

Model for “UPt2Si2”

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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_{1g} , A_{2g} , B_{1g} , B_{2g} , E_g , A_{1u} , A_{2u} , B_{1u} , B_{2u} , E_u]**
 - 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_{1g} , A_{2g} , B_{1g} , B_{2g} , E_g , A_{1u} , A_{2u} , B_{1u} , B_{2u} , E_u]**
 - Spin (s): **[0, 1]**
- Site-cluster selection:
 - Rank: **[0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11]**
 - Irrep.: **[A_{1g} , A_{2g} , B_{1g} , B_{2g} , E_g , A_{1u} , A_{2u} , B_{1u} , B_{2u} , E_u]**
- Bond-cluster selection:
 - Type: **[Q, G, M, T]**
 - Rank: **[0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11]**
 - Irrep.: **[A_{1g} , A_{2g} , B_{1g} , B_{2g} , E_g , A_{1u} , A_{2u} , B_{1u} , B_{2u} , E_u]**
- Max. neighbor: **10**
- Search cell range: **(-2, 3), (-2, 3), (-2, 3)**
- Toroidal priority: **false**

Group and Unit Cell

- Group: SG No. 129 D_{4h}^7 $P4/nmm$ [tetragonal]
- Associated point group: PG No. 129 D_{4h} $4/mmm$ [tetragonal]
- Unit cell:
 - $a = 4.19720$, $b = 4.19720$, $c = 9.69060$, $\alpha = 90.0$, $\beta = 90.0$, $\gamma = 90.0$
- Lattice vectors (conventional cell):
 - $\mathbf{a}_1 = [4.19720, 0.00000, 0.00000]$
 - $\mathbf{a}_2 = [0.00000, 4.19720, 0.00000]$
 - $\mathbf{a}_3 = [0.00000, 0.00000, 9.69060]$

Symmetry Operation

Table 1: Symmetry operation

#	SO	#	SO	#	SO	#	SO	#	SO
1	$\{1 0\}$	2	$\{2_{001} \frac{1}{2}\frac{1}{2}0\}$	3	$\{4_{001}^+ \frac{1}{2}00\}$	4	$\{4_{001}^- 0\frac{1}{2}0\}$	5	$\{2_{010} 0\frac{1}{2}0\}$
6	$\{2_{100} \frac{1}{2}00\}$	7	$\{2_{110} \frac{1}{2}\frac{1}{2}0\}$	8	$\{2_{1-10} 0\}$	9	$\{-1 0\}$	10	$\{m_{001} \frac{1}{2}\frac{1}{2}0\}$
11	$\{-4_{001}^+ \frac{1}{2}00\}$	12	$\{-4_{001}^- 0\frac{1}{2}0\}$	13	$\{m_{010} 0\frac{1}{2}0\}$	14	$\{m_{100} \frac{1}{2}00\}$	15	$\{m_{110} \frac{1}{2}\frac{1}{2}0\}$
16	$\{m_{1-10} 0\}$								

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	$\mathbb{Q}_4(A_{1g}, 1)$	A_{1g}	4	Q, T	1	-	$\frac{\sqrt{21}(x^4 - 3x^2y^2 - 3x^2z^2 + y^4 - 3y^2z^2 + z^4)}{6}$
4	$\mathbb{Q}_4(A_{1g}, 2)$	A_{1g}	4	Q, T	2	-	$-\frac{\sqrt{15}(x^4 - 12x^2y^2 + 6x^2z^2 + y^4 + 6y^2z^2 - 2z^4)}{12}$
5	$\mathbb{G}_5(A_{1g})$	A_{1g}	5	G, M	-	-	$\frac{3\sqrt{35}xyz(x-y)(x+y)}{2}$
6	$\mathbb{Q}_6(A_{1g}, 1)$	A_{1g}	6	Q, T	1	-	$\frac{\sqrt{2}(2x^6 - 15x^4y^2 - 15x^4z^2 - 15x^2y^4 + 180x^2y^2z^2 - 15x^2z^4 + 2y^6 - 15y^4z^2 - 15y^2z^4 + 2z^6)}{8}$

continued ...

Table 2

#	symbol	irrep.	rank	X	multiplicity	component	symmetry
7	$\mathbb{Q}_6(A_{1g}, 2)$	A_{1g}	6	Q, T	2	-	$-\frac{\sqrt{14}(x^6-15x^4z^2+15x^2z^4+y^6-15y^4z^2+15y^2z^4-2z^6)}{8}$
8	$\mathbb{G}_0(A_{1u})$	A_{1u}	0	G, M	-	-	1
9	$\mathbb{G}_2(A_{1u})$	A_{1u}	2	G, M	-	-	$-\frac{x^2}{2} - \frac{y^2}{2} + z^2$
10	$\mathbb{G}_4(A_{1u}, 1)$	A_{1u}	4	G, M	1	-	$\frac{\sqrt{21}(x^4-3x^2y^2-3x^2z^2+y^4-3y^2z^2+z^4)}{6}$
11	$\mathbb{Q}_5(A_{1u})$	A_{1u}	5	Q, T	-	-	$\frac{3\sqrt{35}xyz(x-y)(x+y)}{2}$
12	$\mathbb{G}_1(A_{2g})$	A_{2g}	1	G, M	-	-	z
13	$\mathbb{G}_3(A_{2g})$	A_{2g}	3	G, M	-	-	$-\frac{z(3x^2+3y^2-2z^2)}{2}$
14	$\mathbb{Q}_4(A_{2g})$	A_{2g}	4	Q, T	-	-	$\frac{\sqrt{35}xy(x-y)(x+y)}{2}$
15	$\mathbb{G}_5(A_{2g}, 1)$	A_{2g}	5	G, M	1	-	$\frac{z(15x^4+30x^2y^2-40x^2z^2+15y^4-40y^2z^2+8z^4)}{8}$
16	$\mathbb{G}_5(A_{2g}, 2)$	A_{2g}	5	G, M	2	-	$\frac{3\sqrt{35}z(x^2-2xy-y^2)(x^2+2xy-y^2)}{8}$
17	$\mathbb{Q}_6(A_{2g})$	A_{2g}	6	Q, T	-	-	$-\frac{3\sqrt{7}xy(x-y)(x+y)(x^2+y^2-10z^2)}{4}$
18	$\mathbb{Q}_1(A_{2u})$	A_{2u}	1	Q, T	-	-	z
19	$\mathbb{Q}_3(A_{2u})$	A_{2u}	3	Q, T	-	-	$-\frac{z(3x^2+3y^2-2z^2)}{2}$
20	$\mathbb{Q}_5(A_{2u}, 1)$	A_{2u}	5	Q, T	1	-	$\frac{z(15x^4+30x^2y^2-40x^2z^2+15y^4-40y^2z^2+8z^4)}{8}$
21	$\mathbb{Q}_5(A_{2u}, 2)$	A_{2u}	5	Q, T	2	-	$\frac{3\sqrt{35}z(x^2-2xy-y^2)(x^2+2xy-y^2)}{8}$
22	$\mathbb{Q}_2(B_{1g})$	B_{1g}	2	Q, T	-	-	$\frac{\sqrt{3}(x-y)(x+y)}{2}$
23	$\mathbb{G}_3(B_{1g})$	B_{1g}	3	G, M	-	-	$\sqrt{15}xyz$
24	$\mathbb{Q}_4(B_{1g})$	B_{1g}	4	Q, T	-	-	$\frac{\sqrt{5}(x-y)(x+y)(x^2+y^2-6z^2)}{4}$
25	$\mathbb{G}_5(B_{1g})$	B_{1g}	5	G, M	-	-	$\frac{\sqrt{105}xyz(x^2+y^2-2z^2)}{2}$
26	$\mathbb{Q}_6(B_{1g}, 1)$	B_{1g}	6	Q, T	1	-	$-\frac{\sqrt{2310}(x-y)(x+y)(x-z)(x+z)(y-z)(y+z)}{8}$
27	$\mathbb{Q}_6(B_{1g}, 2)$	B_{1g}	6	Q, T	2	-	$\frac{\sqrt{42}(x-y)(x+y)(x^4-9x^2y^2-5x^2z^2+y^4-5y^2z^2+5z^4)}{8}$

continued ...

Table 2

#	symbol	irrep.	rank	X	multiplicity	component	symmetry
28	$\mathbb{G}_2(B_{1u})$	B_{1u}	2	G, M	-	-	$\frac{\sqrt{3}(x-y)(x+y)}{2}$
29	$\mathbb{Q}_3(B_{1u})$	B_{1u}	3	Q, T	-	-	$\sqrt{15}xyz$
30	$\mathbb{Q}_5(B_{1u})$	B_{1u}	5	Q, T	-	-	$\frac{\sqrt{105}xyz(x^2+y^2-2z^2)}{2}$
31	$\mathbb{Q}_7(B_{1u}, 1)$	B_{1u}	7	Q, T	1	-	$\frac{\sqrt{91}xyz(3x^4-5x^2y^2-5x^2z^2+3y^4-5y^2z^2+3z^4)}{2}$
32	$\mathbb{Q}_2(B_{2g})$	B_{2g}	2	Q, T	-	-	$\sqrt{3}xy$
33	$\mathbb{G}_3(B_{2g})$	B_{2g}	3	G, M	-	-	$\frac{\sqrt{15}z(x-y)(x+y)}{2}$
34	$\mathbb{Q}_4(B_{2g})$	B_{2g}	4	Q, T	-	-	$-\frac{\sqrt{5}xy(x^2+y^2-6z^2)}{2}$
35	$\mathbb{G}_5(B_{2g})$	B_{2g}	5	G, M	-	-	$-\frac{\sqrt{105}z(x-y)(x+y)(x^2+y^2-2z^2)}{4}$
36	$\mathbb{Q}_6(B_{2g}, 1)$	B_{2g}	6	Q, T	1	-	$\frac{\sqrt{462}xy(x^2-3y^2)(3x^2-y^2)}{16}$
37	$\mathbb{Q}_6(B_{2g}, 2)$	B_{2g}	6	Q, T	2	-	$\frac{\sqrt{210}xy(x^4+2x^2y^2-16x^2z^2+y^4-16y^2z^2+16z^4)}{16}$
38	$\mathbb{G}_2(B_{2u})$	B_{2u}	2	G, M	-	-	$\sqrt{3}xy$
39	$\mathbb{Q}_3(B_{2u})$	B_{2u}	3	Q, T	-	-	$\frac{\sqrt{15}z(x-y)(x+y)}{2}$
40	$\mathbb{Q}_5(B_{2u})$	B_{2u}	5	Q, T	-	-	$-\frac{\sqrt{105}z(x-y)(x+y)(x^2+y^2-2z^2)}{4}$
41	$\mathbb{Q}_7(B_{2u}, 1)$	B_{2u}	7	Q, T	1	-	$\frac{\sqrt{6006}z(x-y)(x+y)(x^2-4xy+y^2)(x^2+4xy+y^2)}{32}$
42	$\mathbb{G}_{1,1}(E_g)$	E_g	1	G, M	-	1	x
43	$\mathbb{G}_{1,2}(E_g)$					2	$-y$
44	$\mathbb{Q}_{2,1}(E_g)$	E_g	2	Q, T	-	1	$\sqrt{3}yz$
45	$\mathbb{Q}_{2,2}(E_g)$					2	$\sqrt{3}xz$
46	$\mathbb{G}_{3,1}(E_g, 1)$	E_g	3	G, M	1	1	$\frac{x(2x^2-3y^2-3z^2)}{2}$
47	$\mathbb{G}_{3,2}(E_g, 1)$					2	$\frac{y(3x^2-2y^2+3z^2)}{2}$
48	$\mathbb{G}_{3,1}(E_g, 2)$	E_g	3	G, M	2	1	$\frac{\sqrt{15}x(y-z)(y+z)}{2}$

continued ...

Table 2

#	symbol	irrep.	rank	X	multiplicity	component	symmetry
49	$\mathbb{G}_{3,2}(E_g, 2)$					2	$-\frac{\sqrt{15}y(x-z)(x+z)}{2}$
50	$\mathbb{Q}_{4,1}(E_g, 1)$	E_g	4	Q, T	1	1	$\frac{\sqrt{35}yz(y-z)(y+z)}{2}$
51	$\mathbb{Q}_{4,2}(E_g, 1)$					2	$\frac{\sqrt{35}xz(x-z)(x+z)}{2}$
52	$\mathbb{Q}_{4,1}(E_g, 2)$	E_g	4	Q, T	2	1	$\frac{\sqrt{5}yz(6x^2-y^2-z^2)}{2}$
53	$\mathbb{Q}_{4,2}(E_g, 2)$					2	$-\frac{\sqrt{5}xz(x^2-6y^2+z^2)}{2}$
54	$\mathbb{G}_{5,1}(E_g, 1)$	E_g	5	G, M	1	1	$\frac{x(8x^4-40x^2y^2-40x^2z^2+15y^4+30y^2z^2+15z^4)}{8}$
55	$\mathbb{G}_{5,2}(E_g, 1)$					2	$-\frac{y(15x^4-40x^2y^2+30x^2z^2+8y^4-40y^2z^2+15z^4)}{8}$
56	$\mathbb{G}_{5,1}(E_g, 2)$	E_g	5	G, M	2	1	$\frac{3\sqrt{35}x(y^2-2yz-z^2)(y^2+2yz-z^2)}{8}$
57	$\mathbb{G}_{5,2}(E_g, 2)$					2	$-\frac{3\sqrt{35}y(x^2-2xz-z^2)(x^2+2xz-z^2)}{8}$
58	$\mathbb{G}_{5,1}(E_g, 3)$	E_g	5	G, M	3	1	$\frac{\sqrt{105}x(y-z)(y+z)(2x^2-y^2-z^2)}{4}$
59	$\mathbb{G}_{5,2}(E_g, 3)$					2	$\frac{\sqrt{105}y(x-z)(x+z)(x^2-2y^2+z^2)}{4}$
60	$\mathbb{Q}_{6,1}(E_g, 1)$	E_g	6	Q, T	1	1	$\frac{3\sqrt{7}yz(y-z)(y+z)(10x^2-y^2-z^2)}{4}$
61	$\mathbb{Q}_{6,2}(E_g, 1)$					2	$-\frac{3\sqrt{7}xz(x-z)(x+z)(x^2-10y^2+z^2)}{4}$
62	$\mathbb{Q}_{6,1}(E_g, 2)$	E_g	6	Q, T	2	1	$\frac{\sqrt{462}yz(y^2-3z^2)(3y^2-z^2)}{16}$
63	$\mathbb{Q}_{6,2}(E_g, 2)$					2	$\frac{\sqrt{462}xz(x^2-3z^2)(3x^2-z^2)}{16}$
64	$\mathbb{Q}_{6,1}(E_g, 3)$	E_g	6	Q, T	3	1	$\frac{\sqrt{210}yz(16x^4-16x^2y^2-16x^2z^2+y^4+2y^2z^2+z^4)}{16}$
65	$\mathbb{Q}_{6,2}(E_g, 3)$					2	$\frac{\sqrt{210}xz(x^4-16x^2y^2+2x^2z^2+16y^4-16y^2z^2+z^4)}{16}$
66	$\mathbb{Q}_{1,1}(E_u)$	E_u	1	Q, T	-	1	x
67	$\mathbb{Q}_{1,2}(E_u)$					2	y
68	$\mathbb{G}_{2,1}(E_u)$	E_u	2	G, M	-	1	$\sqrt{3}yz$
69	$\mathbb{G}_{2,2}(E_u)$					2	$-\sqrt{3}xz$

continued ...

Table 2

#	symbol	irrep.	rank	X	multiplicity	component	symmetry
70	$\mathbb{Q}_{3,1}(E_u, 1)$	E_u	3	Q, T	1	1	$\frac{x(2x^2-3y^2-3z^2)}{2}$
71	$\mathbb{Q}_{3,2}(E_u, 1)$					2	$-\frac{y(3x^2-2y^2+3z^2)}{2}$
72	$\mathbb{Q}_{3,1}(E_u, 2)$	E_u	3	Q, T	2	1	$\frac{\sqrt{15}x(y-z)(y+z)}{2}$
73	$\mathbb{Q}_{3,2}(E_u, 2)$					2	$\frac{\sqrt{15}y(x-z)(x+z)}{2}$
74	$\mathbb{Q}_{5,1}(E_u, 1)$	E_u	5	Q, T	1	1	$\frac{x(8x^4-40x^2y^2-40x^2z^2+15y^4+30y^2z^2+15z^4)}{8}$
75	$\mathbb{Q}_{5,2}(E_u, 1)$					2	$\frac{y(15x^4-40x^2y^2+30x^2z^2+8y^4-40y^2z^2+15z^4)}{8}$
76	$\mathbb{Q}_{5,1}(E_u, 2)$	E_u	5	Q, T	2	1	$\frac{3\sqrt{35}x(y^2-2yz-z^2)(y^2+2yz-z^2)}{8}$
77	$\mathbb{Q}_{5,2}(E_u, 2)$					2	$\frac{3\sqrt{35}y(x^2-2xz-z^2)(x^2+2xz-z^2)}{8}$
78	$\mathbb{Q}_{5,1}(E_u, 3)$	E_u	5	Q, T	3	1	$\frac{\sqrt{105}x(y-z)(y+z)(2x^2-y^2-z^2)}{4}$
79	$\mathbb{Q}_{5,2}(E_u, 3)$					2	$-\frac{\sqrt{105}y(x-z)(x+z)(x^2-2y^2+z^2)}{4}$

Basis in full matrix

Table 3: dimension = 46

#	orbital@atom(SL)	#	orbital@atom(SL)	#	orbital@atom(SL)	#	orbital@atom(SL)	#	orbital@atom(SL)
0	$ d_u\rangle @Pt1(1)$	1	$ d_v\rangle @Pt1(1)$	2	$ d_{yz}\rangle @Pt1(1)$	3	$ d_{xz}\rangle @Pt1(1)$	4	$ d_{xy}\rangle @Pt1(1)$
5	$ d_u\rangle @Pt1(2)$	6	$ d_v\rangle @Pt1(2)$	7	$ d_{yz}\rangle @Pt1(2)$	8	$ d_{xz}\rangle @Pt1(2)$	9	$ d_{xy}\rangle @Pt1(2)$
10	$ d_u\rangle @Pt2(1)$	11	$ d_v\rangle @Pt2(1)$	12	$ d_{yz}\rangle @Pt2(1)$	13	$ d_{xz}\rangle @Pt2(1)$	14	$ d_{xy}\rangle @Pt2(1)$

continued ...

Table 3

#	orbital@atom(SL)	#	orbital@atom(SL)	#	orbital@atom(SL)	#	orbital@atom(SL)	#	orbital@atom(SL)
15	$ d_u\rangle @Pt2(2)$	16	$ d_v\rangle @Pt2(2)$	17	$ d_{yz}\rangle @Pt2(2)$	18	$ d_{xz}\rangle @Pt2(2)$	19	$ d_{xy}\rangle @Pt2(2)$
20	$ p_x\rangle @Si1(1)$	21	$ p_y\rangle @Si1(1)$	22	$ p_z\rangle @Si1(1)$	23	$ p_x\rangle @Si1(2)$	24	$ p_y\rangle @Si1(2)$
25	$ p_z\rangle @Si1(2)$	26	$ p_x\rangle @Si2(1)$	27	$ p_y\rangle @Si2(1)$	28	$ p_z\rangle @Si2(1)$	29	$ p_x\rangle @Si2(2)$
30	$ p_y\rangle @Si2(2)$	31	$ p_z\rangle @Si2(2)$	32	$ f_3\rangle @U(1)$	33	$ f_{ax}\rangle @U(1)$	34	$ f_{ay}\rangle @U(1)$
35	$ f_{az}\rangle @U(1)$	36	$ f_{bx}\rangle @U(1)$	37	$ f_{by}\rangle @U(1)$	38	$ f_{bz}\rangle @U(1)$	39	$ f_3\rangle @U(2)$
40	$ f_{ax}\rangle @U(2)$	41	$ f_{ay}\rangle @U(2)$	42	$ f_{az}\rangle @U(2)$	43	$ f_{bx}\rangle @U(2)$	44	$ f_{by}\rangle @U(2)$
45	$ f_{bz}\rangle @U(2)$								

Table 4: Atomic basis (orbital part only)

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

continued ...

