mathbb{T}_{2,1}^{(s)}(E_{2g}) = \left[ 0, \frac{i}{2}, -\frac{i}{2}, 0, \frac{i}{2}, -\frac{i}{2} \right]$$

$$\boxed{\text{y32}} \quad \mathbb{T}_{2,2}^{(s)}(E_{2g}) = \left[ -\frac{\sqrt{3}i}{3}, \frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{6}, -\frac{\sqrt{3}i}{3}, \frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{6} \right]$$

\*\* Wyckoff: 12a012j

$$\boxed{\text{y33}} \quad \mathbb{Q}_0^{(s)}(A_{1g}) = \left[ \frac{\sqrt{3}}{6}, \frac{\sqrt{3}}{6}, \frac{\sqrt{3}}{6}, \frac{\sqrt{3}}{6}, \frac{\sqrt{3}}{6}, \frac{\sqrt{3}}{6}, \frac{\sqrt{3}}{6}, \frac{\sqrt{3}}{6}, \frac{\sqrt{3}}{6}, \frac{\sqrt{3}}{6}, \frac{\sqrt{3}}{6}, \frac{\sqrt{3}}{6} \right]$$

$$\boxed{\text{y34}} \quad \mathbb{T}_0^{(s)}(A_{1g}) = \left[ \frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{6} \right]$$

$$\boxed{\text{y35}} \quad \mathbb{M}_1^{(s)}(A_{2g}) = \left[ \frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{6}, -\frac{\sqrt{3}i}{6}, -\frac{\sqrt{3}i}{6}, -\frac{\sqrt{3}i}{6}, -\frac{\sqrt{3}i}{6}, -\frac{\sqrt{3}i}{6}, -\frac{\sqrt{3}i}{6} \right]$$

$$\boxed{\text{y36}} \quad \mathbb{Q}_6^{(s)}(A_{2g}) = \left[ \frac{\sqrt{3}}{6}, \frac{\sqrt{3}}{6}, \frac{\sqrt{3}}{6}, \frac{\sqrt{3}}{6}, \frac{\sqrt{3}}{6}, \frac{\sqrt{3}}{6}, -\frac{\sqrt{3}}{6}, -\frac{\sqrt{3}}{6}, -\frac{\sqrt{3}}{6}, -\frac{\sqrt{3}}{6}, -\frac{\sqrt{3}}{6}, -\frac{\sqrt{3}}{6} \right]$$

$$\boxed{\text{y37}} \quad \mathbb{Q}_3^{(s)}(B_{1u}) = \left[ \frac{\sqrt{3}}{6}, \frac{\sqrt{3}}{6}, \frac{\sqrt{3}}{6}, -\frac{\sqrt{3}}{6}, -\frac{\sqrt{3}}{6}, -\frac{\sqrt{3}}{6}, -\frac{\sqrt{3}}{6}, -\frac{\sqrt{3}}{6}, -\frac{\sqrt{3}}{6}, -\frac{\sqrt{3}}{6}, \frac{\sqrt{3}}{6}, \frac{\sqrt{3}}{6}, \frac{\sqrt{3}}{6} \right]$$

$$\boxed{\text{y38}} \quad \mathbb{T}_3^{(s)}(B_{1u}) = \left[ \frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{6}, -\frac{\sqrt{3}i}{6}, -\frac{\sqrt{3}i}{6}, -\frac{\sqrt{3}i}{6}, -\frac{\sqrt{3}i}{6}, -\frac{\sqrt{3}i}{6}, -\frac{\sqrt{3}i}{6}, -\frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{6} \right]$$