Table 4

orbital	definition
$ f_3\rangle$	$\sqrt{15}xyz$
$ f_{ax}\rangle$	$\frac{x(2x^2-3y^2-3z^2)}{2}$
$ f_{ay}\rangle$	$\frac{y(-3x^2+2y^2-3z^2)}{2}$
$ f_{az}\rangle$	$\frac{z(-3x^2-3y^2+2z^2)}{2}$
$ f_{bx}\rangle$	$\frac{\sqrt{15}x(y^2-z^2)}{2}$
$ f_{by}\rangle$	$\frac{\sqrt{15}y(-x^2+z^2)}{2}$
$ f_{bz}\rangle$	$\frac{\sqrt{15}z(x^2-y^2)}{2}$

SAMB

380 (all 380) SAMBs

• 'Pt1' site-cluster : **Pt1**

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

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

$$\boxed{\text{z2}} \quad \mathbb{Q}_2^{(c)}(A_{1g}) = \mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_0^{(s)}(A_{1g})$$

$$\boxed{\text{z3}} \quad \mathbb{Q}_4^{(c)}(A_{1g}, 1) = \mathbb{Q}_4^{(a)}(A_{1g}, 1)\mathbb{Q}_0^{(s)}(A_{1g})$$

$$\boxed{\text{z4}} \quad \mathbb{Q}_4^{(c)}(A_{1g}, 2) = \mathbb{Q}_4^{(a)}(A_{1g}, 2)\mathbb{Q}_0^{(s)}(A_{1g})$$

$$\boxed{\text{z35}} \quad \mathbb{Q}_5^{(c)}(A_{1u}, a) = \mathbb{Q}_2^{(a)}(B_{2g})\mathbb{Q}_3^{(s)}(B_{2u})$$

$$\boxed{\text{z53}} \quad \mathbb{Q}_5^{(c)}(A_{1u}, b) = \mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_3^{(s)}(B_{2u})$$

$$\boxed{\text{z54}} \quad \mathbb{Q}_4^{(c)}(A_{2g}) = \mathbb{Q}_4^{(a)}(A_{2g})\mathbb{Q}_0^{(s)}(A_{1g})$$

$$\boxed{\text{z79}} \quad \mathbb{Q}_1^{(c)}(A_{2u}, a) = \mathbb{Q}_2^{(a)}(B_{1g})\mathbb{Q}_3^{(s)}(B_{2u})$$

$$\boxed{\text{z80}} \quad \mathbb{Q}_1^{(c)}(A_{2u}, b) = -\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_3^{(s)}(B_{2u})$$

$$\boxed{\text{z103}} \quad \mathbb{Q}_2^{(c)}(B_{1g}) = \mathbb{Q}_2^{(a)}(B_{1g})\mathbb{Q}_0^{(s)}(A_{1g})$$

$$\boxed{\text{z104}} \quad \mathbb{Q}_4^{(c)}(B_{1g}) = \mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_0^{(s)}(A_{1g})$$

$$\boxed{\text{z105}} \quad \mathbb{Q}_3^{(c)}(B_{1u}) = \mathbb{Q}_4^{(a)}(A_{2g})\mathbb{Q}_3^{(s)}(B_{2u})$$

$$\boxed{\text{z106}} \quad \mathbb{Q}_2^{(c)}(B_{2g}) = \mathbb{Q}_2^{(a)}(B_{2g})\mathbb{Q}_0^{(s)}(A_{1g})$$

$$\boxed{\text{z107}} \quad \mathbb{Q}_4^{(c)}(B_{2g}) = \mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_0^{(s)}(A_{1g})$$

$$\boxed{\text{z108}} \quad \mathbb{Q}_3^{(c)}(B_{2u}, a) = \mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_3^{(s)}(B_{2u})$$

$$\boxed{\text{z191}} \quad \mathbb{Q}_3^{(c)}(B_{2u}, b) = -\frac{\mathbb{Q}_4^{(a)}(A_{1g}, 1)\mathbb{Q}_3^{(s)}(B_{2u})}{6} - \frac{\sqrt{35}\mathbb{Q}_4^{(a)}(A_{1g}, 2)\mathbb{Q}_3^{(s)}(B_{2u})}{6}$$

$$\boxed{\text{z192}} \quad \mathbb{Q}_5^{(c)}(B_{2u}, a) = \mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_3^{(s)}(B_{2u})$$

$$\boxed{\text{z211}} \quad \mathbb{Q}_5^{(c)}(B_{2u}, b) = -\frac{\sqrt{35}\mathbb{Q}_4^{(a)}(A_{1g}, 1)\mathbb{Q}_3^{(s)}(B_{2u})}{6} + \frac{\mathbb{Q}_4^{(a)}(A_{1g}, 2)\mathbb{Q}_3^{(s)}(B_{2u})}{6}$$

$$\boxed{\text{z212}} \quad \mathbb{Q}_{2,1}^{(c)}(E_g) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

$$\boxed{\text{z242}} \quad \mathbb{Q}_{2,2}^{(c)}(E_g) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

$$\boxed{\text{z264}} \quad \mathbb{Q}_{4,1}^{(c)}(E_g, 1) = \frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_g, 1)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

$$\boxed{\text{z265}} \quad \mathbb{Q}_{4,2}^{(c)}(E_g, 1) = \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_g, 1)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

$$\boxed{\text{z266}} \quad \mathbb{Q}_{4,1}^{(c)}(E_g, 2) = \frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_g, 2)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

$$\boxed{\text{z267}} \quad \mathbb{Q}_{4,2}^{(c)}(E_g, 2) = \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_g, 2)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

$$\boxed{\text{z293}} \quad \mathbb{Q}_{1,1}^{(c)}(E_u, a) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_3^{(s)}(B_{2u})}{2}$$

$$\boxed{\text{z294}} \quad \mathbb{Q}_{1,2}^{(c)}(E_u, a) = -\frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_3^{(s)}(B_{2u})}{2}$$

$$\boxed{\text{z295}} \quad \mathbb{Q}_{1,1}^{(c)}(E_u, b) = \frac{\sqrt{14}\mathbb{Q}_{4,2}^{(a)}(E_g, 1)\mathbb{Q}_3^{(s)}(B_{2u})}{8} - \frac{3\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_g, 2)\mathbb{Q}_3^{(s)}(B_{2u})}{8}$$

$$\boxed{\text{z296}} \quad \mathbb{Q}_{1,2}^{(c)}(E_u, b) = -\frac{\sqrt{14}\mathbb{Q}_{4,1}^{(a)}(E_g, 1)\mathbb{Q}_3^{(s)}(B_{2u})}{8} + \frac{3\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_g, 2)\mathbb{Q}_3^{(s)}(B_{2u})}{8}$$

$$\boxed{\text{z297}} \quad \mathbb{Q}_{3,1}^{(c)}(E_u, 1) = \frac{3\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_g, 1)\mathbb{Q}_3^{(s)}(B_{2u})}{8} + \frac{\sqrt{14}\mathbb{Q}_{4,2}^{(a)}(E_g, 2)\mathbb{Q}_3^{(s)}(B_{2u})}{8}$$

$$\boxed{\text{z298}} \quad \mathbb{Q}_{3,2}^{(c)}(E_u, 1) = -\frac{3\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_g, 1)\mathbb{Q}_3^{(s)}(B_{2u})}{8} - \frac{\sqrt{14}\mathbb{Q}_{4,1}^{(a)}(E_g, 2)\mathbb{Q}_3^{(s)}(B_{2u})}{8}$$

• 'Pt2' site-cluster : Pt2

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

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

* wyckoff: 2c

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

$$\boxed{\text{z6}} \quad \mathbb{Q}_2^{(c)}(A_{1g}) = \mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_0^{(s)}(A_{1g})$$

$$\boxed{\text{z7}} \quad \mathbb{Q}_4^{(c)}(A_{1g}, 1) = \mathbb{Q}_4^{(a)}(A_{1g}, 1)\mathbb{Q}_0^{(s)}(A_{1g})$$

$$\boxed{\text{z8}} \quad \mathbb{Q}_4^{(c)}(A_{1g}, 2) = \mathbb{Q}_4^{(a)}(A_{1g}, 2)\mathbb{Q}_0^{(s)}(A_{1g})$$

$$\boxed{\text{z36}} \quad \mathbb{Q}_5^{(c)}(A_{1u}) = \mathbb{Q}_4^{(a)}(A_{2g})\mathbb{Q}_1^{(s)}(A_{2u})$$

$$\boxed{\text{z55}} \quad \mathbb{Q}_4^{(c)}(A_{2g}) = \mathbb{Q}_4^{(a)}(A_{2g})\mathbb{Q}_0^{(s)}(A_{1g})$$

$$\boxed{\text{z56}} \quad \mathbb{Q}_1^{(c)}(A_{2u}, a) = \mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_1^{(s)}(A_{2u})$$

$$\boxed{\text{z81}} \quad \mathbb{Q}_1^{(c)}(A_{2u}, b) = \mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_1^{(s)}(A_{2u})$$

$$\boxed{\text{z82}} \quad \mathbb{Q}_3^{(c)}(A_{2u}) = \frac{\sqrt{21}\mathbb{Q}_4^{(a)}(A_{1g}, 1)\mathbb{Q}_1^{(s)}(A_{2u})}{6} + \frac{\sqrt{15}\mathbb{Q}_4^{(a)}(A_{1g}, 2)\mathbb{Q}_1^{(s)}(A_{2u})}{6}$$

$$\boxed{\text{z109}} \quad \mathbb{Q}_5^{(c)}(A_{2u}, 2) = \frac{\sqrt{15}\mathbb{Q}_4^{(a)}(A_{1g}, 1)\mathbb{Q}_1^{(s)}(A_{2u})}{6} - \frac{\sqrt{21}\mathbb{Q}_4^{(a)}(A_{1g}, 2)\mathbb{Q}_1^{(s)}(A_{2u})}{6}$$

$$\boxed{\text{z110}} \quad \mathbb{Q}_2^{(c)}(B_{1g}) = \mathbb{Q}_2^{(a)}(B_{1g})\mathbb{Q}_0^{(s)}(A_{1g})$$

$$\boxed{\text{z111}} \quad \mathbb{Q}_4^{(c)}(B_{1g}) = \mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_0^{(s)}(A_{1g})$$

$$\boxed{\text{z112}} \quad \mathbb{Q}_3^{(c)}(B_{1u}, a) = \mathbb{Q}_2^{(a)}(B_{2g})\mathbb{Q}_1^{(s)}(A_{2u})$$

$$\boxed{\text{z113}} \quad \mathbb{Q}_3^{(c)}(B_{1u}, b) = \mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_1^{(s)}(A_{2u})$$

$$\boxed{\text{z114}} \quad \mathbb{Q}_2^{(c)}(B_{2g}) = \mathbb{Q}_2^{(a)}(B_{2g})\mathbb{Q}_0^{(s)}(A_{1g})$$

$$\boxed{\text{z193}} \quad \mathbb{Q}_4^{(c)}(B_{2g}) = \mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_0^{(s)}(A_{1g})$$

$$\boxed{\text{z213}} \quad \mathbb{Q}_3^{(c)}(B_{2u}, a) = \mathbb{Q}_2^{(a)}(B_{1g})\mathbb{Q}_1^{(s)}(A_{2u})$$

$$\boxed{\text{z214}} \quad \mathbb{Q}_3^{(c)}(B_{2u}, b) = -\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_1^{(s)}(A_{2u})$$

$$\boxed{\text{z215}} \quad \mathbb{Q}_{2,1}^{(c)}(E_g) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

$$\boxed{\text{z216}} \quad \mathbb{Q}_{2,2}^{(c)}(E_g) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

$$\boxed{\text{z243}} \quad \mathbb{Q}_{4,1}^{(c)}(E_g, 1) = \frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_g, 1)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

$$\boxed{\text{z244}} \quad \mathbb{Q}_{4,2}^{(c)}(E_g, 1) = \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_g, 1)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

$$\boxed{\text{z268}} \quad \mathbb{Q}_{4,1}^{(c)}(E_g, 2) = \frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_g, 2)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

$$\boxed{\text{z269}} \quad \mathbb{Q}_{4,2}^{(c)}(E_g, 2) = \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_g, 2)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

$$\boxed{\text{z299}} \quad \mathbb{Q}_{1,1}^{(c)}(E_u) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_1^{(s)}(A_{2u})}{2}$$

$$\boxed{\text{z300}} \quad \mathbb{Q}_{1,2}^{(c)}(E_u) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_1^{(s)}(A_{2u})}{2}$$

$$\boxed{\text{z301}} \quad \mathbb{Q}_{3,1}^{(c)}(E_u, 1) = \frac{\sqrt{7}\mathbb{Q}_{4,2}^{(a)}(E_g, 1)\mathbb{Q}_1^{(s)}(A_{2u})}{4} - \frac{\mathbb{Q}_{4,2}^{(a)}(E_g, 2)\mathbb{Q}_1^{(s)}(A_{2u})}{4}$$

$$\boxed{\text{z302}} \quad \mathbb{Q}_{3,2}^{(c)}(E_u, 1) = \frac{\sqrt{7}\mathbb{Q}_{4,1}^{(a)}(E_g, 1)\mathbb{Q}_1^{(s)}(A_{2u})}{4} - \frac{\mathbb{Q}_{4,1}^{(a)}(E_g, 2)\mathbb{Q}_1^{(s)}(A_{2u})}{4}$$

$$\boxed{\text{z303}} \quad \mathbb{Q}_{3,1}^{(c)}(E_u, 2) = \frac{\mathbb{Q}_{4,2}^{(a)}(E_g, 1)\mathbb{Q}_1^{(s)}(A_{2u})}{4} + \frac{\sqrt{7}\mathbb{Q}_{4,2}^{(a)}(E_g, 2)\mathbb{Q}_1^{(s)}(A_{2u})}{4}$$

$$\boxed{\text{z304}} \quad \mathbb{Q}_{3,2}^{(c)}(E_u, 2) = \frac{\mathbb{Q}_{4,1}^{(a)}(E_g, 1)\mathbb{Q}_1^{(s)}(A_{2u})}{4} + \frac{\sqrt{7}\mathbb{Q}_{4,1}^{(a)}(E_g, 2)\mathbb{Q}_1^{(s)}(A_{2u})}{4}$$

• 'S11' site-cluster : S11

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

* ket: $|p_x\rangle$, $|p_y\rangle$, $|p_z\rangle$

* wyckoff: 2b

$$\boxed{\text{z9}} \quad \mathbb{Q}_0^{(c)}(A_{1g}) = \mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_0^{(s)}(A_{1g})$$

$$\boxed{\text{z10}} \quad \mathbb{Q}_2^{(c)}(A_{1g}) = \mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_0^{(s)}(A_{1g})$$

$$\boxed{\text{z57}} \quad \mathbb{Q}_5^{(c)}(A_{1u}) = \mathbb{Q}_2^{(a)}(B_{2g})\mathbb{Q}_3^{(s)}(B_{2u})$$

$$\boxed{\text{z83}} \quad \mathbb{Q}_1^{(c)}(A_{2u}) = \mathbb{Q}_2^{(a)}(B_{1g})\mathbb{Q}_3^{(s)}(B_{2u})$$

$$\boxed{\text{z115}} \quad \mathbb{Q}_2^{(c)}(B_{1g}) = \mathbb{Q}_2^{(a)}(B_{1g})\mathbb{Q}_0^{(s)}(A_{1g})$$

$$\boxed{\text{z116}} \quad \mathbb{Q}_2^{(c)}(B_{2g}) = \mathbb{Q}_2^{(a)}(B_{2g})\mathbb{Q}_0^{(s)}(A_{1g})$$

$$\boxed{\text{z194}} \quad \mathbb{Q}_3^{(c)}(B_{2u}) = \mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_3^{(s)}(B_{2u})$$

$$\boxed{\text{z217}} \quad \mathbb{Q}_5^{(c)}(B_{2u}) = \mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_3^{(s)}(B_{2u})$$

$$\boxed{\text{z270}} \quad \mathbb{Q}_{2,1}^{(c)}(E_g) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

$$\boxed{\text{z271}} \quad \mathbb{Q}_{2,2}^{(c)}(E_g) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

$$\boxed{\text{z305}} \quad \mathbb{Q}_{1,1}^{(c)}(E_u) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_3^{(s)}(B_{2u})}{2}$$

$$\boxed{\text{z306}} \quad \mathbb{Q}_{1,2}^{(c)}(E_u) = -\frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_3^{(s)}(B_{2u})}{2}$$

• 'Si2' site-cluster : Si2

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

* ket: $|p_x\rangle$, $|p_y\rangle$, $|p_z\rangle$

* wyckoff: 2c

$$\boxed{\text{z11}} \quad \mathbb{Q}_0^{(c)}(A_{1g}) = \mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_0^{(s)}(A_{1g})$$

$$\boxed{\text{z12}} \quad \mathbb{Q}_2^{(c)}(A_{1g}) = \mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_0^{(s)}(A_{1g})$$

$$\boxed{\text{z58}} \quad \mathbb{Q}_1^{(c)}(A_{2u}, a) = \mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_1^{(s)}(A_{2u})$$

$$\boxed{\text{z84}} \quad \mathbb{Q}_1^{(c)}(A_{2u}, b) = \mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_1^{(s)}(A_{2u})$$

$$\boxed{\text{z117}} \quad \mathbb{Q}_2^{(c)}(B_{1g}) = \mathbb{Q}_2^{(a)}(B_{1g})\mathbb{Q}_0^{(s)}(A_{1g})$$

$$\boxed{\text{z118}} \quad \mathbb{Q}_3^{(c)}(B_{1u}) = \mathbb{Q}_2^{(a)}(B_{2g})\mathbb{Q}_1^{(s)}(A_{2u})$$

$$\boxed{\text{z218}} \quad \mathbb{Q}_2^{(c)}(B_{2g}) = \mathbb{Q}_2^{(a)}(B_{2g})\mathbb{Q}_0^{(s)}(A_{1g})$$

$$\boxed{\text{z219}} \quad \mathbb{Q}_3^{(c)}(B_{2u}) = \mathbb{Q}_2^{(a)}(B_{1g})\mathbb{Q}_1^{(s)}(A_{2u})$$

$$\boxed{\text{z245}} \quad \mathbb{Q}_{2,1}^{(c)}(E_g) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

$$\boxed{\text{z272}} \quad \mathbb{Q}_{2,2}^{(c)}(E_g) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

$$\boxed{\text{z307}} \quad \mathbb{Q}_{1,1}^{(c)}(E_u) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_1^{(s)}(A_{2u})}{2}$$

$$\boxed{\text{z308}} \quad \mathbb{Q}_{1,2}^{(c)}(E_u) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_1^{(s)}(A_{2u})}{2}$$

• 'U' site-cluster : U

* bra: $\langle f_3 |, \langle f_{ax} |, \langle f_{ay} |, \langle f_{az} |, \langle f_{bx} |, \langle f_{by} |, \langle f_{bz} |$

* ket: $|f_3\rangle, |f_{ax}\rangle, |f_{ay}\rangle, |f_{az}\rangle, |f_{bx}\rangle, |f_{by}\rangle, |f_{bz}\rangle$

* wyckoff: 2c

$$\boxed{\text{z13}} \quad \mathbb{Q}_0^{(c)}(A_{1g}) = \mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_0^{(s)}(A_{1g})$$

$$\boxed{\text{z14}} \quad \mathbb{Q}_2^{(c)}(A_{1g}) = \mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_0^{(s)}(A_{1g})$$

$$\boxed{\text{z15}} \quad \mathbb{Q}_4^{(c)}(A_{1g}, 1) = \mathbb{Q}_4^{(a)}(A_{1g}, 1)\mathbb{Q}_0^{(s)}(A_{1g})$$

$$\boxed{\text{z16}} \quad \mathbb{Q}_4^{(c)}(A_{1g}, 2) = \mathbb{Q}_4^{(a)}(A_{1g}, 2)\mathbb{Q}_0^{(s)}(A_{1g})$$

$$\boxed{\text{z17}} \quad \mathbb{Q}_6^{(c)}(A_{1g}, 1) = \mathbb{Q}_6^{(a)}(A_{1g}, 1)\mathbb{Q}_0^{(s)}(A_{1g})$$

$$\boxed{\text{z18}} \quad \mathbb{Q}_6^{(c)}(A_{1g}, 2) = \mathbb{Q}_6^{(a)}(A_{1g}, 2)\mathbb{Q}_0^{(s)}(A_{1g})$$

$$\boxed{\text{z37}} \quad \mathbb{Q}_5^{(c)}(A_{1u}, a) = \mathbb{Q}_4^{(a)}(A_{2g})\mathbb{Q}_1^{(s)}(A_{2u})$$

$$\boxed{\text{z38}} \quad \mathbb{Q}_5^{(c)}(A_{1u}, b) = \mathbb{Q}_6^{(a)}(A_{2g})\mathbb{Q}_1^{(s)}(A_{2u})$$

$$\boxed{\text{z59}} \quad \mathbb{Q}_4^{(c)}(A_{2g}) = \mathbb{Q}_4^{(a)}(A_{2g})\mathbb{Q}_0^{(s)}(A_{1g})$$

$$\boxed{\text{z60}} \quad \mathbb{Q}_6^{(c)}(A_{2g}) = \mathbb{Q}_6^{(a)}(A_{2g})\mathbb{Q}_0^{(s)}(A_{1g})$$

$$\boxed{\text{z61}} \quad \mathbb{Q}_1^{(c)}(A_{2u}, a) = \mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_1^{(s)}(A_{2u})$$

$$\boxed{\text{z62}} \quad \mathbb{Q}_1^{(c)}(A_{2u}, b) = \mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_1^{(s)}(A_{2u})$$

$$\boxed{\text{z85}} \quad \mathbb{Q}_3^{(c)}(A_{2u}) = \frac{\sqrt{21}\mathbb{Q}_4^{(a)}(A_{1g}, 1)\mathbb{Q}_1^{(s)}(A_{2u})}{6} + \frac{\sqrt{15}\mathbb{Q}_4^{(a)}(A_{1g}, 2)\mathbb{Q}_1^{(s)}(A_{2u})}{6}$$

$$\boxed{\text{z86}} \quad \mathbb{Q}_5^{(c)}(A_{2u}, 1) = \frac{\sqrt{2}\mathbb{Q}_6^{(a)}(A_{1g}, 1)\mathbb{Q}_1^{(s)}(A_{2u})}{4} + \frac{\sqrt{14}\mathbb{Q}_6^{(a)}(A_{1g}, 2)\mathbb{Q}_1^{(s)}(A_{2u})}{4}$$

$$\boxed{\text{z87}} \quad \mathbb{Q}_5^{(c)}(A_{2u}, 2a) = \frac{\sqrt{15}\mathbb{Q}_4^{(a)}(A_{1g}, 1)\mathbb{Q}_1^{(s)}(A_{2u})}{6} - \frac{\sqrt{21}\mathbb{Q}_4^{(a)}(A_{1g}, 2)\mathbb{Q}_1^{(s)}(A_{2u})}{6}$$

$$\boxed{\text{z88}} \quad \mathbb{Q}_5^{(c)}(A_{2u}, 2b) = -\frac{\sqrt{14}\mathbb{Q}_6^{(a)}(A_{1g}, 1)\mathbb{Q}_1^{(s)}(A_{2u})}{4} + \frac{\sqrt{2}\mathbb{Q}_6^{(a)}(A_{1g}, 2)\mathbb{Q}_1^{(s)}(A_{2u})}{4}$$

$$\boxed{\text{z119}} \quad \mathbb{Q}_2^{(c)}(B_{1g}) = \mathbb{Q}_2^{(a)}(B_{1g})\mathbb{Q}_0^{(s)}(A_{1g})$$