$$\boxed{\text{y39}} \quad \mathbb{Q}_3^{(s)}(B_{2u}) = \left[ \frac{\sqrt{3}}{6}, \frac{\sqrt{3}}{6}, \frac{\sqrt{3}}{6}, -\frac{\sqrt{3}}{6}, -\frac{\sqrt{3}}{6}, -\frac{\sqrt{3}}{6}, \frac{\sqrt{3}}{6}, \frac{\sqrt{3}}{6}, \frac{\sqrt{3}}{6}, \frac{\sqrt{3}}{6}, -\frac{\sqrt{3}}{6}, -\frac{\sqrt{3}}{6}, -\frac{\sqrt{3}}{6} \right]$$

$$\boxed{\text{y40}} \quad \mathbb{T}_3^{(s)}(B_{2u}) = \left[ \frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{6}, -\frac{\sqrt{3}i}{6}, -\frac{\sqrt{3}i}{6}, -\frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{6}, -\frac{\sqrt{3}i}{6}, -\frac{\sqrt{3}i}{6}, -\frac{\sqrt{3}i}{6} \right]$$

$$\begin{aligned}
\boxed{\text{y41}} \quad \mathbb{Q}_{1,1}^{(s)}(E_{1u}) &= \left[ \frac{5\sqrt{42}}{84}, -\frac{\sqrt{42}}{21}, -\frac{\sqrt{42}}{84}, -\frac{5\sqrt{42}}{84}, \frac{\sqrt{42}}{21}, \frac{\sqrt{42}}{84}, -\frac{\sqrt{42}}{84}, \frac{5\sqrt{42}}{84}, -\frac{\sqrt{42}}{21}, \frac{\sqrt{42}}{84}, -\frac{5\sqrt{42}}{84}, \frac{\sqrt{42}}{21} \right] \\
\boxed{\text{y42}} \quad \mathbb{Q}_{1,2}^{(s)}(E_{1u}) &= \left[ \frac{\sqrt{14}}{28}, \frac{\sqrt{14}}{14}, -\frac{3\sqrt{14}}{28}, -\frac{\sqrt{14}}{28}, -\frac{\sqrt{14}}{14}, \frac{3\sqrt{14}}{28}, \frac{3\sqrt{14}}{28}, -\frac{\sqrt{14}}{28}, -\frac{\sqrt{14}}{14}, -\frac{3\sqrt{14}}{28}, \frac{\sqrt{14}}{28}, \frac{\sqrt{14}}{14} \right] \\
\boxed{\text{y43}} \quad \mathbb{T}_{1,1}^{(s)}(E_{1u}, a) &= \left[ \frac{5\sqrt{42}i}{84}, -\frac{\sqrt{42}i}{21}, -\frac{\sqrt{42}i}{84}, -\frac{5\sqrt{42}i}{84}, \frac{\sqrt{42}i}{21}, \frac{\sqrt{42}i}{84}, -\frac{\sqrt{42}i}{84}, \frac{5\sqrt{42}i}{84}, -\frac{\sqrt{42}i}{21}, \frac{\sqrt{42}i}{84}, -\frac{5\sqrt{42}i}{84}, \frac{\sqrt{42}i}{21} \right] \\
\boxed{\text{y44}} \quad \mathbb{T}_{1,2}^{(s)}(E_{1u}, a) &= \left[ \frac{\sqrt{14}i}{28}, \frac{\sqrt{14}i}{14}, -\frac{3\sqrt{14}i}{28}, -\frac{\sqrt{14}i}{28}, -\frac{\sqrt{14}i}{14}, \frac{3\sqrt{14}i}{28}, \frac{3\sqrt{14}i}{28}, -\frac{\sqrt{14}i}{28}, -\frac{\sqrt{14}i}{14}, -\frac{3\sqrt{14}i}{28}, \frac{\sqrt{14}i}{28}, \frac{\sqrt{14}i}{14} \right] \\
\boxed{\text{y45}} \quad \mathbb{T}_{1,1}^{(s)}(E_{1u}, b) &= \left[ \frac{\sqrt{14}i}{28}, \frac{\sqrt{14}i}{14}, -\frac{3\sqrt{14}i}{28}, -\frac{\sqrt{14}i}{28}, -\frac{\sqrt{14}i}{14}, \frac{3\sqrt{14}i}{28}, -\frac{3\sqrt{14}i}{28}, \frac{\sqrt{14}i}{28}, \frac{\sqrt{14}i}{14}, \frac{3\sqrt{14}i}{28}, -\frac{\sqrt{14}i}{28}, -\frac{\sqrt{14}i}{14} \right] \\
\boxed{\text{y46}} \quad \mathbb{T}_{1,2}^{(s)}(E_{1u}, b) &= \left[ -\frac{5\sqrt{42}i}{84}, \frac{\sqrt{42}i}{21}, \frac{\sqrt{42}i}{84}, \frac{5\sqrt{42}i}{84}, -\frac{\sqrt{42}i}{21}, -\frac{\sqrt{42}i}{84}, -\frac{\sqrt{42}i}{84}, \frac{5\sqrt{42}i}{84}, -\frac{\sqrt{42}i}{21}, \frac{\sqrt{42}i}{84}, -\frac{5\sqrt{42}i}{84}, \frac{\sqrt{42}i}{21} \right] \\