$$\boxed{\text{z120}} \quad \mathbb{Q}_4^{(c)}(B_{1g}) = \mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_0^{(s)}(A_{1g})$$

$$\boxed{\text{z121}} \quad \mathbb{Q}_6^{(c)}(B_{1g}, 1) = \mathbb{Q}_6^{(a)}(B_{1g}, 1)\mathbb{Q}_0^{(s)}(A_{1g})$$

$$\boxed{\text{z122}} \quad \mathbb{Q}_6^{(c)}(B_{1g}, 2) = \mathbb{Q}_6^{(a)}(B_{1g}, 2)\mathbb{Q}_0^{(s)}(A_{1g})$$

$$\boxed{\text{z123}} \quad \mathbb{Q}_3^{(c)}(B_{1u}, a) = \mathbb{Q}_2^{(a)}(B_{2g})\mathbb{Q}_1^{(s)}(A_{2u})$$

$$\boxed{\text{z124}} \quad \mathbb{Q}_3^{(c)}(B_{1u}, b) = \mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_1^{(s)}(A_{2u})$$

$$\boxed{\text{z125}} \quad \mathbb{Q}_5^{(c)}(B_{1u}) = -\mathbb{Q}_6^{(a)}(B_{2g}, 2)\mathbb{Q}_1^{(s)}(A_{2u})$$

$$\boxed{\text{z126}} \quad \mathbb{Q}_7^{(c)}(B_{1u}, 1) = \mathbb{Q}_6^{(a)}(B_{2g}, 1)\mathbb{Q}_1^{(s)}(A_{2u})$$

$$\boxed{\text{z127}} \quad \mathbb{Q}_2^{(c)}(B_{2g}) = \mathbb{Q}_2^{(a)}(B_{2g})\mathbb{Q}_0^{(s)}(A_{1g})$$

$$\boxed{\text{z128}} \quad \mathbb{Q}_4^{(c)}(B_{2g}) = \mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_0^{(s)}(A_{1g})$$

$$\boxed{\text{z129}} \quad \mathbb{Q}_6^{(c)}(B_{2g}, 1) = \mathbb{Q}_6^{(a)}(B_{2g}, 1)\mathbb{Q}_0^{(s)}(A_{1g})$$

$$\boxed{\text{z130}} \quad \mathbb{Q}_6^{(c)}(B_{2g}, 2) = \mathbb{Q}_6^{(a)}(B_{2g}, 2)\mathbb{Q}_0^{(s)}(A_{1g})$$

$$\boxed{\text{z195}} \quad \mathbb{Q}_3^{(c)}(B_{2u}, a) = \mathbb{Q}_2^{(a)}(B_{1g})\mathbb{Q}_1^{(s)}(A_{2u})$$

$$\boxed{\text{z196}} \quad \mathbb{Q}_3^{(c)}(B_{2u}, b) = -\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_1^{(s)}(A_{2u})$$

$$\boxed{\text{z220}} \quad \mathbb{Q}_5^{(c)}(B_{2u}) = -\frac{\sqrt{11}\mathbb{Q}_6^{(a)}(B_{1g}, 1)\mathbb{Q}_1^{(s)}(A_{2u})}{4} + \frac{\sqrt{5}\mathbb{Q}_6^{(a)}(B_{1g}, 2)\mathbb{Q}_1^{(s)}(A_{2u})}{4}$$

$$\boxed{\text{z221}} \quad \mathbb{Q}_7^{(c)}(B_{2u}, 1) = \frac{\sqrt{5}\mathbb{Q}_6^{(a)}(B_{1g}, 1)\mathbb{Q}_1^{(s)}(A_{2u})}{4} + \frac{\sqrt{11}\mathbb{Q}_6^{(a)}(B_{1g}, 2)\mathbb{Q}_1^{(s)}(A_{2u})}{4}$$

$$\boxed{\text{z222}} \quad \mathbb{Q}_{2,1}^{(c)}(E_g) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

$$\boxed{\text{z223}} \quad \mathbb{Q}_{2,2}^{(c)}(E_g) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

$$\boxed{\text{z224}} \quad \mathbb{Q}_{4,1}^{(c)}(E_g, 1) = \frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_g, 1)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

$$\boxed{\text{z225}} \quad \mathbb{Q}_{4,2}^{(c)}(E_g, 1) = \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_g, 1)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

$$\boxed{\text{z246}} \quad \mathbb{Q}_{4,1}^{(c)}(E_g, 2) = \frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_g, 2)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

$$\boxed{\text{z247}} \quad \mathbb{Q}_{4,2}^{(c)}(E_g, 2) = \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_g, 2)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

$$\boxed{\text{z248}} \quad \mathbb{Q}_{6,1}^{(c)}(E_g, 1) = \frac{\sqrt{2}\mathbb{Q}_{6,1}^{(a)}(E_g, 1)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

$$\boxed{\text{z249}} \quad \mathbb{Q}_{6,2}^{(c)}(E_g, 1) = \frac{\sqrt{2}\mathbb{Q}_{6,2}^{(a)}(E_g, 1)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

$$\boxed{\text{z273}} \quad \mathbb{Q}_{6,1}^{(c)}(E_g, 2) = \frac{\sqrt{2}\mathbb{Q}_{6,1}^{(a)}(E_g, 2)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

$$\boxed{\text{z274}} \quad \mathbb{Q}_{6,2}^{(c)}(E_g, 2) = \frac{\sqrt{2}\mathbb{Q}_{6,2}^{(a)}(E_g, 2)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

$$\begin{aligned}
\boxed{\text{z275}} \quad \mathbb{Q}_{6,1}^{(c)}(E_g, 3) &= \frac{\sqrt{2}\mathbb{Q}_{6,1}^{(a)}(E_g, 3)\mathbb{Q}_0^{(s)}(A_{1g})}{2} \\
\boxed{\text{z276}} \quad \mathbb{Q}_{6,2}^{(c)}(E_g, 3) &= \frac{\sqrt{2}\mathbb{Q}_{6,2}^{(a)}(E_g, 3)\mathbb{Q}_0^{(s)}(A_{1g})}{2} \\
\boxed{\text{z309}} \quad \mathbb{Q}_{1,1}^{(c)}(E_u) &= \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_1^{(s)}(A_{2u})}{2} \\
\boxed{\text{z310}} \quad \mathbb{Q}_{1,2}^{(c)}(E_u) &= \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_1^{(s)}(A_{2u})}{2} \\
\boxed{\text{z311}} \quad \mathbb{Q}_{3,1}^{(c)}(E_u, 1) &= \frac{\sqrt{7}\mathbb{Q}_{4,2}^{(a)}(E_g, 1)\mathbb{Q}_1^{(s)}(A_{2u})}{4} - \frac{\mathbb{Q}_{4,2}^{(a)}(E_g, 2)\mathbb{Q}_1^{(s)}(A_{2u})}{4} \\
\boxed{\text{z312}} \quad \mathbb{Q}_{3,2}^{(c)}(E_u, 1) &= \frac{\sqrt{7}\mathbb{Q}_{4,1}^{(a)}(E_g, 1)\mathbb{Q}_1^{(s)}(A_{2u})}{4} - \frac{\mathbb{Q}_{4,1}^{(a)}(E_g, 2)\mathbb{Q}_1^{(s)}(A_{2u})}{4} \\
\boxed{\text{z313}} \quad \mathbb{Q}_{3,1}^{(c)}(E_u, 2) &= \frac{\mathbb{Q}_{4,2}^{(a)}(E_g, 1)\mathbb{Q}_1^{(s)}(A_{2u})}{4} + \frac{\sqrt{7}\mathbb{Q}_{4,2}^{(a)}(E_g, 2)\mathbb{Q}_1^{(s)}(A_{2u})}{4} \\
\boxed{\text{z314}} \quad \mathbb{Q}_{3,2}^{(c)}(E_u, 2) &= \frac{\mathbb{Q}_{4,1}^{(a)}(E_g, 1)\mathbb{Q}_1^{(s)}(A_{2u})}{4} + \frac{\sqrt{7}\mathbb{Q}_{4,1}^{(a)}(E_g, 2)\mathbb{Q}_1^{(s)}(A_{2u})}{4} \\
\boxed{\text{z315}} \quad \mathbb{Q}_{5,1}^{(c)}(E_u, 1) &= -\frac{\sqrt{6}\mathbb{Q}_{6,2}^{(a)}(E_g, 1)\mathbb{Q}_1^{(s)}(A_{2u})}{8} + \frac{3\sqrt{11}\mathbb{Q}_{6,2}^{(a)}(E_g, 2)\mathbb{Q}_1^{(s)}(A_{2u})}{16} + \frac{\sqrt{5}\mathbb{Q}_{6,2}^{(a)}(E_g, 3)\mathbb{Q}_1^{(s)}(A_{2u})}{16} \\
\boxed{\text{z316}} \quad \mathbb{Q}_{5,2}^{(c)}(E_u, 1) &= -\frac{\sqrt{6}\mathbb{Q}_{6,1}^{(a)}(E_g, 1)\mathbb{Q}_1^{(s)}(A_{2u})}{8} + \frac{3\sqrt{11}\mathbb{Q}_{6,1}^{(a)}(E_g, 2)\mathbb{Q}_1^{(s)}(A_{2u})}{16} + \frac{\sqrt{5}\mathbb{Q}_{6,1}^{(a)}(E_g, 3)\mathbb{Q}_1^{(s)}(A_{2u})}{16} \\
\boxed{\text{z317}} \quad \mathbb{Q}_{5,1}^{(c)}(E_u, 2) &= \frac{7\sqrt{290}\mathbb{Q}_{6,2}^{(a)}(E_g, 1)\mathbb{Q}_1^{(s)}(A_{2u})}{232} + \frac{\sqrt{4785}\mathbb{Q}_{6,2}^{(a)}(E_g, 2)\mathbb{Q}_1^{(s)}(A_{2u})}{464} + \frac{23\sqrt{87}\mathbb{Q}_{6,2}^{(a)}(E_g, 3)\mathbb{Q}_1^{(s)}(A_{2u})}{464} \\
\boxed{\text{z318}} \quad \mathbb{Q}_{5,2}^{(c)}(E_u, 2) &= \frac{7\sqrt{290}\mathbb{Q}_{6,1}^{(a)}(E_g, 1)\mathbb{Q}_1^{(s)}(A_{2u})}{232} + \frac{\sqrt{4785}\mathbb{Q}_{6,1}^{(a)}(E_g, 2)\mathbb{Q}_1^{(s)}(A_{2u})}{464} + \frac{23\sqrt{87}\mathbb{Q}_{6,1}^{(a)}(E_g, 3)\mathbb{Q}_1^{(s)}(A_{2u})}{464} \\
\boxed{\text{z319}} \quad \mathbb{Q}_{5,1}^{(c)}(E_u, 3) &= \frac{\sqrt{1914}\mathbb{Q}_{6,2}^{(a)}(E_g, 1)\mathbb{Q}_1^{(s)}(A_{2u})}{116} + \frac{13\sqrt{29}\mathbb{Q}_{6,2}^{(a)}(E_g, 2)\mathbb{Q}_1^{(s)}(A_{2u})}{232} - \frac{3\sqrt{1595}\mathbb{Q}_{6,2}^{(a)}(E_g, 3)\mathbb{Q}_1^{(s)}(A_{2u})}{232} \\
\boxed{\text{z320}} \quad \mathbb{Q}_{5,2}^{(c)}(E_u, 3) &= \frac{\sqrt{1914}\mathbb{Q}_{6,1}^{(a)}(E_g, 1)\mathbb{Q}_1^{(s)}(A_{2u})}{116} + \frac{13\sqrt{29}\mathbb{Q}_{6,1}^{(a)}(E_g, 2)\mathbb{Q}_1^{(s)}(A_{2u})}{232} - \frac{3\sqrt{1595}\mathbb{Q}_{6,1}^{(a)}(E_g, 3)\mathbb{Q}_1^{(s)}(A_{2u})}{232}
\end{aligned}$$

• 'Pt1'-'Si2' bond-cluster : Si2;Pt1_001_1

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

* ket: $|p_x\rangle$, $|p_y\rangle$, $|p_z\rangle$

* wyckoff: 8a@8i

$$\boxed{\text{z27}} \quad \mathbb{Q}_0^{(c)}(A_{1g}, a) = \frac{\sqrt{3}\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_{1,1}^{(b)}(E_u)}{3} + \frac{\sqrt{3}\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_{1,2}^{(b)}(E_u)}{3} + \frac{\sqrt{3}\mathbb{Q}_1^{(a)}(A_{2u})\mathbb{Q}_1^{(b)}(A_{2u})}{3}$$

$$\boxed{\text{z28}} \quad \mathbb{Q}_0^{(c)}(A_{1g}, b) = \mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_3^{(b)}(B_{2u})$$

$$\boxed{\text{z29}} \quad \mathbb{Q}_2^{(c)}(A_{1g}, a) = -\frac{\sqrt{6}\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_{1,1}^{(b)}(E_u)}{6} - \frac{\sqrt{6}\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_{1,2}^{(b)}(E_u)}{6} + \frac{\sqrt{6}\mathbb{Q}_1^{(a)}(A_{2u})\mathbb{Q}_1^{(b)}(A_{2u})}{3}$$

$$\boxed{\text{z30}} \quad \mathbb{Q}_2^{(c)}(A_{1g}, b) = -\frac{\sqrt{21}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_{1,1}^{(b)}(E_u)}{14} - \frac{\sqrt{35}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{1,1}^{(b)}(E_u)}{14} - \frac{\sqrt{21}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_{1,2}^{(b)}(E_u)}{14} - \frac{\sqrt{35}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{1,2}^{(b)}(E_u)}{14} + \frac{\sqrt{21}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_1^{(b)}(A_{2u})}{7}$$

$$\boxed{\text{z31}} \quad \mathbb{Q}_2^{(c)}(A_{1g}, c) = -\frac{\sqrt{2}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_{1,1}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_{1,2}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z32}} \quad \mathbb{Q}_2^{(c)}(A_{1g}, d) = -\mathbb{G}_2^{(a)}(B_{2u})\mathbb{Q}_3^{(b)}(B_{2u})$$

$$\boxed{\text{z33}} \quad \mathbb{Q}_4^{(c)}(A_{1g}, 1) = \frac{\sqrt{3}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_{1,1}^{(b)}(E_u)}{3} + \frac{\sqrt{3}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_{1,2}^{(b)}(E_u)}{3} + \frac{\sqrt{3}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_1^{(b)}(A_{2u})}{3}$$

$$\boxed{\text{z34}} \quad \mathbb{Q}_4^{(c)}(A_{1g}, 2) = -\frac{\sqrt{105}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_{1,1}^{(b)}(E_u)}{42} + \frac{3\sqrt{7}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{1,1}^{(b)}(E_u)}{14} - \frac{\sqrt{105}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_{1,2}^{(b)}(E_u)}{42} + \frac{3\sqrt{7}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{1,2}^{(b)}(E_u)}{14} + \frac{\sqrt{105}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_1^{(b)}(A_{2u})}{21}$$

$$\boxed{\text{z46}} \quad \mathbb{Q}_5^{(c)}(A_{1u}) = \frac{\sqrt{35}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_{2,1}^{(b)}(E_g)}{14} - \frac{\sqrt{21}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{2,1}^{(b)}(E_g)}{14} - \frac{\sqrt{35}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_{2,2}^{(b)}(E_g)}{14} + \frac{\sqrt{21}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{2,2}^{(b)}(E_g)}{14} + \frac{\sqrt{21}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_2^{(b)}(B_{1g})}{7}$$

$$\boxed{\text{z47}} \quad \mathbb{G}_0^{(c)}(A_{1u}) = \frac{\sqrt{3}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{3} - \frac{\sqrt{3}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{3} + \frac{\sqrt{3}\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_2^{(b)}(B_{1g})}{3}$$

$$\boxed{\text{z48}} \quad \mathbb{G}_2^{(c)}(A_{1u}, a) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} - \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z49}} \quad \mathbb{G}_2^{(c)}(A_{1u}, b) = -\frac{\sqrt{7}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_{2,1}^{(b)}(E_g)}{28} - \frac{5\sqrt{105}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{2,1}^{(b)}(E_g)}{84} + \frac{\sqrt{7}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_{2,2}^{(b)}(E_g)}{28} + \frac{5\sqrt{105}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{2,2}^{(b)}(E_g)}{84} - \frac{\sqrt{105}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_2^{(b)}(B_{1g})}{21}$$

$$\boxed{\text{z50}} \quad \mathbb{G}_2^{(c)}(A_{1u}, c) = \mathbb{G}_2^{(a)}(A_{1u})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\begin{aligned}
\boxed{\text{z51}} \quad \mathbb{G}_2^{(c)}(A_{1u}, d) &= \frac{\sqrt{6}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{6} - \frac{\sqrt{6}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{6} - \frac{\sqrt{6}\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_2^{(b)}(B_{1g})}{3} \\
\boxed{\text{z52}} \quad \mathbb{G}_4^{(c)}(A_{1u}, 1) &= -\frac{\sqrt{5}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_{2,1}^{(b)}(E_g)}{4} - \frac{\sqrt{3}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{2,1}^{(b)}(E_g)}{12} + \frac{\sqrt{5}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_{2,2}^{(b)}(E_g)}{4} + \frac{\sqrt{3}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{2,2}^{(b)}(E_g)}{12} + \frac{\sqrt{3}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_2^{(b)}(B_{1g})}{3} \\
\boxed{\text{z71}} \quad \mathbb{Q}_4^{(c)}(A_{2g}, a) &= \frac{\sqrt{5}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_{1,2}^{(b)}(E_u)}{4} - \frac{\sqrt{3}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{1,2}^{(b)}(E_u)}{4} - \frac{\sqrt{5}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_{1,1}^{(b)}(E_u)}{4} + \frac{\sqrt{3}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{1,1}^{(b)}(E_u)}{4} \\
\boxed{\text{z72}} \quad \mathbb{Q}_4^{(c)}(A_{2g}, b) &= \mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_3^{(b)}(B_{2u}) \\
\boxed{\text{z73}} \quad \mathbb{Q}_4^{(c)}(A_{2g}, c) &= -\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_3^{(b)}(B_{2u}) \\
\boxed{\text{z74}} \quad \mathbb{G}_1^{(c)}(A_{2g}, a) &= \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_{1,2}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_{1,1}^{(b)}(E_u)}{2} \\
\boxed{\text{z75}} \quad \mathbb{G}_1^{(c)}(A_{2g}, b) &= \frac{\sqrt{30}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_{1,2}^{(b)}(E_u)}{10} - \frac{\sqrt{30}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_{1,1}^{(b)}(E_u)}{10} + \frac{\sqrt{10}\mathbb{G}_2^{(a)}(A_{1u})\mathbb{Q}_1^{(b)}(A_{2u})}{5} \\
\boxed{\text{z76}} \quad \mathbb{G}_3^{(c)}(A_{2g}, a) &= -\frac{\sqrt{3}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_{1,2}^{(b)}(E_u)}{4} - \frac{\sqrt{5}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{1,2}^{(b)}(E_u)}{4} + \frac{\sqrt{3}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_{1,1}^{(b)}(E_u)}{4} + \frac{\sqrt{5}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{1,1}^{(b)}(E_u)}{4} \\
\boxed{\text{z77}} \quad \mathbb{G}_3^{(c)}(A_{2g}, b) &= -\frac{\sqrt{5}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_{1,2}^{(b)}(E_u)}{5} + \frac{\sqrt{5}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_{1,1}^{(b)}(E_u)}{5} + \frac{\sqrt{15}\mathbb{G}_2^{(a)}(A_{1u})\mathbb{Q}_1^{(b)}(A_{2u})}{5} \\
\boxed{\text{z78}} \quad \mathbb{Q}_1^{(c)}(A_{2u}, a) &= \mathbb{Q}_1^{(a)}(A_{2u})\mathbb{Q}_0^{(b)}(A_{1g}) \\
\boxed{\text{z96}} \quad \mathbb{Q}_1^{(c)}(A_{2u}, b) &= \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2} + \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} \\
\boxed{\text{z97}} \quad \mathbb{Q}_1^{(c)}(A_{2u}, c) &= -\frac{\sqrt{7}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_{2,2}^{(b)}(E_g)}{7} - \frac{\sqrt{105}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{2,2}^{(b)}(E_g)}{21} - \frac{\sqrt{7}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_{2,1}^{(b)}(E_g)}{7} - \frac{\sqrt{105}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{2,1}^{(b)}(E_g)}{21} + \frac{\sqrt{105}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_2^{(b)}(B_{1g})}{21} \\
\boxed{\text{z98}} \quad \mathbb{Q}_1^{(c)}(A_{2u}, d) &= -\frac{\sqrt{6}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{6} - \frac{\sqrt{6}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{6} - \frac{\sqrt{6}\mathbb{G}_2^{(a)}(B_{2u})\mathbb{Q}_2^{(b)}(B_{1g})}{3} \\
\boxed{\text{z99}} \quad \mathbb{Q}_3^{(c)}(A_{2u}, a) &= \mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_0^{(b)}(A_{1g}) \\
\boxed{\text{z100}} \quad \mathbb{Q}_3^{(c)}(A_{2u}, b) &= -\frac{\sqrt{35}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_{2,2}^{(b)}(E_g)}{28} - \frac{5\sqrt{21}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{2,2}^{(b)}(E_g)}{84} - \frac{\sqrt{35}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_{2,1}^{(b)}(E_g)}{28} - \frac{5\sqrt{21}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{2,1}^{(b)}(E_g)}{84} - \frac{4\sqrt{21}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_2^{(b)}(B_{1g})}{21}
\end{aligned}$$