\boxed{\text{y47}} \quad \mathbb{Q}_{5,1}^{(s)}(E_{1u}, 1) &= \left[ \frac{\sqrt{14}}{28}, \frac{\sqrt{14}}{14}, -\frac{3\sqrt{14}}{28}, -\frac{\sqrt{14}}{28}, -\frac{\sqrt{14}}{14}, \frac{3\sqrt{14}}{28}, -\frac{3\sqrt{14}}{28}, \frac{\sqrt{14}}{28}, \frac{\sqrt{14}}{14}, \frac{3\sqrt{14}}{28}, -\frac{\sqrt{14}}{28}, -\frac{\sqrt{14}}{14} \right] \\
\boxed{\text{y48}} \quad \mathbb{Q}_{5,2}^{(s)}(E_{1u}, 1) &= \left[ -\frac{5\sqrt{42}}{84}, \frac{\sqrt{42}}{21}, \frac{\sqrt{42}}{84}, \frac{5\sqrt{42}}{84}, -\frac{\sqrt{42}}{21}, -\frac{\sqrt{42}}{84}, -\frac{\sqrt{42}}{84}, \frac{5\sqrt{42}}{84}, -\frac{\sqrt{42}}{21}, \frac{\sqrt{42}}{84}, -\frac{5\sqrt{42}}{84}, \frac{\sqrt{42}}{21} \right] \\
\boxed{\text{y49}} \quad \mathbb{Q}_{2,1}^{(s)}(E_{2g}) &= \left[ \frac{11\sqrt{6}}{84}, \frac{\sqrt{6}}{42}, -\frac{13\sqrt{6}}{84}, \frac{11\sqrt{6}}{84}, \frac{\sqrt{6}}{42}, -\frac{13\sqrt{6}}{84}, -\frac{13\sqrt{6}}{84}, \frac{11\sqrt{6}}{84}, \frac{\sqrt{6}}{42}, -\frac{13\sqrt{6}}{84}, \frac{11\sqrt{6}}{84}, \frac{\sqrt{6}}{42} \right] \\
\boxed{\text{y50}} \quad \mathbb{Q}_{2,2}^{(s)}(E_{2g}) &= \left[ -\frac{5\sqrt{2}}{28}, \frac{2\sqrt{2}}{7}, -\frac{3\sqrt{2}}{28}, -\frac{5\sqrt{2}}{28}, \frac{2\sqrt{2}}{7}, -\frac{3\sqrt{2}}{28}, \frac{3\sqrt{2}}{28}, \frac{5\sqrt{2}}{28}, -\frac{2\sqrt{2}}{7}, \frac{3\sqrt{2}}{28}, \frac{5\sqrt{2}}{28}, -\frac{2\sqrt{2}}{7} \right] \\
\boxed{\text{y51}} \quad \mathbb{T}_{2,1}^{(s)}(E_{2g}, a) &= \left[ \frac{11\sqrt{6}i}{84}, \frac{\sqrt{6}i}{42}, -\frac{13\sqrt{6}i}{84}, \frac{11\sqrt{6}i}{84}, \frac{\sqrt{6}i}{42}, -\frac{13\sqrt{6}i}{84}, -\frac{13\sqrt{6}i}{84}, \frac{11\sqrt{6}i}{84}, \frac{\sqrt{6}i}{42}, -\frac{13\sqrt{6}i}{84}, \frac{11\sqrt{6}i}{84}, \frac{\sqrt{6}i}{42} \right] \\
\boxed{\text{y52}} \quad \mathbb{T}_{2,2}^{(s)}(E_{2g}, a) &= \left[ -\frac{5\sqrt{2}i}{28}, \frac{2\sqrt{2}i}{7}, -\frac{3\sqrt{2}i}{28}, -\frac{5\sqrt{2}i}{28}, \frac{2\sqrt{2}i}{7}, -\frac{3\sqrt{2}i}{28}, \frac{3\sqrt{2}i}{28}, \frac{5\sqrt{2}i}{28}, -\frac{2\sqrt{2}i}{7}, \frac{3\sqrt{2}i}{28}, \frac{5\sqrt{2}i}{28}, -\frac{2\sqrt{2}i}{7} \right] \\
\boxed{\text{y53}} \quad \mathbb{T}_{2,1}^{(s)}(E_{2g}, b) &= \left[ \frac{5\sqrt{2}i}{28}, -\frac{2\sqrt{2}i}{7}, \frac{3\sqrt{2}i}{28}, \frac{5\sqrt{2}i}{28}, -\frac{2\sqrt{2}i}{7}, \frac{3\sqrt{2}i}{28}, \frac{3\sqrt{2}i}{28}, \frac{5\sqrt{2}i}{28}, -\frac{2\sqrt{2}i}{7}, \frac{3\sqrt{2}i}{28}, \frac{5\sqrt{2}i}{28}, -\frac{2\sqrt{2}i}{7} \right]
\end{aligned}$$