$$\begin{aligned}
\text{z101} \quad \mathbb{Q}_3^{(c)}(A_{2u}, c) &= -\frac{\sqrt{3}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{3} - \frac{\sqrt{3}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{3} + \frac{\sqrt{3}\mathbb{G}_2^{(a)}(B_{2u})\mathbb{Q}_2^{(b)}(B_{1g})}{3} \\
\text{z102} \quad \mathbb{Q}_5^{(c)}(A_{2u}, 2) &= \frac{\sqrt{5}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_{2,2}^{(b)}(E_g)}{4} - \frac{\sqrt{3}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{2,2}^{(b)}(E_g)}{4} + \frac{\sqrt{5}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_{2,1}^{(b)}(E_g)}{4} - \frac{\sqrt{3}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{2,1}^{(b)}(E_g)}{4} \\
\text{z161} \quad \mathbb{Q}_2^{(c)}(B_{1g}, a) &= \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_{1,1}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_{1,2}^{(b)}(E_u)}{2} \\
\text{z162} \quad \mathbb{Q}_2^{(c)}(B_{1g}, b) &= \mathbb{Q}_1^{(a)}(A_{2u})\mathbb{Q}_3^{(b)}(B_{2u}) \\
\text{z163} \quad \mathbb{Q}_2^{(c)}(B_{1g}, c) &= \frac{3\sqrt{7}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_{1,1}^{(b)}(E_u)}{14} - \frac{\sqrt{105}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{1,1}^{(b)}(E_u)}{42} - \frac{3\sqrt{7}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_{1,2}^{(b)}(E_u)}{14} + \frac{\sqrt{105}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{1,2}^{(b)}(E_u)}{42} + \frac{\sqrt{105}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_1^{(b)}(A_{2u})}{21} \\
\text{z164} \quad \mathbb{Q}_2^{(c)}(B_{1g}, d) &= -\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_3^{(b)}(B_{2u}) \\
\text{z165} \quad \mathbb{Q}_2^{(c)}(B_{1g}, e) &= -\frac{\sqrt{6}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_{1,1}^{(b)}(E_u)}{6} + \frac{\sqrt{6}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_{1,2}^{(b)}(E_u)}{6} + \frac{\sqrt{6}\mathbb{G}_2^{(a)}(B_{2u})\mathbb{Q}_1^{(b)}(A_{2u})}{3} \\
\text{z166} \quad \mathbb{Q}_4^{(c)}(B_{1g}) &= \frac{\sqrt{35}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_{1,1}^{(b)}(E_u)}{14} + \frac{\sqrt{21}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{1,1}^{(b)}(E_u)}{14} - \frac{\sqrt{35}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_{1,2}^{(b)}(E_u)}{14} - \frac{\sqrt{21}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{1,2}^{(b)}(E_u)}{14} - \frac{\sqrt{21}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_1^{(b)}(A_{2u})}{7} \\
\text{z167} \quad \mathbb{G}_3^{(c)}(B_{1g}, a) &= -\frac{\sqrt{3}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{1,1}^{(b)}(E_u)}{3} + \frac{\sqrt{3}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{1,2}^{(b)}(E_u)}{3} - \frac{\sqrt{3}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_1^{(b)}(A_{2u})}{3} \\
\text{z168} \quad \mathbb{G}_3^{(c)}(B_{1g}, b) &= \frac{\sqrt{3}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_{1,1}^{(b)}(E_u)}{3} - \frac{\sqrt{3}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_{1,2}^{(b)}(E_u)}{3} + \frac{\sqrt{3}\mathbb{G}_2^{(a)}(B_{2u})\mathbb{Q}_1^{(b)}(A_{2u})}{3} \\
\text{z169} \quad \mathbb{Q}_3^{(c)}(B_{1u}, a) &= \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} + \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2} \\
\text{z170} \quad \mathbb{Q}_3^{(c)}(B_{1u}, b) &= \mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_0^{(b)}(A_{1g}) \\
\text{z171} \quad \mathbb{Q}_3^{(c)}(B_{1u}, c) &= -\frac{\sqrt{2}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} - \frac{\sqrt{2}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2} \\
\text{z172} \quad \mathbb{Q}_3^{(c)}(B_{1u}, d) &= \mathbb{G}_2^{(a)}(A_{1u})\mathbb{Q}_2^{(b)}(B_{1g}) \\
\text{z173} \quad \mathbb{Q}_5^{(c)}(B_{1u}) &= \frac{\sqrt{2}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} + \frac{\sqrt{2}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}
\end{aligned}$$

$$\begin{aligned}
\text{z174} \quad \mathbb{G}_2^{(c)}(B_{1u}, a) &= \mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_0^{(b)}(A_{1g}) \\
\text{z175} \quad \mathbb{G}_2^{(c)}(B_{1u}, b) &= -\frac{\sqrt{2}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} - \frac{\sqrt{2}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2} \\
\text{z176} \quad \mathbb{Q}_2^{(c)}(B_{2g}, a) &= \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_{1,2}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_{1,1}^{(b)}(E_u)}{2} \\
\text{z177} \quad \mathbb{Q}_2^{(c)}(B_{2g}, b) &= -\frac{\sqrt{7}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_{1,2}^{(b)}(E_u)}{7} + \frac{\sqrt{105}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{1,2}^{(b)}(E_u)}{21} - \frac{\sqrt{7}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_{1,1}^{(b)}(E_u)}{7} + \frac{\sqrt{105}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{1,1}^{(b)}(E_u)}{21} + \frac{\sqrt{105}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_1^{(b)}(A_{2u})}{21} \\
\text{z178} \quad \mathbb{Q}_2^{(c)}(B_{2g}, c) &= -\frac{\sqrt{6}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_{1,2}^{(b)}(E_u)}{6} - \frac{\sqrt{6}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_{1,1}^{(b)}(E_u)}{6} - \frac{\sqrt{6}\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_1^{(b)}(A_{2u})}{3} \\
\text{z179} \quad \mathbb{Q}_2^{(c)}(B_{2g}, d) &= \mathbb{G}_2^{(a)}(A_{1u})\mathbb{Q}_3^{(b)}(B_{2u}) \\
\text{z180} \quad \mathbb{Q}_4^{(c)}(B_{2g}) &= -\frac{\sqrt{35}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_{1,2}^{(b)}(E_u)}{28} - \frac{3\sqrt{21}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{1,2}^{(b)}(E_u)}{28} - \frac{\sqrt{35}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_{1,1}^{(b)}(E_u)}{28} - \frac{3\sqrt{21}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{1,1}^{(b)}(E_u)}{28} + \frac{\sqrt{21}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_1^{(b)}(A_{2u})}{7} \\
\text{z181} \quad \mathbb{G}_3^{(c)}(B_{2g}, a) &= \frac{\sqrt{5}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_{1,2}^{(b)}(E_u)}{4} + \frac{\sqrt{3}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{1,2}^{(b)}(E_u)}{12} + \frac{\sqrt{5}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_{1,1}^{(b)}(E_u)}{4} + \frac{\sqrt{3}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{1,1}^{(b)}(E_u)}{12} + \frac{\sqrt{3}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_1^{(b)}(A_{2u})}{3} \\
\text{z182} \quad \mathbb{G}_3^{(c)}(B_{2g}, b) &= -\frac{\sqrt{3}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_{1,2}^{(b)}(E_u)}{3} - \frac{\sqrt{3}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_{1,1}^{(b)}(E_u)}{3} + \frac{\sqrt{3}\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_1^{(b)}(A_{2u})}{3} \\
\text{z183} \quad \mathbb{Q}_3^{(c)}(B_{2u}, a) &= \frac{\sqrt{3}\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{3} - \frac{\sqrt{3}\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{3} + \frac{\sqrt{3}\mathbb{Q}_1^{(a)}(A_{2u})\mathbb{Q}_2^{(b)}(B_{1g})}{3} \\
\text{z184} \quad \mathbb{Q}_3^{(c)}(B_{2u}, b) &= \mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_0^{(b)}(A_{1g}) \\
\text{z185} \quad \mathbb{Q}_3^{(c)}(B_{2u}, c) &= \frac{\sqrt{3}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_{2,2}^{(b)}(E_g)}{12} - \frac{\sqrt{5}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{2,2}^{(b)}(E_g)}{4} - \frac{\sqrt{3}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_{2,1}^{(b)}(E_g)}{12} + \frac{\sqrt{5}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{2,1}^{(b)}(E_g)}{4} - \frac{\sqrt{3}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_2^{(b)}(B_{1g})}{3} \\
\text{z186} \quad \mathbb{Q}_5^{(c)}(B_{2u}) &= -\frac{\sqrt{105}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_{2,2}^{(b)}(E_g)}{21} - \frac{\sqrt{7}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{2,2}^{(b)}(E_g)}{7} + \frac{\sqrt{105}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_{2,1}^{(b)}(E_g)}{21} + \frac{\sqrt{7}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{2,1}^{(b)}(E_g)}{7} + \frac{\sqrt{105}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_2^{(b)}(B_{1g})}{21} \\
\text{z187} \quad \mathbb{G}_2^{(c)}(B_{2u}, a) &= -\frac{\sqrt{6}\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{6} + \frac{\sqrt{6}\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{6} + \frac{\sqrt{6}\mathbb{Q}_1^{(a)}(A_{2u})\mathbb{Q}_2^{(b)}(B_{1g})}{3}
\end{aligned}$$

$$\boxed{\text{z188}} \quad \mathbb{G}_2^{(c)}(B_{2u}, b) = -\frac{3\sqrt{21}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_{2,2}^{(b)}(E_g)}{28} + \frac{\sqrt{35}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{2,2}^{(b)}(E_g)}{28} + \frac{3\sqrt{21}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_{2,1}^{(b)}(E_g)}{28} - \frac{\sqrt{35}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{2,1}^{(b)}(E_g)}{28} - \frac{\sqrt{21}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_2^{(b)}(B_{1g})}{7}$$

$$\boxed{\text{z189}} \quad \mathbb{G}_2^{(c)}(B_{2u}, c) = \mathbb{G}_2^{(a)}(B_{2u})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z190}} \quad \mathbb{G}_2^{(c)}(B_{2u}, d) = \frac{\sqrt{2}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2} - \frac{\sqrt{2}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z204}} \quad \mathbb{Q}_{2,1}^{(c)}(E_g, a) = \frac{\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_1^{(b)}(A_{2u})}{2} + \frac{\mathbb{Q}_1^{(a)}(A_{2u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z205}} \quad \mathbb{Q}_{2,2}^{(c)}(E_g, a) = \frac{\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_1^{(b)}(A_{2u})}{2} + \frac{\mathbb{Q}_1^{(a)}(A_{2u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z206}} \quad \mathbb{Q}_{2,1}^{(c)}(E_g, b) = -\frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_3^{(b)}(B_{2u})}{2}$$

$$\boxed{\text{z207}} \quad \mathbb{Q}_{2,2}^{(c)}(E_g, b) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_3^{(b)}(B_{2u})}{2}$$

$$\boxed{\text{z208}} \quad \mathbb{Q}_{2,1}^{(c)}(E_g, c) = -\frac{\sqrt{14}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_1^{(b)}(A_{2u})}{14} - \frac{\sqrt{210}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_1^{(b)}(A_{2u})}{42} - \frac{\sqrt{14}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{14} + \frac{\sqrt{210}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{42} - \frac{\sqrt{210}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{42}$$

$$\boxed{\text{z209}} \quad \mathbb{Q}_{2,2}^{(c)}(E_g, c) = -\frac{\sqrt{14}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_1^{(b)}(A_{2u})}{14} - \frac{\sqrt{210}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_1^{(b)}(A_{2u})}{42} - \frac{\sqrt{14}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{14} + \frac{\sqrt{210}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{42} + \frac{\sqrt{210}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{42}$$

$$\boxed{\text{z210}} \quad \mathbb{Q}_{2,1}^{(c)}(E_g, d) = -\frac{\sqrt{2}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_3^{(b)}(B_{2u})}{8} + \frac{\sqrt{30}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_3^{(b)}(B_{2u})}{8}$$

$$\boxed{\text{z234}} \quad \mathbb{Q}_{2,2}^{(c)}(E_g, d) = \frac{\sqrt{2}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_3^{(b)}(B_{2u})}{8} - \frac{\sqrt{30}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_3^{(b)}(B_{2u})}{8}$$

$$\boxed{\text{z235}} \quad \mathbb{Q}_{2,1}^{(c)}(E_g, e) = \frac{\sqrt{3}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_1^{(b)}(A_{2u})}{6} + \frac{\mathbb{G}_2^{(a)}(A_{1u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{2} + \frac{\sqrt{3}\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{6} + \frac{\sqrt{3}\mathbb{G}_2^{(a)}(B_{2u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{6}$$

$$\boxed{\text{z236}} \quad \mathbb{Q}_{2,2}^{(c)}(E_g, e) = \frac{\sqrt{3}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_1^{(b)}(A_{2u})}{6} - \frac{\mathbb{G}_2^{(a)}(A_{1u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{2} + \frac{\sqrt{3}\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{6} - \frac{\sqrt{3}\mathbb{G}_2^{(a)}(B_{2u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{6}$$

$$\boxed{\text{z237}} \quad \mathbb{Q}_{4,1}^{(c)}(E_g, 1a) = \frac{\sqrt{10}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_1^{(b)}(A_{2u})}{8} + \frac{\sqrt{6}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_1^{(b)}(A_{2u})}{8} - \frac{\sqrt{10}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{8} - \frac{\sqrt{6}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{8}$$

$$\begin{aligned}
\text{z238} \quad \mathbb{Q}_{4,2}^{(c)}(E_g, 1a) &= \frac{\sqrt{10}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_1^{(b)}(A_{2u})}{8} + \frac{\sqrt{6}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_1^{(b)}(A_{2u})}{8} - \frac{\sqrt{10}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{8} + \frac{\sqrt{6}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{8} \\
\text{z239} \quad \mathbb{Q}_{4,1}^{(c)}(E_g, 1b) &= -\frac{\sqrt{30}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_3^{(b)}(B_{2u})}{8} - \frac{\sqrt{2}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_3^{(b)}(B_{2u})}{8} \\
\text{z240} \quad \mathbb{Q}_{4,2}^{(c)}(E_g, 1b) &= \frac{\sqrt{30}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_3^{(b)}(B_{2u})}{8} + \frac{\sqrt{2}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_3^{(b)}(B_{2u})}{8} \\
\text{z241} \quad \mathbb{Q}_{4,1}^{(c)}(E_g, 1c) &= -\frac{\sqrt{2}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_3^{(b)}(B_{2u})}{2} \\
\text{z257} \quad \mathbb{Q}_{4,2}^{(c)}(E_g, 1c) &= \frac{\sqrt{2}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_3^{(b)}(B_{2u})}{2} \\
\text{z258} \quad \mathbb{Q}_{4,1}^{(c)}(E_g, 2) &= -\frac{\sqrt{70}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_1^{(b)}(A_{2u})}{56} + \frac{3\sqrt{42}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_1^{(b)}(A_{2u})}{56} - \frac{\sqrt{70}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{56} + \frac{\sqrt{42}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{14} + \frac{3\sqrt{42}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{56} \\
\text{z259} \quad \mathbb{Q}_{4,2}^{(c)}(E_g, 2) &= -\frac{\sqrt{70}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_1^{(b)}(A_{2u})}{56} + \frac{3\sqrt{42}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_1^{(b)}(A_{2u})}{56} - \frac{\sqrt{70}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{56} + \frac{\sqrt{42}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{14} - \frac{3\sqrt{42}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{56} \\
\text{z260} \quad \mathbb{G}_{1,1}^{(c)}(E_g, a) &= \frac{\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_1^{(b)}(A_{2u})}{2} - \frac{\mathbb{Q}_1^{(a)}(A_{2u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{2} \\
\text{z261} \quad \mathbb{G}_{1,2}^{(c)}(E_g, a) &= \frac{\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_1^{(b)}(A_{2u})}{2} - \frac{\mathbb{Q}_1^{(a)}(A_{2u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{2} \\
\text{z262} \quad \mathbb{G}_{1,1}^{(c)}(E_g, b) &= -\frac{\sqrt{15}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_1^{(b)}(A_{2u})}{10} - \frac{\sqrt{5}\mathbb{G}_2^{(a)}(A_{1u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{10} + \frac{\sqrt{15}\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{10} + \frac{\sqrt{15}\mathbb{G}_2^{(a)}(B_{2u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{10} \\
\text{z263} \quad \mathbb{G}_{1,2}^{(c)}(E_g, b) &= -\frac{\sqrt{15}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_1^{(b)}(A_{2u})}{10} + \frac{\sqrt{5}\mathbb{G}_2^{(a)}(A_{1u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{10} + \frac{\sqrt{15}\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{10} - \frac{\sqrt{15}\mathbb{G}_2^{(a)}(B_{2u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{10} \\
\text{z285} \quad \mathbb{G}_{3,1}^{(c)}(E_g, 1a) &= -\frac{\sqrt{6}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_1^{(b)}(A_{2u})}{8} + \frac{\sqrt{10}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_1^{(b)}(A_{2u})}{8} + \frac{\sqrt{6}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{8} - \frac{\sqrt{10}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{8} \\
\text{z286} \quad \mathbb{G}_{3,2}^{(c)}(E_g, 1a) &= -\frac{\sqrt{6}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_1^{(b)}(A_{2u})}{8} + \frac{\sqrt{10}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_1^{(b)}(A_{2u})}{8} + \frac{\sqrt{6}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{8} + \frac{\sqrt{10}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{8} \\
\text{z287} \quad \mathbb{G}_{3,1}^{(c)}(E_g, 1b) &= \frac{\sqrt{10}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_1^{(b)}(A_{2u})}{10} - \frac{\sqrt{30}\mathbb{G}_2^{(a)}(A_{1u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{20} + \frac{3\sqrt{10}\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{20} - \frac{\sqrt{10}\mathbb{G}_2^{(a)}(B_{2u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{10}
\end{aligned}$$

$$\begin{aligned}
\text{z288} \quad \mathbb{G}_{3,2}^{(c)}(E_g, 1b) &= \frac{\sqrt{10}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_1^{(b)}(A_{2u})}{10} + \frac{\sqrt{30}\mathbb{G}_2^{(a)}(A_{1u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{20} + \frac{3\sqrt{10}\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{20} + \frac{\sqrt{10}\mathbb{G}_2^{(a)}(B_{2u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{10} \\
\text{z289} \quad \mathbb{G}_{3,1}^{(c)}(E_g, 2a) &= \frac{\sqrt{10}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_1^{(b)}(A_{2u})}{8} - \frac{\sqrt{6}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_1^{(b)}(A_{2u})}{24} + \frac{\sqrt{10}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{8} + \frac{\sqrt{6}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{6} - \frac{\sqrt{6}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{24} \\
\text{z290} \quad \mathbb{G}_{3,2}^{(c)}(E_g, 2a) &= \frac{\sqrt{10}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_1^{(b)}(A_{2u})}{8} - \frac{\sqrt{6}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_1^{(b)}(A_{2u})}{24} + \frac{\sqrt{10}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{8} + \frac{\sqrt{6}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{6} + \frac{\sqrt{6}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{24} \\
\text{z291} \quad \mathbb{G}_{3,1}^{(c)}(E_g, 2b) &= \frac{\sqrt{6}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_1^{(b)}(A_{2u})}{6} - \frac{\sqrt{2}\mathbb{G}_2^{(a)}(A_{1u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{4} - \frac{\sqrt{6}\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{12} + \frac{\sqrt{6}\mathbb{G}_2^{(a)}(B_{2u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{6} \\
\text{z292} \quad \mathbb{G}_{3,2}^{(c)}(E_g, 2b) &= \frac{\sqrt{6}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_1^{(b)}(A_{2u})}{6} + \frac{\sqrt{2}\mathbb{G}_2^{(a)}(A_{1u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{4} - \frac{\sqrt{6}\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{12} - \frac{\sqrt{6}\mathbb{G}_2^{(a)}(B_{2u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{6} \\
\text{z351} \quad \mathbb{Q}_{1,1}^{(c)}(E_u, a) &= \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_0^{(b)}(A_{1g})}{2} \\
\text{z352} \quad \mathbb{Q}_{1,2}^{(c)}(E_u, a) &= \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_0^{(b)}(A_{1g})}{2} \\
\text{z353} \quad \mathbb{Q}_{1,1}^{(c)}(E_u, b) &= \frac{\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_2^{(b)}(B_{1g})}{2} + \frac{\mathbb{Q}_1^{(a)}(A_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2} \\
\text{z354} \quad \mathbb{Q}_{1,2}^{(c)}(E_u, b) &= -\frac{\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_2^{(b)}(B_{1g})}{2} + \frac{\mathbb{Q}_1^{(a)}(A_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} \\
\text{z355} \quad \mathbb{Q}_{1,1}^{(c)}(E_u, c) &= \frac{3\sqrt{14}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_2^{(b)}(B_{1g})}{28} - \frac{\sqrt{210}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_2^{(b)}(B_{1g})}{84} - \frac{\sqrt{14}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{14} + \frac{\sqrt{210}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{42} + \frac{\sqrt{210}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{42} \\
\text{z356} \quad \mathbb{Q}_{1,2}^{(c)}(E_u, c) &= -\frac{3\sqrt{14}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_2^{(b)}(B_{1g})}{28} + \frac{\sqrt{210}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_2^{(b)}(B_{1g})}{84} - \frac{\sqrt{14}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{14} + \frac{\sqrt{210}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{42} - \frac{\sqrt{210}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{42} \\
\text{z357} \quad \mathbb{Q}_{1,1}^{(c)}(E_u, d) &= \frac{\sqrt{3}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_2^{(b)}(B_{1g})}{6} - \frac{\mathbb{G}_2^{(a)}(A_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} - \frac{\sqrt{3}\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{6} + \frac{\sqrt{3}\mathbb{G}_2^{(a)}(B_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{6} \\
\text{z358} \quad \mathbb{Q}_{1,2}^{(c)}(E_u, d) &= -\frac{\sqrt{3}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_2^{(b)}(B_{1g})}{6} + \frac{\mathbb{G}_2^{(a)}(A_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2} - \frac{\sqrt{3}\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{6} - \frac{\sqrt{3}\mathbb{G}_2^{(a)}(B_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{6} \\
\text{z359} \quad \mathbb{Q}_{3,1}^{(c)}(E_u, 1a) &= \frac{\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_2^{(b)}(B_{1g})}{2} - \frac{\mathbb{Q}_1^{(a)}(A_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}
\end{aligned}$$