$$\boxed{\text{y54}} \quad \mathbb{T}_{2,2}^{(s)}(E_{2g}, b) = \left[ \frac{11\sqrt{6}i}{84}, \frac{\sqrt{6}i}{42}, -\frac{13\sqrt{6}i}{84}, \frac{11\sqrt{6}i}{84}, \frac{\sqrt{6}i}{42}, -\frac{13\sqrt{6}i}{84}, \frac{13\sqrt{6}i}{84}, -\frac{11\sqrt{6}i}{84}, -\frac{\sqrt{6}i}{42}, \frac{13\sqrt{6}i}{84}, -\frac{11\sqrt{6}i}{84}, -\frac{\sqrt{6}i}{42} \right]$$

$$\boxed{\text{y55}} \quad \mathbb{Q}_{4,1}^{(s)}(E_{2g}, 1) = \left[ \frac{5\sqrt{2}}{28}, -\frac{2\sqrt{2}}{7}, \frac{3\sqrt{2}}{28}, \frac{5\sqrt{2}}{28}, -\frac{2\sqrt{2}}{7}, \frac{3\sqrt{2}}{28}, \frac{3\sqrt{2}}{28}, \frac{5\sqrt{2}}{28}, -\frac{2\sqrt{2}}{7}, \frac{3\sqrt{2}}{28}, \frac{5\sqrt{2}}{28}, -\frac{2\sqrt{2}}{7} \right]$$

$$\boxed{\text{y56}} \quad \mathbb{Q}_{4,2}^{(s)}(E_{2g}, 1) = \left[ \frac{11\sqrt{6}}{84}, \frac{\sqrt{6}}{42}, -\frac{13\sqrt{6}}{84}, \frac{11\sqrt{6}}{84}, \frac{\sqrt{6}}{42}, -\frac{13\sqrt{6}}{84}, \frac{13\sqrt{6}}{84}, -\frac{11\sqrt{6}}{84}, -\frac{\sqrt{6}}{42}, \frac{13\sqrt{6}}{84}, -\frac{11\sqrt{6}}{84}, -\frac{\sqrt{6}}{42} \right]$$