$$\boxed{\text{z360}} \quad \mathbb{Q}_{3,2}^{(c)}(E_u, 1a) = -\frac{\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_2^{(b)}(B_{1g})}{2} - \frac{\mathbb{Q}_1^{(a)}(A_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z361}} \quad \mathbb{Q}_{3,1}^{(c)}(E_u, 1b) = \frac{\sqrt{2}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z362}} \quad \mathbb{Q}_{3,2}^{(c)}(E_u, 1b) = \frac{\sqrt{2}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z363}} \quad \mathbb{Q}_{3,1}^{(c)}(E_u, 1c) = \frac{33\sqrt{1834}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_2^{(b)}(B_{1g})}{3668} + \frac{17\sqrt{27510}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_2^{(b)}(B_{1g})}{11004} - \frac{2\sqrt{1834}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{917} - \frac{17\sqrt{27510}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{5502} + \frac{2\sqrt{27510}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2751}$$

$$\boxed{\text{z364}} \quad \mathbb{Q}_{3,2}^{(c)}(E_u, 1c) = -\frac{33\sqrt{1834}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_2^{(b)}(B_{1g})}{3668} - \frac{17\sqrt{27510}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_2^{(b)}(B_{1g})}{11004} - \frac{2\sqrt{1834}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{917} - \frac{17\sqrt{27510}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{5502} - \frac{2\sqrt{27510}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2751}$$

$$\boxed{\text{z365}} \quad \mathbb{Q}_{3,1}^{(c)}(E_u, 1d) = -\frac{\sqrt{15}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_2^{(b)}(B_{1g})}{30} + \frac{\sqrt{5}\mathbb{G}_2^{(a)}(A_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{10} + \frac{\sqrt{15}\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{30} + \frac{\sqrt{15}\mathbb{G}_2^{(a)}(B_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{6}$$

$$\boxed{\text{z366}} \quad \mathbb{Q}_{3,2}^{(c)}(E_u, 1d) = \frac{\sqrt{15}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_2^{(b)}(B_{1g})}{30} - \frac{\sqrt{5}\mathbb{G}_2^{(a)}(A_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{10} + \frac{\sqrt{15}\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{30} - \frac{\sqrt{15}\mathbb{G}_2^{(a)}(B_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{6}$$

$$\boxed{\text{z367}} \quad \mathbb{Q}_{3,1}^{(c)}(E_u, 2a) = \frac{\sqrt{2}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z368}} \quad \mathbb{Q}_{3,2}^{(c)}(E_u, 2a) = \frac{\sqrt{2}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z369}} \quad \mathbb{Q}_{3,1}^{(c)}(E_u, 2b) = \frac{25\sqrt{655}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_2^{(b)}(B_{1g})}{2096} - \frac{5\sqrt{393}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_2^{(b)}(B_{1g})}{2096} - \frac{7\sqrt{655}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{1048} + \frac{5\sqrt{393}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{1048} - \frac{4\sqrt{393}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{131}$$

$$\boxed{\text{z370}} \quad \mathbb{Q}_{3,2}^{(c)}(E_u, 2b) = -\frac{25\sqrt{655}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_2^{(b)}(B_{1g})}{2096} + \frac{5\sqrt{393}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_2^{(b)}(B_{1g})}{2096} - \frac{7\sqrt{655}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{1048} + \frac{5\sqrt{393}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{1048} + \frac{4\sqrt{393}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{131}$$

$$\boxed{\text{z371}} \quad \mathbb{Q}_{3,1}^{(c)}(E_u, 2c) = \frac{\sqrt{15}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_2^{(b)}(B_{1g})}{10} + \frac{\sqrt{5}\mathbb{G}_2^{(a)}(A_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{5} - \frac{\sqrt{15}\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{10}$$

$$\boxed{\text{z372}} \quad \mathbb{Q}_{3,2}^{(c)}(E_u, 2c) = -\frac{\sqrt{15}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_2^{(b)}(B_{1g})}{10} - \frac{\sqrt{5}\mathbb{G}_2^{(a)}(A_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{5} - \frac{\sqrt{15}\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{10}$$

$$\boxed{\text{z373}} \quad \mathbb{Q}_{5,1}^{(c)}(E_u, 1) = \frac{5\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_2^{(b)}(B_{1g})}{16} - \frac{\sqrt{15}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_2^{(b)}(B_{1g})}{80} + \frac{5\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{8} + \frac{\sqrt{15}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{40}$$

$$\boxed{\text{z374}} \quad \mathbb{Q}_{5,2}^{(c)}(E_u, 1) = -\frac{5\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_2^{(b)}(B_{1g})}{16} + \frac{\sqrt{15}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_2^{(b)}(B_{1g})}{80} + \frac{5\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{8} + \frac{\sqrt{15}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{40}$$

$$\boxed{\text{z375}} \quad \mathbb{Q}_{5,1}^{(c)}(E_u, 2) = -\frac{\sqrt{10}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_2^{(b)}(B_{1g})}{5} - \frac{\sqrt{10}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{10}$$

$$\boxed{\text{z376}} \quad \mathbb{Q}_{5,2}^{(c)}(E_u, 2) = \frac{\sqrt{10}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_2^{(b)}(B_{1g})}{5} - \frac{\sqrt{10}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{10}$$

$$\boxed{\text{z377}} \quad \mathbb{G}_{2,1}^{(c)}(E_u, a) = \frac{\sqrt{2}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z378}} \quad \mathbb{G}_{2,2}^{(c)}(E_u, a) = \frac{\sqrt{2}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z379}} \quad \mathbb{G}_{2,1}^{(c)}(E_u, b) = -\frac{\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_2^{(b)}(B_{1g})}{2} - \frac{\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z380}} \quad \mathbb{G}_{2,2}^{(c)}(E_u, b) = \frac{\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_2^{(b)}(B_{1g})}{2} - \frac{\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$$

• 'Pt2'-'Si1' bond-cluster : Si1;Pt2_001_1

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

* ket: $|p_x\rangle$, $|p_y\rangle$, $|p_z\rangle$

* wyckoff: 8a@8i

$$\boxed{\text{z19}} \quad \mathbb{Q}_0^{(c)}(A_{1g}, a) = \frac{\sqrt{3}\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_{1,1}^{(b)}(E_u)}{3} + \frac{\sqrt{3}\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_{1,2}^{(b)}(E_u)}{3} + \frac{\sqrt{3}\mathbb{Q}_1^{(a)}(A_{2u})\mathbb{Q}_1^{(b)}(A_{2u})}{3}$$

$$\boxed{\text{z20}} \quad \mathbb{Q}_0^{(c)}(A_{1g}, b) = \mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_3^{(b)}(B_{2u})$$

$$\boxed{\text{z21}} \quad \mathbb{Q}_2^{(c)}(A_{1g}, a) = -\frac{\sqrt{6}\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_{1,1}^{(b)}(E_u)}{6} - \frac{\sqrt{6}\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_{1,2}^{(b)}(E_u)}{6} + \frac{\sqrt{6}\mathbb{Q}_1^{(a)}(A_{2u})\mathbb{Q}_1^{(b)}(A_{2u})}{3}$$

$$\boxed{\text{z22}} \quad \mathbb{Q}_2^{(c)}(A_{1g}, b) = -\frac{\sqrt{21}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_{1,1}^{(b)}(E_u)}{14} - \frac{\sqrt{35}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{1,1}^{(b)}(E_u)}{14} - \frac{\sqrt{21}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_{1,2}^{(b)}(E_u)}{14} - \frac{\sqrt{35}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{1,2}^{(b)}(E_u)}{14} + \frac{\sqrt{21}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_1^{(b)}(A_{2u})}{7}$$

$$\boxed{\text{z23}} \quad \mathbb{Q}_2^{(c)}(A_{1g}, c) = -\frac{\sqrt{2}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_{1,1}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_{1,2}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z24}} \quad \mathbb{Q}_2^{(c)}(A_{1g}, d) = -\mathbb{G}_2^{(a)}(B_{2u})\mathbb{Q}_3^{(b)}(B_{2u})$$

$$\boxed{\text{z25}} \quad \mathbb{Q}_4^{(c)}(A_{1g}, 1) = \frac{\sqrt{3}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_{1,1}^{(b)}(E_u)}{3} + \frac{\sqrt{3}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_{1,2}^{(b)}(E_u)}{3} + \frac{\sqrt{3}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_1^{(b)}(A_{2u})}{3}$$

$$\boxed{\text{z26}} \quad \mathbb{Q}_4^{(c)}(A_{1g}, 2) = -\frac{\sqrt{105}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_{1,1}^{(b)}(E_u)}{42} + \frac{3\sqrt{7}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{1,1}^{(b)}(E_u)}{14} - \frac{\sqrt{105}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_{1,2}^{(b)}(E_u)}{42} + \frac{3\sqrt{7}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{1,2}^{(b)}(E_u)}{14} + \frac{\sqrt{105}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_1^{(b)}(A_{2u})}{21}$$

$$\boxed{\text{z39}} \quad \mathbb{Q}_5^{(c)}(A_{1u}) = \frac{\sqrt{35}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_{2,1}^{(b)}(E_g)}{14} - \frac{\sqrt{21}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{2,1}^{(b)}(E_g)}{14} - \frac{\sqrt{35}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_{2,2}^{(b)}(E_g)}{14} + \frac{\sqrt{21}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{2,2}^{(b)}(E_g)}{14} + \frac{\sqrt{21}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_2^{(b)}(B_{1g})}{7}$$

$$\boxed{\text{z40}} \quad \mathbb{G}_0^{(c)}(A_{1u}) = \frac{\sqrt{3}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{3} - \frac{\sqrt{3}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{3} + \frac{\sqrt{3}\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_2^{(b)}(B_{1g})}{3}$$

$$\boxed{\text{z41}} \quad \mathbb{G}_2^{(c)}(A_{1u}, a) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} - \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z42}} \quad \mathbb{G}_2^{(c)}(A_{1u}, b) = -\frac{\sqrt{7}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_{2,1}^{(b)}(E_g)}{28} - \frac{5\sqrt{105}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{2,1}^{(b)}(E_g)}{84} + \frac{\sqrt{7}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_{2,2}^{(b)}(E_g)}{28} + \frac{5\sqrt{105}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{2,2}^{(b)}(E_g)}{84} - \frac{\sqrt{105}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_2^{(b)}(B_{1g})}{21}$$

$$\boxed{\text{z43}} \quad \mathbb{G}_2^{(c)}(A_{1u}, c) = \mathbb{G}_2^{(a)}(A_{1u})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z44}} \quad \mathbb{G}_2^{(c)}(A_{1u}, d) = \frac{\sqrt{6}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{6} - \frac{\sqrt{6}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{6} - \frac{\sqrt{6}\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_2^{(b)}(B_{1g})}{3}$$

$$\boxed{\text{z45}} \quad \mathbb{G}_4^{(c)}(A_{1u}, 1) = -\frac{\sqrt{5}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_{2,1}^{(b)}(E_g)}{4} - \frac{\sqrt{3}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{2,1}^{(b)}(E_g)}{12} + \frac{\sqrt{5}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_{2,2}^{(b)}(E_g)}{4} + \frac{\sqrt{3}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{2,2}^{(b)}(E_g)}{12} + \frac{\sqrt{3}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_2^{(b)}(B_{1g})}{3}$$

$$\boxed{\text{z63}} \quad \mathbb{Q}_4^{(c)}(A_{2g}, a) = \frac{\sqrt{5}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_{1,2}^{(b)}(E_u)}{4} - \frac{\sqrt{3}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{1,2}^{(b)}(E_u)}{4} - \frac{\sqrt{5}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_{1,1}^{(b)}(E_u)}{4} + \frac{\sqrt{3}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{1,1}^{(b)}(E_u)}{4}$$

$$\boxed{\text{z64}} \quad \mathbb{Q}_4^{(c)}(A_{2g}, b) = \mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_3^{(b)}(B_{2u})$$

$$\boxed{\text{z65}} \quad \mathbb{Q}_4^{(c)}(A_{2g}, c) = -\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_3^{(b)}(B_{2u})$$

$$\boxed{\text{z66}} \quad \mathbb{G}_1^{(c)}(A_{2g}, a) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_{1,2}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_{1,1}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z67}} \quad \mathbb{G}_1^{(c)}(A_{2g}, b) = \frac{\sqrt{30}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_{1,2}^{(b)}(E_u)}{10} - \frac{\sqrt{30}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_{1,1}^{(b)}(E_u)}{10} + \frac{\sqrt{10}\mathbb{G}_2^{(a)}(A_{1u})\mathbb{Q}_1^{(b)}(A_{2u})}{5}$$

$$\boxed{\text{z68}} \quad \mathbb{G}_3^{(c)}(A_{2g}, a) = -\frac{\sqrt{3}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_{1,2}^{(b)}(E_u)}{4} - \frac{\sqrt{5}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{1,2}^{(b)}(E_u)}{4} + \frac{\sqrt{3}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_{1,1}^{(b)}(E_u)}{4} + \frac{\sqrt{5}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{1,1}^{(b)}(E_u)}{4}$$

$$\boxed{\text{z69}} \quad \mathbb{G}_3^{(c)}(A_{2g}, b) = -\frac{\sqrt{5}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_{1,2}^{(b)}(E_u)}{5} + \frac{\sqrt{5}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_{1,1}^{(b)}(E_u)}{5} + \frac{\sqrt{15}\mathbb{G}_2^{(a)}(A_{1u})\mathbb{Q}_1^{(b)}(A_{2u})}{5}$$

$$\boxed{\text{z70}} \quad \mathbb{Q}_1^{(c)}(A_{2u}, a) = \mathbb{Q}_1^{(a)}(A_{2u})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z89}} \quad \mathbb{Q}_1^{(c)}(A_{2u}, b) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2} + \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z90}} \quad \mathbb{Q}_1^{(c)}(A_{2u}, c) = -\frac{\sqrt{7}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_{2,2}^{(b)}(E_g)}{7} - \frac{\sqrt{105}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{2,2}^{(b)}(E_g)}{21} - \frac{\sqrt{7}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_{2,1}^{(b)}(E_g)}{7} - \frac{\sqrt{105}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{2,1}^{(b)}(E_g)}{21} + \frac{\sqrt{105}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_2^{(b)}(B_{1g})}{21}$$

$$\boxed{\text{z91}} \quad \mathbb{Q}_1^{(c)}(A_{2u}, d) = -\frac{\sqrt{6}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{6} - \frac{\sqrt{6}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{6} - \frac{\sqrt{6}\mathbb{G}_2^{(a)}(B_{2u})\mathbb{Q}_2^{(b)}(B_{1g})}{3}$$

$$\boxed{\text{z92}} \quad \mathbb{Q}_3^{(c)}(A_{2u}, a) = \mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z93}} \quad \mathbb{Q}_3^{(c)}(A_{2u}, b) = -\frac{\sqrt{35}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_{2,2}^{(b)}(E_g)}{28} - \frac{5\sqrt{21}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{2,2}^{(b)}(E_g)}{84} - \frac{\sqrt{35}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_{2,1}^{(b)}(E_g)}{28} - \frac{5\sqrt{21}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{2,1}^{(b)}(E_g)}{84} - \frac{4\sqrt{21}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_2^{(b)}(B_{1g})}{21}$$

$$\boxed{\text{z94}} \quad \mathbb{Q}_3^{(c)}(A_{2u}, c) = -\frac{\sqrt{3}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{3} - \frac{\sqrt{3}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{3} + \frac{\sqrt{3}\mathbb{G}_2^{(a)}(B_{2u})\mathbb{Q}_2^{(b)}(B_{1g})}{3}$$

$$\boxed{\text{z95}} \quad \mathbb{Q}_5^{(c)}(A_{2u}, 2) = \frac{\sqrt{5}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_{2,2}^{(b)}(E_g)}{4} - \frac{\sqrt{3}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{2,2}^{(b)}(E_g)}{4} + \frac{\sqrt{5}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_{2,1}^{(b)}(E_g)}{4} - \frac{\sqrt{3}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{2,1}^{(b)}(E_g)}{4}$$

$$\boxed{\text{z131}} \quad \mathbb{Q}_2^{(c)}(B_{1g}, a) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_{1,1}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_{1,2}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z132}} \quad \mathbb{Q}_2^{(c)}(B_{1g}, b) = \mathbb{Q}_1^{(a)}(A_{2u})\mathbb{Q}_3^{(b)}(B_{2u})$$

$$\boxed{\text{z133}} \quad \mathbb{Q}_2^{(c)}(B_{1g}, c) = \frac{3\sqrt{7}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_{1,1}^{(b)}(E_u)}{14} - \frac{\sqrt{105}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{1,1}^{(b)}(E_u)}{42} - \frac{3\sqrt{7}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_{1,2}^{(b)}(E_u)}{14} + \frac{\sqrt{105}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{1,2}^{(b)}(E_u)}{42} + \frac{\sqrt{105}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_1^{(b)}(A_{2u})}{21}$$

$$\boxed{\text{z134}} \quad \mathbb{Q}_2^{(c)}(B_{1g}, d) = -\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_3^{(b)}(B_{2u})$$

$$\boxed{\text{z135}} \quad \mathbb{Q}_2^{(c)}(B_{1g}, e) = -\frac{\sqrt{6}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_{1,1}^{(b)}(E_u)}{6} + \frac{\sqrt{6}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_{1,2}^{(b)}(E_u)}{6} + \frac{\sqrt{6}\mathbb{G}_2^{(a)}(B_{2u})\mathbb{Q}_1^{(b)}(A_{2u})}{3}$$

$$\begin{aligned}
\text{z136} \quad \mathbb{Q}_4^{(c)}(B_{1g}) &= \frac{\sqrt{35}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_{1,1}^{(b)}(E_u)}{14} + \frac{\sqrt{21}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{1,1}^{(b)}(E_u)}{14} - \frac{\sqrt{35}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_{1,2}^{(b)}(E_u)}{14} - \frac{\sqrt{21}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{1,2}^{(b)}(E_u)}{14} - \frac{\sqrt{21}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_1^{(b)}(A_{2u})}{7} \\
\text{z137} \quad \mathbb{G}_3^{(c)}(B_{1g}, a) &= -\frac{\sqrt{3}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{1,1}^{(b)}(E_u)}{3} + \frac{\sqrt{3}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{1,2}^{(b)}(E_u)}{3} - \frac{\sqrt{3}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_1^{(b)}(A_{2u})}{3} \\
\text{z138} \quad \mathbb{G}_3^{(c)}(B_{1g}, b) &= \frac{\sqrt{3}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_{1,1}^{(b)}(E_u)}{3} - \frac{\sqrt{3}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_{1,2}^{(b)}(E_u)}{3} + \frac{\sqrt{3}\mathbb{G}_2^{(a)}(B_{2u})\mathbb{Q}_1^{(b)}(A_{2u})}{3} \\
\text{z139} \quad \mathbb{Q}_3^{(c)}(B_{1u}, a) &= \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} + \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2} \\
\text{z140} \quad \mathbb{Q}_3^{(c)}(B_{1u}, b) &= \mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_0^{(b)}(A_{1g}) \\
\text{z141} \quad \mathbb{Q}_3^{(c)}(B_{1u}, c) &= -\frac{\sqrt{2}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} - \frac{\sqrt{2}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2} \\
\text{z142} \quad \mathbb{Q}_3^{(c)}(B_{1u}, d) &= \mathbb{G}_2^{(a)}(A_{1u})\mathbb{Q}_2^{(b)}(B_{1g}) \\
\text{z143} \quad \mathbb{Q}_5^{(c)}(B_{1u}) &= \frac{\sqrt{2}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} + \frac{\sqrt{2}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2} \\
\text{z144} \quad \mathbb{G}_2^{(c)}(B_{1u}, a) &= \mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_0^{(b)}(A_{1g}) \\
\text{z145} \quad \mathbb{G}_2^{(c)}(B_{1u}, b) &= -\frac{\sqrt{2}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} - \frac{\sqrt{2}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2} \\
\text{z146} \quad \mathbb{Q}_2^{(c)}(B_{2g}, a) &= \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_{1,2}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_{1,1}^{(b)}(E_u)}{2} \\
\text{z147} \quad \mathbb{Q}_2^{(c)}(B_{2g}, b) &= -\frac{\sqrt{7}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_{1,2}^{(b)}(E_u)}{7} + \frac{\sqrt{105}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{1,2}^{(b)}(E_u)}{21} - \frac{\sqrt{7}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_{1,1}^{(b)}(E_u)}{7} + \frac{\sqrt{105}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{1,1}^{(b)}(E_u)}{21} + \frac{\sqrt{105}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_1^{(b)}(A_{2u})}{21} \\
\text{z148} \quad \mathbb{Q}_2^{(c)}(B_{2g}, c) &= -\frac{\sqrt{6}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_{1,2}^{(b)}(E_u)}{6} - \frac{\sqrt{6}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_{1,1}^{(b)}(E_u)}{6} - \frac{\sqrt{6}\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_1^{(b)}(A_{2u})}{3} \\
\text{z149} \quad \mathbb{Q}_2^{(c)}(B_{2g}, d) &= \mathbb{G}_2^{(a)}(A_{1u})\mathbb{Q}_3^{(b)}(B_{2u}) \\
\text{z150} \quad \mathbb{Q}_4^{(c)}(B_{2g}) &= -\frac{\sqrt{35}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_{1,2}^{(b)}(E_u)}{28} - \frac{3\sqrt{21}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{1,2}^{(b)}(E_u)}{28} - \frac{\sqrt{35}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_{1,1}^{(b)}(E_u)}{28} - \frac{3\sqrt{21}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{1,1}^{(b)}(E_u)}{28} + \frac{\sqrt{21}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_1^{(b)}(A_{2u})}{7}
\end{aligned}$$

$$\boxed{\text{z151}} \quad \mathbb{G}_3^{(c)}(B_{2g}, a) = \frac{\sqrt{5}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_{1,2}^{(b)}(E_u)}{4} + \frac{\sqrt{3}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{1,2}^{(b)}(E_u)}{12} + \frac{\sqrt{5}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_{1,1}^{(b)}(E_u)}{4} + \frac{\sqrt{3}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{1,1}^{(b)}(E_u)}{12} + \frac{\sqrt{3}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_1^{(b)}(A_{2u})}{3}$$

$$\boxed{\text{z152}} \quad \mathbb{G}_3^{(c)}(B_{2g}, b) = -\frac{\sqrt{3}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_{1,2}^{(b)}(E_u)}{3} - \frac{\sqrt{3}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_{1,1}^{(b)}(E_u)}{3} + \frac{\sqrt{3}\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_1^{(b)}(A_{2u})}{3}$$

$$\boxed{\text{z153}} \quad \mathbb{Q}_3^{(c)}(B_{2u}, a) = \frac{\sqrt{3}\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{3} - \frac{\sqrt{3}\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{3} + \frac{\sqrt{3}\mathbb{Q}_1^{(a)}(A_{2u})\mathbb{Q}_2^{(b)}(B_{1g})}{3}$$

$$\boxed{\text{z154}} \quad \mathbb{Q}_3^{(c)}(B_{2u}, b) = \mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z155}} \quad \mathbb{Q}_3^{(c)}(B_{2u}, c) = \frac{\sqrt{3}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_{2,2}^{(b)}(E_g)}{12} - \frac{\sqrt{5}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{2,2}^{(b)}(E_g)}{4} - \frac{\sqrt{3}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_{2,1}^{(b)}(E_g)}{12} + \frac{\sqrt{5}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{2,1}^{(b)}(E_g)}{4} - \frac{\sqrt{3}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_2^{(b)}(B_{1g})}{3}$$

$$\boxed{\text{z156}} \quad \mathbb{Q}_5^{(c)}(B_{2u}) = -\frac{\sqrt{105}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_{2,2}^{(b)}(E_g)}{21} - \frac{\sqrt{7}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{2,2}^{(b)}(E_g)}{7} + \frac{\sqrt{105}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_{2,1}^{(b)}(E_g)}{21} + \frac{\sqrt{7}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{2,1}^{(b)}(E_g)}{7} + \frac{\sqrt{105}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_2^{(b)}(B_{1g})}{21}$$

$$\boxed{\text{z157}} \quad \mathbb{G}_2^{(c)}(B_{2u}, a) = -\frac{\sqrt{6}\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{6} + \frac{\sqrt{6}\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{6} + \frac{\sqrt{6}\mathbb{Q}_1^{(a)}(A_{2u})\mathbb{Q}_2^{(b)}(B_{1g})}{3}$$

$$\boxed{\text{z158}} \quad \mathbb{G}_2^{(c)}(B_{2u}, b) = -\frac{3\sqrt{21}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_{2,2}^{(b)}(E_g)}{28} + \frac{\sqrt{35}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{2,2}^{(b)}(E_g)}{28} + \frac{3\sqrt{21}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_{2,1}^{(b)}(E_g)}{28} - \frac{\sqrt{35}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{2,1}^{(b)}(E_g)}{28} - \frac{\sqrt{21}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_2^{(b)}(B_{1g})}{7}$$

$$\boxed{\text{z159}} \quad \mathbb{G}_2^{(c)}(B_{2u}, c) = \mathbb{G}_2^{(a)}(B_{2u})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z160}} \quad \mathbb{G}_2^{(c)}(B_{2u}, d) = \frac{\sqrt{2}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2} - \frac{\sqrt{2}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z197}} \quad \mathbb{Q}_{2,1}^{(c)}(E_g, a) = \frac{\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_1^{(b)}(A_{2u})}{2} + \frac{\mathbb{Q}_1^{(a)}(A_{2u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z198}} \quad \mathbb{Q}_{2,2}^{(c)}(E_g, a) = \frac{\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_1^{(b)}(A_{2u})}{2} + \frac{\mathbb{Q}_1^{(a)}(A_{2u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z199}} \quad \mathbb{Q}_{2,1}^{(c)}(E_g, b) = -\frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_3^{(b)}(B_{2u})}{2}$$

$$\boxed{\text{z200}} \quad \mathbb{Q}_{2,2}^{(c)}(E_g, b) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_3^{(b)}(B_{2u})}{2}$$

$$\begin{aligned}
\text{z201} \quad \mathbb{Q}_{2,1}^{(c)}(E_g, c) &= -\frac{\sqrt{14}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_1^{(b)}(A_{2u})}{14} - \frac{\sqrt{210}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_1^{(b)}(A_{2u})}{42} - \frac{\sqrt{14}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{14} + \frac{\sqrt{210}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{42} - \frac{\sqrt{210}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{42} \\
\text{z202} \quad \mathbb{Q}_{2,2}^{(c)}(E_g, c) &= -\frac{\sqrt{14}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_1^{(b)}(A_{2u})}{14} - \frac{\sqrt{210}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_1^{(b)}(A_{2u})}{42} - \frac{\sqrt{14}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{14} + \frac{\sqrt{210}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{42} + \frac{\sqrt{210}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{42} \\
\text{z203} \quad \mathbb{Q}_{2,1}^{(c)}(E_g, d) &= -\frac{\sqrt{2}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_3^{(b)}(B_{2u})}{8} + \frac{\sqrt{30}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_3^{(b)}(B_{2u})}{8} \\
\text{z226} \quad \mathbb{Q}_{2,2}^{(c)}(E_g, d) &= \frac{\sqrt{2}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_3^{(b)}(B_{2u})}{8} - \frac{\sqrt{30}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_3^{(b)}(B_{2u})}{8} \\
\text{z227} \quad \mathbb{Q}_{2,1}^{(c)}(E_g, e) &= \frac{\sqrt{3}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_1^{(b)}(A_{2u})}{6} + \frac{\mathbb{G}_2^{(a)}(A_{1u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{2} + \frac{\sqrt{3}\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{6} + \frac{\sqrt{3}\mathbb{G}_2^{(a)}(B_{2u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{6} \\
\text{z228} \quad \mathbb{Q}_{2,2}^{(c)}(E_g, e) &= \frac{\sqrt{3}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_1^{(b)}(A_{2u})}{6} - \frac{\mathbb{G}_2^{(a)}(A_{1u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{2} + \frac{\sqrt{3}\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{6} - \frac{\sqrt{3}\mathbb{G}_2^{(a)}(B_{2u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{6} \\
\text{z229} \quad \mathbb{Q}_{4,1}^{(c)}(E_g, 1a) &= \frac{\sqrt{10}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_1^{(b)}(A_{2u})}{8} + \frac{\sqrt{6}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_1^{(b)}(A_{2u})}{8} - \frac{\sqrt{10}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{8} - \frac{\sqrt{6}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{8} \\
\text{z230} \quad \mathbb{Q}_{4,2}^{(c)}(E_g, 1a) &= \frac{\sqrt{10}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_1^{(b)}(A_{2u})}{8} + \frac{\sqrt{6}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_1^{(b)}(A_{2u})}{8} - \frac{\sqrt{10}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{8} + \frac{\sqrt{6}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{8} \\
\text{z231} \quad \mathbb{Q}_{4,1}^{(c)}(E_g, 1b) &= -\frac{\sqrt{30}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_3^{(b)}(B_{2u})}{8} - \frac{\sqrt{2}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_3^{(b)}(B_{2u})}{8} \\
\text{z232} \quad \mathbb{Q}_{4,2}^{(c)}(E_g, 1b) &= \frac{\sqrt{30}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_3^{(b)}(B_{2u})}{8} + \frac{\sqrt{2}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_3^{(b)}(B_{2u})}{8} \\
\text{z233} \quad \mathbb{Q}_{4,1}^{(c)}(E_g, 1c) &= -\frac{\sqrt{2}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_3^{(b)}(B_{2u})}{2} \\
\text{z250} \quad \mathbb{Q}_{4,2}^{(c)}(E_g, 1c) &= \frac{\sqrt{2}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_3^{(b)}(B_{2u})}{2} \\
\text{z251} \quad \mathbb{Q}_{4,1}^{(c)}(E_g, 2) &= -\frac{\sqrt{70}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_1^{(b)}(A_{2u})}{56} + \frac{3\sqrt{42}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_1^{(b)}(A_{2u})}{56} - \frac{\sqrt{70}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{56} + \frac{\sqrt{42}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{14} + \frac{3\sqrt{42}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{56} \\
\text{z252} \quad \mathbb{Q}_{4,2}^{(c)}(E_g, 2) &= -\frac{\sqrt{70}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_1^{(b)}(A_{2u})}{56} + \frac{3\sqrt{42}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_1^{(b)}(A_{2u})}{56} - \frac{\sqrt{70}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{56} + \frac{\sqrt{42}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{14} - \frac{3\sqrt{42}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{56}
\end{aligned}$$

$$\begin{aligned}
\boxed{\text{z253}} \quad \mathbb{G}_{1,1}^{(c)}(E_g, a) &= \frac{\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_1^{(b)}(A_{2u})}{2} - \frac{\mathbb{Q}_1^{(a)}(A_{2u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{2} \\
\boxed{\text{z254}} \quad \mathbb{G}_{1,2}^{(c)}(E_g, a) &= \frac{\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_1^{(b)}(A_{2u})}{2} - \frac{\mathbb{Q}_1^{(a)}(A_{2u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{2} \\
\boxed{\text{z255}} \quad \mathbb{G}_{1,1}^{(c)}(E_g, b) &= -\frac{\sqrt{15}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_1^{(b)}(A_{2u})}{10} - \frac{\sqrt{5}\mathbb{G}_2^{(a)}(A_{1u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{10} + \frac{\sqrt{15}\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{10} + \frac{\sqrt{15}\mathbb{G}_2^{(a)}(B_{2u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{10} \\
\boxed{\text{z256}} \quad \mathbb{G}_{1,2}^{(c)}(E_g, b) &= -\frac{\sqrt{15}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_1^{(b)}(A_{2u})}{10} + \frac{\sqrt{5}\mathbb{G}_2^{(a)}(A_{1u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{10} + \frac{\sqrt{15}\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{10} - \frac{\sqrt{15}\mathbb{G}_2^{(a)}(B_{2u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{10} \\
\boxed{\text{z277}} \quad \mathbb{G}_{3,1}^{(c)}(E_g, 1a) &= -\frac{\sqrt{6}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_1^{(b)}(A_{2u})}{8} + \frac{\sqrt{10}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_1^{(b)}(A_{2u})}{8} + \frac{\sqrt{6}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{8} - \frac{\sqrt{10}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{8} \\
\boxed{\text{z278}} \quad \mathbb{G}_{3,2}^{(c)}(E_g, 1a) &= -\frac{\sqrt{6}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_1^{(b)}(A_{2u})}{8} + \frac{\sqrt{10}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_1^{(b)}(A_{2u})}{8} + \frac{\sqrt{6}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{8} + \frac{\sqrt{10}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{8} \\
\boxed{\text{z279}} \quad \mathbb{G}_{3,1}^{(c)}(E_g, 1b) &= \frac{\sqrt{10}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_1^{(b)}(A_{2u})}{10} - \frac{\sqrt{30}\mathbb{G}_2^{(a)}(A_{1u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{20} + \frac{3\sqrt{10}\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{20} - \frac{\sqrt{10}\mathbb{G}_2^{(a)}(B_{2u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{10} \\
\boxed{\text{z280}} \quad \mathbb{G}_{3,2}^{(c)}(E_g, 1b) &= \frac{\sqrt{10}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_1^{(b)}(A_{2u})}{10} + \frac{\sqrt{30}\mathbb{G}_2^{(a)}(A_{1u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{20} + \frac{3\sqrt{10}\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{20} + \frac{\sqrt{10}\mathbb{G}_2^{(a)}(B_{2u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{10} \\
\boxed{\text{z281}} \quad \mathbb{G}_{3,1}^{(c)}(E_g, 2a) &= \frac{\sqrt{10}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_1^{(b)}(A_{2u})}{8} - \frac{\sqrt{6}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_1^{(b)}(A_{2u})}{24} + \frac{\sqrt{10}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{8} + \frac{\sqrt{6}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{6} - \frac{\sqrt{6}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{24} \\
\boxed{\text{z282}} \quad \mathbb{G}_{3,2}^{(c)}(E_g, 2a) &= \frac{\sqrt{10}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_1^{(b)}(A_{2u})}{8} - \frac{\sqrt{6}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_1^{(b)}(A_{2u})}{24} + \frac{\sqrt{10}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{8} + \frac{\sqrt{6}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{6} + \frac{\sqrt{6}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{24} \\
\boxed{\text{z283}} \quad \mathbb{G}_{3,1}^{(c)}(E_g, 2b) &= \frac{\sqrt{6}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_1^{(b)}(A_{2u})}{6} - \frac{\sqrt{2}\mathbb{G}_2^{(a)}(A_{1u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{4} - \frac{\sqrt{6}\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{12} + \frac{\sqrt{6}\mathbb{G}_2^{(a)}(B_{2u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{6} \\
\boxed{\text{z284}} \quad \mathbb{G}_{3,2}^{(c)}(E_g, 2b) &= \frac{\sqrt{6}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_1^{(b)}(A_{2u})}{6} + \frac{\sqrt{2}\mathbb{G}_2^{(a)}(A_{1u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{4} - \frac{\sqrt{6}\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{12} - \frac{\sqrt{6}\mathbb{G}_2^{(a)}(B_{2u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{6} \\
\boxed{\text{z321}} \quad \mathbb{Q}_{1,1}^{(c)}(E_u, a) &= \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_0^{(b)}(A_{1g})}{2} \\
\boxed{\text{z322}} \quad \mathbb{Q}_{1,2}^{(c)}(E_u, a) &= \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_0^{(b)}(A_{1g})}{2}
\end{aligned}$$

$$\boxed{\text{z323}} \quad \mathbb{Q}_{1,1}^{(c)}(E_u, b) = \frac{\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_2^{(b)}(B_{1g})}{2} + \frac{\mathbb{Q}_1^{(a)}(A_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z324}} \quad \mathbb{Q}_{1,2}^{(c)}(E_u, b) = -\frac{\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_2^{(b)}(B_{1g})}{2} + \frac{\mathbb{Q}_1^{(a)}(A_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z325}} \quad \mathbb{Q}_{1,1}^{(c)}(E_u, c) = \frac{3\sqrt{14}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_2^{(b)}(B_{1g})}{28} - \frac{\sqrt{210}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_2^{(b)}(B_{1g})}{84} - \frac{\sqrt{14}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{14} + \frac{\sqrt{210}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{42} + \frac{\sqrt{210}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{42}$$

$$\boxed{\text{z326}} \quad \mathbb{Q}_{1,2}^{(c)}(E_u, c) = -\frac{3\sqrt{14}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_2^{(b)}(B_{1g})}{28} + \frac{\sqrt{210}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_2^{(b)}(B_{1g})}{84} - \frac{\sqrt{14}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{14} + \frac{\sqrt{210}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{42} - \frac{\sqrt{210}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{42}$$

$$\boxed{\text{z327}} \quad \mathbb{Q}_{1,1}^{(c)}(E_u, d) = \frac{\sqrt{3}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_2^{(b)}(B_{1g})}{6} - \frac{\mathbb{G}_2^{(a)}(A_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} - \frac{\sqrt{3}\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{6} + \frac{\sqrt{3}\mathbb{G}_2^{(a)}(B_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{6}$$

$$\boxed{\text{z328}} \quad \mathbb{Q}_{1,2}^{(c)}(E_u, d) = -\frac{\sqrt{3}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_2^{(b)}(B_{1g})}{6} + \frac{\mathbb{G}_2^{(a)}(A_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2} - \frac{\sqrt{3}\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{6} - \frac{\sqrt{3}\mathbb{G}_2^{(a)}(B_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{6}$$

$$\boxed{\text{z329}} \quad \mathbb{Q}_{3,1}^{(c)}(E_u, 1a) = \frac{\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_2^{(b)}(B_{1g})}{2} - \frac{\mathbb{Q}_1^{(a)}(A_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z330}} \quad \mathbb{Q}_{3,2}^{(c)}(E_u, 1a) = -\frac{\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_2^{(b)}(B_{1g})}{2} - \frac{\mathbb{Q}_1^{(a)}(A_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z331}} \quad \mathbb{Q}_{3,1}^{(c)}(E_u, 1b) = \frac{\sqrt{2}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z332}} \quad \mathbb{Q}_{3,2}^{(c)}(E_u, 1b) = \frac{\sqrt{2}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z333}} \quad \mathbb{Q}_{3,1}^{(c)}(E_u, 1c) = \frac{33\sqrt{1834}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_2^{(b)}(B_{1g})}{3668} + \frac{17\sqrt{27510}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_2^{(b)}(B_{1g})}{11004} - \frac{2\sqrt{1834}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{917} - \frac{17\sqrt{27510}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{5502} + \frac{2\sqrt{27510}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2751}$$

$$\boxed{\text{z334}} \quad \mathbb{Q}_{3,2}^{(c)}(E_u, 1c) = -\frac{33\sqrt{1834}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_2^{(b)}(B_{1g})}{3668} - \frac{17\sqrt{27510}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_2^{(b)}(B_{1g})}{11004} - \frac{2\sqrt{1834}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{917} - \frac{17\sqrt{27510}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{5502} - \frac{2\sqrt{27510}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2751}$$

$$\boxed{\text{z335}} \quad \mathbb{Q}_{3,1}^{(c)}(E_u, 1d) = -\frac{\sqrt{15}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_2^{(b)}(B_{1g})}{30} + \frac{\sqrt{5}\mathbb{G}_2^{(a)}(A_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{10} + \frac{\sqrt{15}\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{30} + \frac{\sqrt{15}\mathbb{G}_2^{(a)}(B_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{6}$$

$$\boxed{\text{z336}} \quad \mathbb{Q}_{3,2}^{(c)}(E_u, 1d) = \frac{\sqrt{15}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_2^{(b)}(B_{1g})}{30} - \frac{\sqrt{5}\mathbb{G}_2^{(a)}(A_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{10} + \frac{\sqrt{15}\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{30} - \frac{\sqrt{15}\mathbb{G}_2^{(a)}(B_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{6}$$

$$\begin{aligned}
\boxed{\text{z337}} \quad \mathbb{Q}_{3,1}^{(c)}(E_u, 2a) &= \frac{\sqrt{2}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_0^{(b)}(A_{1g})}{2} \\
\boxed{\text{z338}} \quad \mathbb{Q}_{3,2}^{(c)}(E_u, 2a) &= \frac{\sqrt{2}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_0^{(b)}(A_{1g})}{2} \\
\boxed{\text{z339}} \quad \mathbb{Q}_{3,1}^{(c)}(E_u, 2b) &= \frac{25\sqrt{655}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_2^{(b)}(B_{1g})}{2096} - \frac{5\sqrt{393}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_2^{(b)}(B_{1g})}{2096} - \frac{7\sqrt{655}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{1048} + \frac{5\sqrt{393}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{1048} - \frac{4\sqrt{393}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{131} \\
\boxed{\text{z340}} \quad \mathbb{Q}_{3,2}^{(c)}(E_u, 2b) &= -\frac{25\sqrt{655}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_2^{(b)}(B_{1g})}{2096} + \frac{5\sqrt{393}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_2^{(b)}(B_{1g})}{2096} - \frac{7\sqrt{655}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{1048} + \frac{5\sqrt{393}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{1048} + \frac{4\sqrt{393}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{131} \\
\boxed{\text{z341}} \quad \mathbb{Q}_{3,1}^{(c)}(E_u, 2c) &= \frac{\sqrt{15}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_2^{(b)}(B_{1g})}{10} + \frac{\sqrt{5}\mathbb{G}_2^{(a)}(A_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{5} - \frac{\sqrt{15}\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{10} \\
\boxed{\text{z342}} \quad \mathbb{Q}_{3,2}^{(c)}(E_u, 2c) &= -\frac{\sqrt{15}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_2^{(b)}(B_{1g})}{10} - \frac{\sqrt{5}\mathbb{G}_2^{(a)}(A_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{5} - \frac{\sqrt{15}\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{10} \\
\boxed{\text{z343}} \quad \mathbb{Q}_{5,1}^{(c)}(E_u, 1) &= \frac{5\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_2^{(b)}(B_{1g})}{16} - \frac{\sqrt{15}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_2^{(b)}(B_{1g})}{80} + \frac{5\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{8} + \frac{\sqrt{15}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{40} \\
\boxed{\text{z344}} \quad \mathbb{Q}_{5,2}^{(c)}(E_u, 1) &= -\frac{5\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_2^{(b)}(B_{1g})}{16} + \frac{\sqrt{15}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_2^{(b)}(B_{1g})}{80} + \frac{5\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{8} + \frac{\sqrt{15}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{40} \\
\boxed{\text{z345}} \quad \mathbb{Q}_{5,1}^{(c)}(E_u, 2) &= -\frac{\sqrt{10}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_2^{(b)}(B_{1g})}{5} - \frac{\sqrt{10}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{10} \\
\boxed{\text{z346}} \quad \mathbb{Q}_{5,2}^{(c)}(E_u, 2) &= \frac{\sqrt{10}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_2^{(b)}(B_{1g})}{5} - \frac{\sqrt{10}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{10} \\
\boxed{\text{z347}} \quad \mathbb{G}_{2,1}^{(c)}(E_u, a) &= \frac{\sqrt{2}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_0^{(b)}(A_{1g})}{2} \\
\boxed{\text{z348}} \quad \mathbb{G}_{2,2}^{(c)}(E_u, a) &= \frac{\sqrt{2}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_0^{(b)}(A_{1g})}{2} \\
\boxed{\text{z349}} \quad \mathbb{G}_{2,1}^{(c)}(E_u, b) &= -\frac{\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_2^{(b)}(B_{1g})}{2} - \frac{\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} \\
\boxed{\text{z350}} \quad \mathbb{G}_{2,2}^{(c)}(E_u, b) &= \frac{\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_2^{(b)}(B_{1g})}{2} - \frac{\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}
\end{aligned}$$