---

### Site and Bond

---

Table 5: Orbital of each site

#	site	orbital
1	Mn	$ d_v\rangle,  d_{xy}\rangle,  d_{xz}\rangle,  d_{yz}\rangle,  d_u\rangle$
2	Sn	$ d_v\rangle,  d_{xy}\rangle,  d_{xz}\rangle,  d_{yz}\rangle,  d_u\rangle$

Table 6: Neighbor and bra-ket of each bond

#	head	tail	neighbor	head (bra)	tail (ket)
1	Mn	Mn	[1]	[d]	[d]
2	Mn	Sn	[1]	[d]	[d]
3	Sn	Sn	[1]	[d]	[d]

---

### Site in Unit Cell

---

Sites in (conventional) cell (no plus set), SL = sublattice

Table 7: 'Mn' (#1) site cluster (6h), mm2

SL	position ( $s$ )	mapping
1	[ 0.83880, 0.67760, 0.25000]	[1,11,16,20]
2	[ 0.32240, 0.16120, 0.25000]	[2,10,17,19]
3	[ 0.83880, 0.16120, 0.25000]	[3,12,18,21]
4	[ 0.16120, 0.32240, 0.75000]	[4,8,13,23]
5	[ 0.67760, 0.83880, 0.75000]	[5,7,14,22]
6	[ 0.16120, 0.83880, 0.75000]	[6,9,15,24]

Table 8: 'Sn' (#2) site cluster (2c), -6m2

SL	position ( $s$ )	mapping
1	[ 0.33333, 0.66667, 0.25000]	[1,2,3,10,11,12,16,17,18,19,20,21]
2	[ 0.66667, 0.33333, 0.75000]	[4,5,6,7,8,9,13,14,15,22,23,24]

## — Bond in Unit Cell —

Bonds in (conventional) cell (no plus set): tail, head = (SL, plus set), (N)D = (non)directional (listed up to 5th neighbor at most)

Table 9: 1-th 'Mn'-'Mn' [1] (#1) bond cluster (6b@6h), ND,  $|\mathbf{v}|=0.4836$  (cartesian)

SL	vector ( $\mathbf{v}$ )	center ( $\mathbf{c}$ )	mapping	head	tail	$\mathbf{R}$ (primitive)
1	[-0.48360, 0.00000, 0.00000]	[ 0.08060, 0.16120, 0.25000]	[1,-11,16,-20]	(3,1)	(2,1)	[1,0,0]
2	[ 0.00000,-0.48360, 0.00000]	[ 0.83880, 0.91940, 0.25000]	[2,-10,17,-19]	(1,1)	(3,1)	[0,1,0]
3	[ 0.48360, 0.48360, 0.00000]	[ 0.08060, 0.91940, 0.25000]	[3,-12,18,-21]	(2,1)	(1,1)	[-1,-1,0]
4	[ 0.48360, 0.00000, 0.00000]	[ 0.91940, 0.83880, 0.75000]	[4,-8,13,-23]	(6,1)	(5,1)	[-1,0,0]
5	[ 0.00000, 0.48360, 0.00000]	[ 0.16120, 0.08060, 0.75000]	[5,-7,14,-22]	(4,1)	(6,1)	[0,-1,0]
6	[-0.48360,-0.48360, 0.00000]	[ 0.91940, 0.08060, 0.75000]	[6,-9,15,-24]	(5,1)	(4,1)	[1,1,0]

Table 10: 1-th 'Mn'-'Sn' [1] (#2) bond cluster (12a@12j), D,  $|\mathbf{v}|=0.50009$  (cartesian)

SL	vector ( $\mathbf{v}$ )	center ( $\mathbf{c}$ )	mapping	head	tail	$\mathbf{R}$ (primitive)
1	[-0.49453, 0.01093, 0.00000]	[ 0.08607, 0.67213, 0.25000]	[1,16]	(1,1)	(1,1)	[1,0,0]
2	[-0.01093,-0.50547, 0.00000]	[ 0.32787, 0.41393, 0.25000]	[2,17]	(2,1)	(1,1)	[0,0,0]
3	[ 0.50547, 0.49453, 0.00000]	[ 0.58607, 0.91393, 0.25000]	[3,18]	(3,1)	(1,1)	[0,-1,0]
4	[ 0.49453,-0.01093, 0.00000]	[ 0.91393, 0.32787, 0.75000]	[4,13]	(4,1)	(2,1)	[-1,0,0]
5	[ 0.01093, 0.50547, 0.00000]	[ 0.67213, 0.58607, 0.75000]	[5,14]	(5,1)	(2,1)	[0,0,0]
6	[-0.50547,-0.49453, 0.00000]	[ 0.41393, 0.08607, 0.75000]	[6,15]	(6,1)	(2,1)	[0,1,0]
7	[ 0.01093,-0.49453, 0.00000]	[ 0.67213, 0.08607, 0.75000]	[7,22]	(5,1)	(2,1)	[0,1,0]
8	[-0.50547,-0.01093, 0.00000]	[ 0.41393, 0.32787, 0.75000]	[8,23]	(4,1)	(2,1)	[0,0,0]
9	[ 0.49453, 0.50547, 0.00000]	[ 0.91393, 0.58607, 0.75000]	[9,24]	(6,1)	(2,1)	[-1,0,0]

*continued ...*



Table 10

SL	vector ( $\boldsymbol{v}$ )	center ( $\boldsymbol{c}$ )	mapping	head	tail	$\boldsymbol{R}$ (primitive)
10	[-0.01093, 0.49453, 0.00000]	[ 0.32787, 0.91393, 0.25000]	[10,19]	(2,1)	(1,1)	[0,-1,0]
11	[ 0.50547, 0.01093, 0.00000]	[ 0.58607, 0.67213, 0.25000]	[11,20]	(1,1)	(1,1)	[0,0,0]
12	[-0.49453,-0.50547, 0.00000]	[ 0.08607, 0.41393, 0.25000]	[12,21]	(3,1)	(1,1)	[1,0,0]

Table 11: 1-th 'Sn'-'Sn' [1] (#3) bond cluster (6a06g), ND,  $|\boldsymbol{v}|=0.76376$  (cartesian)

SL	vector ( $\boldsymbol{v}$ )	center ( $\boldsymbol{c}$ )	mapping	head	tail	$\boldsymbol{R}$ (primitive)
1	[ 0.33333, 0.66667,-0.50000]	[ 0.50000, 0.00000, 0.00000]	[1,-8,-13,20]	(2,1)	(1,1)	[0,-1,1]
2	[-0.66667,-0.33333,-0.50000]	[ 0.00000, 0.50000, 0.00000]	[2,-7,-14,19]	(2,1)	(1,1)	[1,0,1]
3	[ 0.33333,-0.33333,-0.50000]	[ 0.50000, 0.50000, 0.00000]	[3,-9,-15,21]	(2,1)	(1,1)	[0,0,1]
4	[-0.33333,-0.66667,-0.50000]	[ 0.50000, 0.00000, 0.50000]	[4,-11,-16,23]	(1,1)	(2,1)	[0,1,0]
5	[ 0.66667, 0.33333,-0.50000]	[ 0.00000, 0.50000, 0.50000]	[5,-10,-17,22]	(1,1)	(2,1)	[-1,0,0]
6	[-0.33333, 0.33333,-0.50000]	[ 0.50000, 0.50000, 0.50000]	[6,-12,-18,24]	(1,1)	(2,1)	[0,0,0]