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

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

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

$$\boxed{\text{x3}} \quad \mathbb{Q}_4^{(a)}(A_{1g}, 1) = \begin{bmatrix} \frac{\sqrt{30}}{10} & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{30}}{10} & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{30}}{15} & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{30}}{15} & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{30}}{15} \end{bmatrix}$$

$$\boxed{\text{x4}} \quad \mathbb{Q}_4^{(a)}(A_{1g}, 2) = \begin{bmatrix} \frac{\sqrt{42}}{14} & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{42}}{14} & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{42}}{21} & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{42}}{21} & 0 \\ 0 & 0 & 0 & 0 & \frac{2\sqrt{42}}{21} \end{bmatrix}$$

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

$$\boxed{\text{x6}} \quad \mathbb{Q}_2^{(a)}(B_{1g}) = \begin{bmatrix} 0 & -\frac{\sqrt{14}}{7} & 0 & 0 & 0 \\ -\frac{\sqrt{14}}{7} & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{42}}{14} & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{42}}{14} & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x7}} \quad \mathbb{Q}_4^{(a)}(B_{1g}) = \begin{bmatrix} 0 & -\frac{\sqrt{42}}{14} & 0 & 0 & 0 \\ -\frac{\sqrt{42}}{14} & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{14}}{7} & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{14}}{7} & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x8}} \quad \mathbb{Q}_2^{(a)}(B_{2g}) = \begin{bmatrix} 0 & 0 & 0 & 0 & -\frac{\sqrt{14}}{7} \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{42}}{14} & 0 \\ 0 & 0 & \frac{\sqrt{42}}{14} & 0 & 0 \\ -\frac{\sqrt{14}}{7} & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x9}} \quad \mathbb{Q}_4^{(a)}(B_{2g}) = \begin{bmatrix} 0 & 0 & 0 & 0 & \frac{\sqrt{42}}{14} \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{14}}{7} & 0 \\ 0 & 0 & \frac{\sqrt{14}}{7} & 0 & 0 \\ \frac{\sqrt{42}}{14} & 0 & 0 & 0 & 0 \end{bmatrix}$$

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

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

$$\boxed{\text{x12}} \quad \mathbb{Q}_{4,1}^{(a)}(E_g, 1) = \begin{bmatrix} 0 & 0 & -\frac{\sqrt{6}}{4} & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{2}}{4} & 0 & 0 \\ -\frac{\sqrt{6}}{4} & -\frac{\sqrt{2}}{4} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x13}} \quad \mathbb{Q}_{4,2}^{(a)}(E_g, 1) = \begin{bmatrix} 0 & 0 & 0 & -\frac{\sqrt{6}}{4} & 0 \\ 0 & 0 & 0 & \frac{\sqrt{2}}{4} & 0 \\ 0 & 0 & 0 & 0 & 0 \\ -\frac{\sqrt{6}}{4} & \frac{\sqrt{2}}{4} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x14}} \quad \mathbb{Q}_{4,1}^{(a)}(E_g, 2) = \begin{bmatrix} 0 & 0 & -\frac{\sqrt{42}}{28} & 0 & 0 \\ 0 & 0 & \frac{3\sqrt{14}}{28} & 0 & 0 \\ -\frac{\sqrt{42}}{28} & \frac{3\sqrt{14}}{28} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{14}}{7} \\ 0 & 0 & 0 & \frac{\sqrt{14}}{7} & 0 \end{bmatrix}$$

$$\boxed{\text{x15}} \quad \mathbb{Q}_{4,2}^{(a)}(E_g, 2) = \begin{bmatrix} 0 & 0 & 0 & -\frac{\sqrt{42}}{28} & 0 \\ 0 & 0 & 0 & -\frac{3\sqrt{14}}{28} & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{14}}{7} \\ -\frac{\sqrt{42}}{28} & -\frac{3\sqrt{14}}{28} & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{14}}{7} & 0 & 0 \end{bmatrix}$$

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

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

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

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

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

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

$$\boxed{\text{x22}} \quad \mathbb{M}_{3,1}^{(a)}(E_g, 1) = \begin{bmatrix} 0 & 0 & -\frac{\sqrt{30}i}{20} & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{10}i}{20} & 0 & 0 \\ \frac{\sqrt{30}i}{20} & \frac{\sqrt{10}i}{20} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{10}i}{5} \\ 0 & 0 & 0 & -\frac{\sqrt{10}i}{5} & 0 \end{bmatrix}$$

$$\boxed{\text{x23}} \quad \mathbb{M}_{3,2}^{(a)}(E_g, 1) = \begin{bmatrix} 0 & 0 & 0 & -\frac{\sqrt{30}i}{20} & 0 \\ 0 & 0 & 0 & \frac{\sqrt{10}i}{20} & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{10}i}{5} \\ \frac{\sqrt{30}i}{20} & -\frac{\sqrt{10}i}{20} & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{10}i}{5} & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x24}} \quad \mathbb{M}_{3,1}^{(a)}(E_g, 2) = \begin{bmatrix} 0 & 0 & -\frac{\sqrt{2}i}{4} & 0 & 0 \\ 0 & 0 & \frac{\sqrt{6}i}{4} & 0 & 0 \\ \frac{\sqrt{2}i}{4} & -\frac{\sqrt{6}i}{4} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x25}} \quad \mathbb{M}_{3,2}^{(a)}(E_g, 2) = \begin{bmatrix} 0 & 0 & 0 & -\frac{\sqrt{2}i}{4} & 0 \\ 0 & 0 & 0 & \frac{\sqrt{6}i}{4} & 0 \\ 0 & 0 & 0 & 0 & 0 \\ \frac{\sqrt{2}i}{4} & \frac{\sqrt{6}i}{4} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

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

$$\boxed{\text{x26}} \quad \mathbb{Q}_0^{(a)}(A_{1g}) = \begin{bmatrix} \frac{\sqrt{3}}{3} & 0 & 0 \\ 0 & \frac{\sqrt{3}}{3} & 0 \\ 0 & 0 & \frac{\sqrt{3}}{3} \end{bmatrix}$$

$$\boxed{\text{x27}} \quad \mathbb{Q}_2^{(a)}(A_{1g}) = \begin{bmatrix} -\frac{\sqrt{6}}{6} & 0 & 0 \\ 0 & -\frac{\sqrt{6}}{6} & 0 \\ 0 & 0 & \frac{\sqrt{6}}{3} \end{bmatrix}$$

$$\boxed{\text{x28}} \quad \mathbb{Q}_2^{(a)}(B_{1g}) = \begin{bmatrix} \frac{\sqrt{2}}{2} & 0 & 0 \\ 0 & -\frac{\sqrt{2}}{2} & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x29}} \quad \mathbb{Q}_2^{(a)}(B_{2g}) = \begin{bmatrix} 0 & \frac{\sqrt{2}}{2} & 0 \\ \frac{\sqrt{2}}{2} & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x30}} \quad \mathbb{Q}_{2,1}^{(a)}(E_g) = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{2}}{2} \\ 0 & \frac{\sqrt{2}}{2} & 0 \end{bmatrix}$$

$$\boxed{\text{x31}} \quad \mathbb{Q}_{2,2}^{(a)}(E_g) = \begin{bmatrix} 0 & 0 & \frac{\sqrt{2}}{2} \\ 0 & 0 & 0 \\ \frac{\sqrt{2}}{2} & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x32}} \quad \mathbb{M}_1^{(a)}(A_{2g}) = \begin{bmatrix} 0 & -\frac{\sqrt{2}i}{2} & 0 \\ \frac{\sqrt{2}i}{2} & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x33}} \quad \mathbb{M}_{1,1}^{(a)}(E_g) = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{2}i}{2} \\ 0 & \frac{\sqrt{2}i}{2} & 0 \end{bmatrix}$$

$$\boxed{\text{x34}} \quad \mathbb{M}_{1,2}^{(a)}(E_g) = \begin{bmatrix} 0 & 0 & -\frac{\sqrt{2}i}{2} \\ 0 & 0 & 0 \\ \frac{\sqrt{2}i}{2} & 0 & 0 \end{bmatrix}$$

- bra: $\langle f_3|, \langle f_{ax}|, \langle f_{ay}|, \langle f_{az}|, \langle f_{bx}|, \langle f_{by}|, \langle f_{bz}|$
- ket: $|f_3\rangle, |f_{ax}\rangle, |f_{ay}\rangle, |f_{az}\rangle, |f_{bx}\rangle, |f_{by}\rangle, |f_{bz}\rangle$

$$\boxed{\text{x35}} \quad \mathbb{Q}_0^{(a)}(A_{1g}) = \begin{bmatrix} \frac{\sqrt{7}}{7} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{7}}{7} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{7}}{7} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{7}}{7} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{7}}{7} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{7}}{7} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{7}}{7} \end{bmatrix}$$

$$\boxed{\text{x36}} \quad \mathbb{Q}_2^{(a)}(A_{1g}) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{21}}{21} & 0 & 0 & \frac{\sqrt{35}}{14} & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{21}}{21} & 0 & 0 & -\frac{\sqrt{35}}{14} & 0 \\ 0 & 0 & 0 & \frac{2\sqrt{21}}{21} & 0 & 0 & 0 \\ 0 & \frac{\sqrt{35}}{14} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{35}}{14} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x37}} \quad \mathbb{Q}_4^{(a)}(A_{1g}, 1) = \begin{bmatrix} -\frac{\sqrt{66}}{11} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{66}}{22} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{66}}{22} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{66}}{22} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{66}}{66} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{66}}{66} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{66}}{66} \end{bmatrix}$$

$$\boxed{\text{x38}} \quad \mathbb{Q}_4^{(a)}(A_{1g}, 2) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{2310}}{308} & 0 & 0 & -\frac{3\sqrt{154}}{308} & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{2310}}{308} & 0 & 0 & \frac{3\sqrt{154}}{308} & 0 \\ 0 & 0 & 0 & \frac{\sqrt{2310}}{154} & 0 & 0 & 0 \\ 0 & -\frac{3\sqrt{154}}{308} & 0 & 0 & \frac{\sqrt{2310}}{132} & 0 & 0 \\ 0 & 0 & \frac{3\sqrt{154}}{308} & 0 & 0 & \frac{\sqrt{2310}}{132} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{2310}}{66} \end{bmatrix}$$

$$\boxed{\text{x39}} \quad \mathbb{Q}_6^{(a)}(A_{1g}, 1) = \begin{bmatrix} \frac{2\sqrt{462}}{77} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{5\sqrt{462}}{462} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{5\sqrt{462}}{462} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{5\sqrt{462}}{462} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{3\sqrt{462}}{154} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{3\sqrt{462}}{154} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\frac{3\sqrt{462}}{154} \end{bmatrix}$$

$$\boxed{\text{x40}} \quad \mathbb{Q}_6^{(a)}(A_{1g}, 2) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{5\sqrt{66}}{132} & 0 & 0 & -\frac{\sqrt{110}}{44} & 0 & 0 \\ 0 & 0 & -\frac{5\sqrt{66}}{132} & 0 & 0 & \frac{\sqrt{110}}{44} & 0 \\ 0 & 0 & 0 & \frac{5\sqrt{66}}{66} & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{110}}{44} & 0 & 0 & -\frac{\sqrt{66}}{44} & 0 & 0 \\ 0 & 0 & \frac{\sqrt{110}}{44} & 0 & 0 & -\frac{\sqrt{66}}{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{66}}{22} \end{bmatrix}$$

$$\boxed{\text{x41}} \quad \mathbb{Q}_4^{(a)}(A_{2g}) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{110}}{22} \\ 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{66}}{22} & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{66}}{22} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{66}}{22} & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{66}}{22} & 0 & 0 & 0 & 0 & 0 \\ \frac{\sqrt{110}}{22} & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x42}} \quad \mathbb{Q}_6^{(a)}(A_{2g}) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{33}}{11} \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{55}}{22} & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{55}}{22} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{55}}{22} & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{55}}{22} & 0 & 0 & 0 & 0 & 0 \\ \frac{\sqrt{33}}{11} & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x43}} \quad \mathbb{Q}_2^{(a)}(B_{1g}) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{7}}{7} & 0 & 0 & \frac{\sqrt{105}}{42} & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{7}}{7} & 0 & 0 & \frac{\sqrt{105}}{42} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{105}}{21} \\ 0 & \frac{\sqrt{105}}{42} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{105}}{42} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{105}}{21} & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x44}} \quad \mathbb{Q}_4^{(a)}(B_{1g}) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{3\sqrt{770}}{308} & 0 & 0 & -\frac{\sqrt{462}}{308} & 0 & 0 \\ 0 & 0 & -\frac{3\sqrt{770}}{308} & 0 & 0 & -\frac{\sqrt{462}}{308} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{462}}{154} \\ 0 & -\frac{\sqrt{462}}{308} & 0 & 0 & -\frac{\sqrt{770}}{44} & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{462}}{308} & 0 & 0 & \frac{\sqrt{770}}{44} & 0 \\ 0 & 0 & 0 & \frac{\sqrt{462}}{154} & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x45}} \quad \mathbb{Q}_6^{(a)}(B_{1g}, 1) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{6}}{6} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{6}}{6} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{6}}{6} \\ 0 & -\frac{\sqrt{6}}{6} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{6}}{6} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{6}}{6} & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x46}} \quad \mathbb{Q}_6^{(a)}(B_{1g}, 2) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{5\sqrt{22}}{44} & 0 & 0 & -\frac{\sqrt{330}}{132} & 0 & 0 \\ 0 & 0 & -\frac{5\sqrt{22}}{44} & 0 & 0 & -\frac{\sqrt{330}}{132} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{330}}{66} \\ 0 & -\frac{\sqrt{330}}{132} & 0 & 0 & \frac{3\sqrt{22}}{44} & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{330}}{132} & 0 & 0 & -\frac{3\sqrt{22}}{44} & 0 \\ 0 & 0 & 0 & \frac{\sqrt{330}}{66} & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x47}} \quad \mathbb{Q}_2^{(a)}(B_{2g}) = \begin{bmatrix} 0 & 0 & 0 & -\frac{\sqrt{105}}{21} & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{7}}{28} & 0 & 0 & -\frac{\sqrt{105}}{84} & 0 \\ 0 & -\frac{\sqrt{7}}{28} & 0 & 0 & \frac{\sqrt{105}}{84} & 0 & 0 \\ -\frac{\sqrt{105}}{21} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{105}}{84} & 0 & 0 & -\frac{5\sqrt{7}}{28} & 0 \\ 0 & -\frac{\sqrt{105}}{84} & 0 & 0 & -\frac{5\sqrt{7}}{28} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x48}} \quad \mathbb{Q}_4^{(a)}(B_{2g}) = \begin{bmatrix} 0 & 0 & 0 & -\frac{\sqrt{462}}{154} & 0 & 0 & 0 \\ 0 & 0 & \frac{3\sqrt{770}}{154} & 0 & 0 & -\frac{\sqrt{462}}{77} & 0 \\ 0 & \frac{3\sqrt{770}}{154} & 0 & 0 & \frac{\sqrt{462}}{77} & 0 & 0 \\ -\frac{\sqrt{462}}{154} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{462}}{77} & 0 & 0 & \frac{\sqrt{770}}{154} & 0 \\ 0 & -\frac{\sqrt{462}}{77} & 0 & 0 & \frac{\sqrt{770}}{154} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x49}} \quad \mathbb{Q}_6^{(a)}(B_{2g}, 1) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{5\sqrt{2}}{16} & 0 & 0 & -\frac{\sqrt{30}}{16} & 0 \\ 0 & -\frac{5\sqrt{2}}{16} & 0 & 0 & \frac{\sqrt{30}}{16} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{30}}{16} & 0 & 0 & \frac{3\sqrt{2}}{16} & 0 \\ 0 & -\frac{\sqrt{30}}{16} & 0 & 0 & \frac{3\sqrt{2}}{16} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x50}} \quad \mathbb{Q}_6^{(a)}(B_{2g}, 2) = \begin{bmatrix} 0 & 0 & 0 & \frac{2\sqrt{66}}{33} & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{110}}{176} & 0 & 0 & -\frac{13\sqrt{66}}{528} & 0 \\ 0 & \frac{\sqrt{110}}{176} & 0 & 0 & \frac{13\sqrt{66}}{528} & 0 & 0 \\ \frac{2\sqrt{66}}{33} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{13\sqrt{66}}{528} & 0 & 0 & -\frac{7\sqrt{110}}{176} & 0 \\ 0 & -\frac{13\sqrt{66}}{528} & 0 & 0 & -\frac{7\sqrt{110}}{176} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x51}} \quad \mathbb{Q}_{2,1}^{(a)}(E_g) = \begin{bmatrix} 0 & -\frac{\sqrt{105}}{21} & 0 & 0 & 0 & 0 & 0 \\ -\frac{\sqrt{105}}{21} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{7}}{28} & 0 & 0 & -\frac{\sqrt{105}}{84} \\ 0 & 0 & -\frac{\sqrt{7}}{28} & 0 & 0 & \frac{\sqrt{105}}{84} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{105}}{84} & 0 & 0 & -\frac{5\sqrt{7}}{28} \\ 0 & 0 & -\frac{\sqrt{105}}{84} & 0 & 0 & -\frac{5\sqrt{7}}{28} & 0 \end{bmatrix}$$

$$\boxed{\text{x52}} \quad \mathbb{Q}_{2,2}^{(a)}(E_g) = \begin{bmatrix} 0 & 0 & -\frac{\sqrt{105}}{21} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{7}}{28} & 0 & 0 & \frac{\sqrt{105}}{84} \\ -\frac{\sqrt{105}}{21} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{7}}{28} & 0 & 0 & -\frac{\sqrt{105}}{84} & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{105}}{84} & 0 & 0 & -\frac{5\sqrt{7}}{28} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{105}}{84} & 0 & 0 & -\frac{5\sqrt{7}}{28} & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x53}} \quad \mathbb{Q}_{4,1}^{(a)}(E_g, 1) = \begin{bmatrix} 0 & 0 & 0 & 0 & \frac{\sqrt{110}}{22} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{66}}{22} \\ 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{66}}{22} & 0 \\ \frac{\sqrt{110}}{22} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{66}}{22} & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{66}}{22} & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x54}} \quad \mathbb{Q}_{4,2}^{(a)}(E_g, 1) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{110}}{22} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{66}}{22} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{66}}{22} & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{66}}{22} & 0 & 0 & 0 \\ -\frac{\sqrt{110}}{22} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{66}}{22} & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x55}} \quad \mathbb{Q}_{4,1}^{(a)}(E_g, 2) = \begin{bmatrix} 0 & -\frac{\sqrt{462}}{154} & 0 & 0 & 0 & 0 & 0 \\ -\frac{\sqrt{462}}{154} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{3\sqrt{770}}{154} & 0 & 0 & -\frac{\sqrt{462}}{77} \\ 0 & 0 & \frac{3\sqrt{770}}{154} & 0 & 0 & \frac{\sqrt{462}}{77} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{462}}{77} & 0 & 0 & \frac{\sqrt{770}}{154} \\ 0 & 0 & -\frac{\sqrt{462}}{77} & 0 & 0 & \frac{\sqrt{770}}{154} & 0 \end{bmatrix}$$

$$\boxed{\text{x56}} \quad \mathbb{Q}_{4,2}^{(a)}(E_g, 2) = \begin{bmatrix} 0 & 0 & -\frac{\sqrt{462}}{154} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{3\sqrt{770}}{154} & 0 & 0 & \frac{\sqrt{462}}{77} \\ -\frac{\sqrt{462}}{154} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{3\sqrt{770}}{154} & 0 & 0 & -\frac{\sqrt{462}}{77} & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{462}}{77} & 0 & 0 & \frac{\sqrt{770}}{154} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{462}}{77} & 0 & 0 & \frac{\sqrt{770}}{154} & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x57}} \quad \mathbb{Q}_{6,1}^{(a)}(E_g, 1) = \begin{bmatrix} 0 & 0 & 0 & 0 & \frac{\sqrt{33}}{11} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{55}}{22} \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{55}}{22} & 0 \\ \frac{\sqrt{33}}{11} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{55}}{22} & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{55}}{22} & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x58}} \quad \mathbb{Q}_{6,2}^{(a)}(E_g, 1) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{33}}{11} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{55}}{22} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{55}}{22} & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{55}}{22} & 0 & 0 & 0 \\ -\frac{\sqrt{33}}{11} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{55}}{22} & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x59}} \quad \mathbb{Q}_{6,1}^{(a)}(E_g, 2) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{5\sqrt{2}}{16} & 0 & 0 & -\frac{\sqrt{30}}{16} \\ 0 & 0 & -\frac{5\sqrt{2}}{16} & 0 & 0 & \frac{\sqrt{30}}{16} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{30}}{16} & 0 & 0 & \frac{3\sqrt{2}}{16} \\ 0 & 0 & -\frac{\sqrt{30}}{16} & 0 & 0 & \frac{3\sqrt{2}}{16} & 0 \end{bmatrix}$$

$$\boxed{\text{x60}} \quad \mathbb{Q}_{6,2}^{(a)}(E_g, 2) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{5\sqrt{2}}{16} & 0 & 0 & \frac{\sqrt{30}}{16} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{5\sqrt{2}}{16} & 0 & 0 & -\frac{\sqrt{30}}{16} & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{30}}{16} & 0 & 0 & \frac{3\sqrt{2}}{16} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{30}}{16} & 0 & 0 & \frac{3\sqrt{2}}{16} & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x61}} \quad \mathbb{Q}_{6,1}^{(a)}(E_g, 3) = \begin{bmatrix} 0 & \frac{2\sqrt{66}}{33} & 0 & 0 & 0 & 0 & 0 \\ \frac{2\sqrt{66}}{33} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{110}}{176} & 0 & 0 & -\frac{13\sqrt{66}}{528} \\ 0 & 0 & \frac{\sqrt{110}}{176} & 0 & 0 & \frac{13\sqrt{66}}{528} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{13\sqrt{66}}{528} & 0 & 0 & -\frac{7\sqrt{110}}{176} \\ 0 & 0 & -\frac{13\sqrt{66}}{528} & 0 & 0 & -\frac{7\sqrt{110}}{176} & 0 \end{bmatrix}$$

$$\boxed{\text{x62}} \quad \mathbb{Q}_{6,2}^{(a)}(E_g, 3) = \begin{bmatrix} 0 & 0 & \frac{2\sqrt{66}}{33} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{110}}{176} & 0 & 0 & \frac{13\sqrt{66}}{528} \\ \frac{2\sqrt{66}}{33} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{110}}{176} & 0 & 0 & -\frac{13\sqrt{66}}{528} & 0 & 0 \\ 0 & 0 & 0 & -\frac{13\sqrt{66}}{528} & 0 & 0 & -\frac{7\sqrt{110}}{176} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{13\sqrt{66}}{528} & 0 & 0 & -\frac{7\sqrt{110}}{176} & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x63}} \quad \mathbb{M}_5^{(a)}(A_{1g}) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{i}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{i}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{i}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{i}{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x64}} \quad \mathbb{M}_1^{(a)}(A_{2g}) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{7}i}{7} \\ 0 & 0 & \frac{3\sqrt{7}i}{28} & 0 & 0 & \frac{\sqrt{105}i}{28} & 0 \\ 0 & -\frac{3\sqrt{7}i}{28} & 0 & 0 & \frac{\sqrt{105}i}{28} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{105}i}{28} & 0 & 0 & -\frac{\sqrt{7}i}{28} & 0 \\ 0 & -\frac{\sqrt{105}i}{28} & 0 & 0 & \frac{\sqrt{7}i}{28} & 0 & 0 \\ -\frac{\sqrt{7}i}{7} & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x65}} \quad \mathbb{M}_3^{(a)}(A_{2g}) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{6}i}{6} \\ 0 & 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{6}i}{6} & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 \\ -\frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x66}} \quad \mathbb{M}_5^{(a)}(A_{2g}, 1) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & -\frac{2\sqrt{21}i}{21} \\ 0 & 0 & -\frac{5\sqrt{21}i}{168} & 0 & 0 & \frac{3\sqrt{35}i}{56} & 0 \\ 0 & \frac{5\sqrt{21}i}{168} & 0 & 0 & \frac{3\sqrt{35}i}{56} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{3\sqrt{35}i}{56} & 0 & 0 & \frac{11\sqrt{21}i}{168} & 0 \\ 0 & -\frac{3\sqrt{35}i}{56} & 0 & 0 & -\frac{11\sqrt{21}i}{168} & 0 & 0 \\ \frac{2\sqrt{21}i}{21} & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x67}} \quad \mathbb{M}_5^{(a)}(A_{2g}, 2) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{15}i}{8} & 0 & 0 & -\frac{i}{8} & 0 \\ 0 & -\frac{\sqrt{15}i}{8} & 0 & 0 & -\frac{i}{8} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{i}{8} & 0 & 0 & \frac{\sqrt{15}i}{8} & 0 \\ 0 & \frac{i}{8} & 0 & 0 & -\frac{\sqrt{15}i}{8} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x68}} \quad \mathbb{M}_3^{(a)}(B_{1g}) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{6}i}{6} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{6}i}{6} \\ 0 & \frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{6}i}{6} & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x69}} \quad \mathbb{M}_5^{(a)}(B_{1g}) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{3}i}{6} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{3}i}{6} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{3}i}{3} \\ 0 & \frac{\sqrt{3}i}{6} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{3}i}{6} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{3}i}{3} & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x70}} \quad \mathbb{M}_3^{(a)}(B_{2g}) = \begin{bmatrix} 0 & 0 & 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{6}i}{6} & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 \\ \frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x71}} \quad \mathbb{M}_5^{(a)}(B_{2g}) = \begin{bmatrix} 0 & 0 & 0 & -\frac{\sqrt{3}i}{3} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{3}i}{6} & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{3}i}{6} & 0 & 0 \\ \frac{\sqrt{3}i}{3} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{3}i}{6} & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{3}i}{6} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x72}} \quad \mathbb{M}_{1,1}^{(a)}(E_g) = \begin{bmatrix} 0 & 0 & 0 & 0 & \frac{\sqrt{7}i}{7} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{3\sqrt{7}i}{28} & 0 & 0 & \frac{\sqrt{105}i}{28} \\ 0 & 0 & -\frac{3\sqrt{7}i}{28} & 0 & 0 & \frac{\sqrt{105}i}{28} & 0 \\ -\frac{\sqrt{7}i}{7} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{105}i}{28} & 0 & 0 & -\frac{\sqrt{7}i}{28} \\ 0 & 0 & -\frac{\sqrt{105}i}{28} & 0 & 0 & \frac{\sqrt{7}i}{28} & 0 \end{bmatrix}$$

$$\boxed{\text{x73}} \quad \mathbb{M}_{1,2}^{(a)}(E_g) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{7}i}{7} & 0 \\ 0 & 0 & 0 & \frac{3\sqrt{7}i}{28} & 0 & 0 & -\frac{\sqrt{105}i}{28} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{3\sqrt{7}i}{28} & 0 & 0 & -\frac{\sqrt{105}i}{28} & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{105}i}{28} & 0 & 0 & -\frac{\sqrt{7}i}{28} \\ \frac{\sqrt{7}i}{7} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{105}i}{28} & 0 & 0 & \frac{\sqrt{7}i}{28} & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x74}} \quad \mathbb{M}_{3,1}^{(a)}(E_g, 1) = \begin{bmatrix} 0 & 0 & 0 & 0 & \frac{\sqrt{6}i}{6} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 \\ -\frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{6}i}{6} \\ 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{6}i}{6} & 0 \end{bmatrix}$$

$$\boxed{\text{x75}} \quad \mathbb{M}_{3,2}^{(a)}(E_g, 1) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{6}i}{6} & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{6}i}{6} \\ \frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x76}} \quad \mathbb{M}_{3,1}^{(a)}(E_g, 2) = \begin{bmatrix} 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 & 0 \\ \frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{6}i}{6} \\ 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{6}i}{6} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{6}i}{6} & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x77}} \quad \mathbb{M}_{3,2}^{(a)}(E_g, 2) = \begin{bmatrix} 0 & 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{6}i}{6} \\ \frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{6}i}{6} & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x78}} \quad \mathbb{M}_{5,1}^{(a)}(E_g, 1) = \begin{bmatrix} 0 & 0 & 0 & 0 & -\frac{2\sqrt{21}i}{21} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{5\sqrt{21}i}{168} & 0 & 0 & \frac{3\sqrt{35}i}{56} \\ 0 & 0 & \frac{5\sqrt{21}i}{168} & 0 & 0 & \frac{3\sqrt{35}i}{56} & 0 \\ \frac{2\sqrt{21}i}{21} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{3\sqrt{35}i}{56} & 0 & 0 & \frac{11\sqrt{21}i}{168} \\ 0 & 0 & -\frac{3\sqrt{35}i}{56} & 0 & 0 & -\frac{11\sqrt{21}i}{168} & 0 \end{bmatrix}$$

$$\boxed{\text{x79}} \quad \mathbb{M}_{5,2}^{(a)}(E_g, 1) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & \frac{2\sqrt{21}i}{21} & 0 \\ 0 & 0 & 0 & -\frac{5\sqrt{21}i}{168} & 0 & 0 & -\frac{3\sqrt{35}i}{56} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{5\sqrt{21}i}{168} & 0 & 0 & -\frac{3\sqrt{35}i}{56} & 0 & 0 \\ 0 & 0 & 0 & \frac{3\sqrt{35}i}{56} & 0 & 0 & \frac{11\sqrt{21}i}{168} \\ -\frac{2\sqrt{21}i}{21} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{3\sqrt{35}i}{56} & 0 & 0 & -\frac{11\sqrt{21}i}{168} & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x80}} \quad \mathbb{M}_{5,1}^{(a)}(E_g, 2) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{15}i}{8} & 0 & 0 & -\frac{i}{8} \\ 0 & 0 & -\frac{\sqrt{15}i}{8} & 0 & 0 & -\frac{i}{8} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{i}{8} & 0 & 0 & \frac{\sqrt{15}i}{8} \\ 0 & 0 & \frac{i}{8} & 0 & 0 & -\frac{\sqrt{15}i}{8} & 0 \end{bmatrix}$$

$$\boxed{\text{x81}} \quad \mathbb{M}_{5,2}^{(a)}(E_g, 2) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{15}i}{8} & 0 & 0 & \frac{i}{8} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{15}i}{8} & 0 & 0 & \frac{i}{8} & 0 & 0 \\ 0 & 0 & 0 & -\frac{i}{8} & 0 & 0 & \frac{\sqrt{15}i}{8} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{i}{8} & 0 & 0 & -\frac{\sqrt{15}i}{8} & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x82}} \quad \mathbb{M}_{5,1}^{(a)}(E_g, 3) = \begin{bmatrix} 0 & -\frac{\sqrt{3}i}{3} & 0 & 0 & 0 & 0 & 0 \\ \frac{\sqrt{3}i}{3} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{3}i}{6} \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{3}i}{6} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{3}i}{6} & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{3}i}{6} & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x83}} \quad \mathbb{M}_{5,2}^{(a)}(E_g, 3) = \begin{bmatrix} 0 & 0 & -\frac{\sqrt{3}i}{3} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{3}i}{6} \\ \frac{\sqrt{3}i}{3} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{3}i}{6} & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{3}i}{6} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{3}i}{6} & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

Cluster SAMB

- Site cluster

** Wyckoff: 2a

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

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

** Wyckoff: 2c

$$\boxed{\text{y3}} \quad \mathbb{Q}_0^{(s)}(A_{1g}) = \left[\frac{\sqrt{2}}{2}, \frac{\sqrt{2}}{2} \right]$$

$$\boxed{\text{y4}} \quad \mathbb{Q}_1^{(s)}(A_{2u}) = \left[\frac{\sqrt{2}}{2}, -\frac{\sqrt{2}}{2} \right]$$

** Wyckoff: 2b

$$\boxed{\text{y5}} \quad \mathbb{Q}_0^{(s)}(A_{1g}) = \left[\frac{\sqrt{2}}{2}, \frac{\sqrt{2}}{2} \right]$$

$$\boxed{\text{y6}} \quad \mathbb{Q}_3^{(s)}(B_{2u}) = \left[\frac{\sqrt{2}}{2}, -\frac{\sqrt{2}}{2} \right]$$

- Bond cluster

** Wyckoff: 8a@8i

$$\boxed{\text{y7}} \quad \mathbb{Q}_0^{(s)}(A_{1g}) = \left[\frac{\sqrt{2}}{4}, \frac{\sqrt{2}}{4}, \frac{\sqrt{2}}{4}, \frac{\sqrt{2}}{4}, \frac{\sqrt{2}}{4}, \frac{\sqrt{2}}{4}, \frac{\sqrt{2}}{4}, \frac{\sqrt{2}}{4} \right]$$

$$\boxed{\text{y8}} \quad \mathbb{T}_0^{(s)}(A_{1g}) = \left[\frac{\sqrt{2}i}{4}, \frac{\sqrt{2}i}{4}, \frac{\sqrt{2}i}{4}, \frac{\sqrt{2}i}{4}, \frac{\sqrt{2}i}{4}, \frac{\sqrt{2}i}{4}, \frac{\sqrt{2}i}{4}, \frac{\sqrt{2}i}{4} \right]$$

$$\begin{aligned}
\boxed{\text{y9}} \quad \mathbb{Q}_1^{(s)}(A_{2u}) &= \left[\frac{\sqrt{2}}{4}, \frac{\sqrt{2}}{4}, \frac{\sqrt{2}}{4}, \frac{\sqrt{2}}{4}, -\frac{\sqrt{2}}{4}, -\frac{\sqrt{2}}{4}, -\frac{\sqrt{2}}{4}, -\frac{\sqrt{2}}{4} \right] \\
\boxed{\text{y10}} \quad \mathbb{T}_1^{(s)}(A_{2u}) &= \left[\frac{\sqrt{2}i}{4}, \frac{\sqrt{2}i}{4}, \frac{\sqrt{2}i}{4}, \frac{\sqrt{2}i}{4}, -\frac{\sqrt{2}i}{4}, -\frac{\sqrt{2}i}{4}, -\frac{\sqrt{2}i}{4}, -\frac{\sqrt{2}i}{4} \right] \\
\boxed{\text{y11}} \quad \mathbb{Q}_2^{(s)}(B_{1g}) &= \left[\frac{\sqrt{2}}{4}, \frac{\sqrt{2}}{4}, -\frac{\sqrt{2}}{4}, -\frac{\sqrt{2}}{4}, \frac{\sqrt{2}}{4}, \frac{\sqrt{2}}{4}, -\frac{\sqrt{2}}{4}, -\frac{\sqrt{2}}{4} \right] \\
\boxed{\text{y12}} \quad \mathbb{T}_2^{(s)}(B_{1g}) &= \left[\frac{\sqrt{2}i}{4}, \frac{\sqrt{2}i}{4}, -\frac{\sqrt{2}i}{4}, -\frac{\sqrt{2}i}{4}, \frac{\sqrt{2}i}{4}, \frac{\sqrt{2}i}{4}, -\frac{\sqrt{2}i}{4}, -\frac{\sqrt{2}i}{4} \right] \\
\boxed{\text{y13}} \quad \mathbb{M}_2^{(s)}(B_{2u}) &= \left[\frac{\sqrt{2}i}{4}, \frac{\sqrt{2}i}{4}, -\frac{\sqrt{2}i}{4}, -\frac{\sqrt{2}i}{4}, -\frac{\sqrt{2}i}{4}, -\frac{\sqrt{2}i}{4}, \frac{\sqrt{2}i}{4}, \frac{\sqrt{2}i}{4} \right] \\
\boxed{\text{y14}} \quad \mathbb{Q}_3^{(s)}(B_{2u}) &= \left[\frac{\sqrt{2}}{4}, \frac{\sqrt{2}}{4}, -\frac{\sqrt{2}}{4}, -\frac{\sqrt{2}}{4}, -\frac{\sqrt{2}}{4}, -\frac{\sqrt{2}}{4}, \frac{\sqrt{2}}{4}, \frac{\sqrt{2}}{4} \right] \\
\boxed{\text{y15}} \quad \mathbb{Q}_{2,1}^{(s)}(E_g) &= \left[\frac{1}{2}, -\frac{1}{2}, 0, 0, -\frac{1}{2}, \frac{1}{2}, 0, 0 \right] \\
\boxed{\text{y16}} \quad \mathbb{Q}_{2,2}^{(s)}(E_g) &= \left[0, 0, -\frac{1}{2}, \frac{1}{2}, 0, 0, -\frac{1}{2}, \frac{1}{2} \right] \\
\boxed{\text{y17}} \quad \mathbb{T}_{2,1}^{(s)}(E_g) &= \left[\frac{i}{2}, -\frac{i}{2}, 0, 0, -\frac{i}{2}, \frac{i}{2}, 0, 0 \right] \\
\boxed{\text{y18}} \quad \mathbb{T}_{2,2}^{(s)}(E_g) &= \left[0, 0, -\frac{i}{2}, \frac{i}{2}, 0, 0, -\frac{i}{2}, \frac{i}{2} \right] \\
\boxed{\text{y19}} \quad \mathbb{Q}_{1,1}^{(s)}(E_u) &= \left[0, 0, -\frac{1}{2}, \frac{1}{2}, 0, 0, \frac{1}{2}, -\frac{1}{2} \right] \\
\boxed{\text{y20}} \quad \mathbb{Q}_{1,2}^{(s)}(E_u) &= \left[\frac{1}{2}, -\frac{1}{2}, 0, 0, \frac{1}{2}, -\frac{1}{2}, 0, 0 \right] \\
\boxed{\text{y21}} \quad \mathbb{T}_{1,1}^{(s)}(E_u) &= \left[0, 0, -\frac{i}{2}, \frac{i}{2}, 0, 0, \frac{i}{2}, -\frac{i}{2} \right] \\
\boxed{\text{y22}} \quad \mathbb{T}_{1,2}^{(s)}(E_u) &= \left[\frac{i}{2}, -\frac{i}{2}, 0, 0, \frac{i}{2}, -\frac{i}{2}, 0, 0 \right]
\end{aligned}$$

Table 5: Orbital of each site

#	site	orbital
1	Pt1	$ d_u\rangle, d_v\rangle, d_{yz}\rangle, d_{xz}\rangle, d_{xy}\rangle$
2	Pt2	$ d_u\rangle, d_v\rangle, d_{yz}\rangle, d_{xz}\rangle, d_{xy}\rangle$
3	Si1	$ p_x\rangle, p_y\rangle, p_z\rangle$
4	Si2	$ p_x\rangle, p_y\rangle, p_z\rangle$
5	U	$ f_3\rangle, f_{ax}\rangle, f_{ay}\rangle, f_{az}\rangle, f_{bx}\rangle, f_{by}\rangle, f_{bz}\rangle$

Table 6: Neighbor and bra-ket of each bond

#	head	tail	neighbor	head (bra)	tail (ket)
1	Pt1	Si2	[1]	[d]	[p]
2	Pt2	Si1	[1]	[d]	[p]

Site in Unit Cell

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

Table 7: 'Pt1' (#1) site cluster (2a), $\bar{4}m2$

SL	position (\mathbf{s})	mapping
1	[0.75000, 0.25000, 0.00000]	[1,2,7,8,11,12,13,14]
2	[0.25000, 0.75000, 0.00000]	[3,4,5,6,9,10,15,16]

Table 8: 'Pt2' (#2) site cluster (2c), $4mm$

SL	position (\mathbf{s})	mapping
1	[0.25000, 0.25000, 0.37850]	[1,2,3,4,13,14,15,16]
2	[0.75000, 0.75000, 0.62150]	[5,6,7,8,9,10,11,12]

Table 9: 'Si1' (#3) site cluster (2b), $\bar{4}m2$

SL	position (\mathbf{s})	mapping
1	[0.75000, 0.25000, 0.50000]	[1,2,7,8,11,12,13,14]
2	[0.25000, 0.75000, 0.50000]	[3,4,5,6,9,10,15,16]

Table 10: 'Si2' (#4) site cluster (2c), $4mm$

SL	position (s)	mapping
1	[0.25000, 0.25000, 0.13300]	[1,2,3,4,13,14,15,16]
2	[0.75000, 0.75000, 0.86700]	[5,6,7,8,9,10,11,12]

Table 11: 'U' (#5) site cluster (2c), $4mm$

SL	position (s)	mapping
1	[0.25000, 0.25000, 0.74840]	[1,2,3,4,13,14,15,16]
2	[0.75000, 0.75000, 0.25160]	[5,6,7,8,9,10,11,12]

--- 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 12: 1-th 'Pt1'-'Si2' [1] (#1) bond cluster (8a08i), D, $|\mathbf{v}|=2.46277$ (cartesian)

SL	vector (\mathbf{v})	center (\mathbf{c})	mapping	head	tail	\mathbf{R} (primitive)
1	[0.00000, 0.50000, -0.13300]	[0.25000, 0.50000, 0.06650]	[1,14]	(2,1)	(1,1)	[0,0,0]
2	[0.00000, -0.50000, -0.13300]	[0.25000, 0.00000, 0.06650]	[2,13]	(2,1)	(1,1)	[0,1,0]
3	[-0.50000, 0.00000, -0.13300]	[0.00000, 0.25000, 0.06650]	[3,15]	(1,1)	(1,1)	[1,0,0]
4	[0.50000, 0.00000, -0.13300]	[0.50000, 0.25000, 0.06650]	[4,16]	(1,1)	(1,1)	[0,0,0]
5	[0.00000, 0.50000, 0.13300]	[0.75000, 0.00000, 0.93350]	[5,10]	(1,1)	(2,1)	[0,-1,-1]
6	[0.00000, -0.50000, 0.13300]	[0.75000, 0.50000, 0.93350]	[6,9]	(1,1)	(2,1)	[0,0,-1]
7	[0.50000, 0.00000, 0.13300]	[0.00000, 0.75000, 0.93350]	[7,11]	(2,1)	(2,1)	[-1,0,-1]
8	[-0.50000, 0.00000, 0.13300]	[0.50000, 0.75000, 0.93350]	[8,12]	(2,1)	(2,1)	[0,0,-1]

Table 13: 1-th 'Pt2'-'Si1' [1] (#2) bond cluster (8a08i), D, $|\mathbf{v}|=2.40633$ (cartesian)

SL	vector (\mathbf{v})	center (\mathbf{c})	mapping	head	tail	\mathbf{R} (primitive)
1	[0.00000, 0.50000, -0.12150]	[0.25000, 0.00000, 0.43925]	[1,14]	(1,1)	(2,1)	[0,-1,0]
2	[0.00000, -0.50000, -0.12150]	[0.25000, 0.50000, 0.43925]	[2,13]	(1,1)	(2,1)	[0,0,0]
3	[-0.50000, 0.00000, -0.12150]	[0.50000, 0.25000, 0.43925]	[3,15]	(1,1)	(1,1)	[0,0,0]
4	[0.50000, 0.00000, -0.12150]	[0.00000, 0.25000, 0.43925]	[4,16]	(1,1)	(1,1)	[-1,0,0]
5	[0.00000, 0.50000, 0.12150]	[0.75000, 0.50000, 0.56075]	[5,10]	(2,1)	(1,1)	[0,0,0]

continued ...

Table 13

SL	vector (\boldsymbol{v})	center (\boldsymbol{c})	mapping	head	tail	\boldsymbol{R} (primitive)
6	[0.00000, -0.50000, 0.12150]	[0.75000, 0.00000, 0.56075]	[6,9]	(2,1)	(1,1)	[0,1,0]
7	[0.50000, 0.00000, 0.12150]	[0.50000, 0.75000, 0.56075]	[7,11]	(2,1)	(2,1)	[0,0,0]
8	[-0.50000, 0.00000, 0.12150]	[0.00000, 0.75000, 0.56075]	[8,12]	(2,1)	(2,1)	[1,0,0]