

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]
- 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 ½½0}	3	{4 ₀₀₁ ⁺ ½00}	4	{4 ₀₀₁ ⁻ 0½0}	5	{2 ₀₁₀ 0½0}

continued ...

Table 1

#	SO	#	SO	#	SO	#	SO	#	SO
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	-	$\frac{\sqrt{2}(2x^6 - 15x^4y^2 - 15x^4z^2 - 15x^2y^4 + 180x^2y^2z^2 - 15x^2z^4 + 2y^6 - 15y^4z^2 - 15y^2z^4 + 2z^6)}{8}$
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	-	-	$-\frac{x^2}{2} - \frac{y^2}{2} + z^2$

continued ...

Table 2

#	symbol	irrep.	rank	X	multiplicity	component	symmetry
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	-	$\frac{\sqrt{42}(x-y)(x+y)(x^4 - 9x^2y^2 - 5x^2z^2 + y^4 - 5y^2z^2 + 5z^4)}{8}$
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	-	-	$\frac{\sqrt{105}xyz(x^2 + y^2 - 2z^2)}{2}$

continued ...

Table 2

#	symbol	irrep.	rank	X	multiplicity	component	symmetry
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	$\frac{\sqrt{15}x(y-z)(y+z)}{2}$
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	$\frac{\sqrt{35}xz(x-z)(x+z)}{2}$

continued ...

Table 2

#	symbol	irrep.	rank	X	multiplicity	component	symmetry
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	$-\sqrt{3}xz$
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	$\frac{\sqrt{15}x(y-z)(y+z)}{2}$

continued ...

Table 2

#	symbol	irrep.	rank	X	multiplicity	component	symmetry
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)
1	$ d_u\rangle @Pt1(1)$	2	$ d_v\rangle @Pt1(1)$	3	$ d_{yz}\rangle @Pt1(1)$	4	$ d_{xz}\rangle @Pt1(1)$	5	$ d_{xy}\rangle @Pt1(1)$
6	$ d_u\rangle @Pt1(2)$	7	$ d_v\rangle @Pt1(2)$	8	$ d_{yz}\rangle @Pt1(2)$	9	$ d_{xz}\rangle @Pt1(2)$	10	$ d_{xy}\rangle @Pt1(2)$
11	$ d_u\rangle @Pt2(1)$	12	$ d_v\rangle @Pt2(1)$	13	$ d_{yz}\rangle @Pt2(1)$	14	$ d_{xz}\rangle @Pt2(1)$	15	$ d_{xy}\rangle @Pt2(1)$
16	$ d_u\rangle @Pt2(2)$	17	$ d_v\rangle @Pt2(2)$	18	$ d_{yz}\rangle @Pt2(2)$	19	$ d_{xz}\rangle @Pt2(2)$	20	$ d_{xy}\rangle @Pt2(2)$
21	$ p_x\rangle @Si1(1)$	22	$ p_y\rangle @Si1(1)$	23	$ p_z\rangle @Si1(1)$	24	$ p_x\rangle @Si1(2)$	25	$ p_y\rangle @Si1(2)$
26	$ p_z\rangle @Si1(2)$	27	$ p_x\rangle @Si2(1)$	28	$ p_y\rangle @Si2(1)$	29	$ p_z\rangle @Si2(1)$	30	$ p_x\rangle @Si2(2)$

continued ...

Table 3

#	orbital@atom(SL)								
31	$ p_y\rangle @\text{Si}2(2)$	32	$ p_z\rangle @\text{Si}2(2)$	33	$ f_3\rangle @\text{U}(1)$	34	$ f_{ax}\rangle @\text{U}(1)$	35	$ f_{ay}\rangle @\text{U}(1)$
36	$ f_{az}\rangle @\text{U}(1)$	37	$ f_{bx}\rangle @\text{U}(1)$	38	$ f_{by}\rangle @\text{U}(1)$	39	$ f_{bz}\rangle @\text{U}(1)$	40	$ f_3\rangle @\text{U}(2)$
41	$ f_{ax}\rangle @\text{U}(2)$	42	$ f_{ay}\rangle @\text{U}(2)$	43	$ f_{az}\rangle @\text{U}(2)$	44	$ f_{bx}\rangle @\text{U}(2)$	45	$ f_{by}\rangle @\text{U}(2)$
46	$ f_{bz}\rangle @\text{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$	$\sqrt{3}xy$
$ f_3\rangle$	$\sqrt{15}xyz$
$ f_{ax}\rangle$	$\frac{x(2x^2-3y^2-3z^2)}{2}$
$ f_{ay}\rangle$	$\frac{y(-3x^2+2y^2-3z^2)}{2}$

continued ...

Table 4

orbital	definition
$ 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 —

292 (all 380) SAMBs

- 'Pt1' site-cluster
 - * 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

[z1] $\mathbb{Q}_0^{(c)}(A_{1g}) = \mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_0^{(s)}(A_{1g})$

[z2] $\mathbb{Q}_2^{(c)}(A_{1g}) = \mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_0^{(s)}(A_{1g})$

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- 'Pt2' site-cluster

* 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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- 'Si1' site-cluster

* 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

* 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

- * 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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

$$\boxed{\text{z275}} \quad \mathbb{Q}_{6,1}^{(c)}(E_g, 3) = \frac{\sqrt{2}\mathbb{Q}_{6,1}^{(a)}(E_g, 3)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

$$\boxed{\text{z276}} \quad \mathbb{Q}_{6,2}^{(c)}(E_g, 3) = \frac{\sqrt{2}\mathbb{Q}_{6,2}^{(a)}(E_g, 3)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

$$\boxed{\text{z309}} \quad \mathbb{Q}_{1,1}^{(c)}(E_u) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_1^{(s)}(A_{2u})}{2}$$

$$\boxed{\text{z310}} \quad \mathbb{Q}_{1,2}^{(c)}(E_u) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_1^{(s)}(A_{2u})}{2}$$

$$\boxed{\text{z311}} \quad \mathbb{Q}_{3,1}^{(c)}(E_u, 1) = \frac{\sqrt{7}\mathbb{Q}_{4,2}^{(a)}(E_g, 1)\mathbb{Q}_1^{(s)}(A_{2u})}{4} - \frac{\mathbb{Q}_{4,2}^{(a)}(E_g, 2)\mathbb{Q}_1^{(s)}(A_{2u})}{4}$$

$$\boxed{\text{z312}} \quad \mathbb{Q}_{3,2}^{(c)}(E_u, 1) = \frac{\sqrt{7}\mathbb{Q}_{4,1}^{(a)}(E_g, 1)\mathbb{Q}_1^{(s)}(A_{2u})}{4} - \frac{\mathbb{Q}_{4,1}^{(a)}(E_g, 2)\mathbb{Q}_1^{(s)}(A_{2u})}{4}$$

$$\boxed{\text{z313}} \quad \mathbb{Q}_{3,1}^{(c)}(E_u, 2) = \frac{\mathbb{Q}_{4,2}^{(a)}(E_g, 1)\mathbb{Q}_1^{(s)}(A_{2u})}{4} + \frac{\sqrt{7}\mathbb{Q}_{4,2}^{(a)}(E_g, 2)\mathbb{Q}_1^{(s)}(A_{2u})}{4}$$

$$\boxed{\text{z314}} \quad \mathbb{Q}_{3,2}^{(c)}(E_u, 2) = \frac{\mathbb{Q}_{4,1}^{(a)}(E_g, 1)\mathbb{Q}_1^{(s)}(A_{2u})}{4} + \frac{\sqrt{7}\mathbb{Q}_{4,1}^{(a)}(E_g, 2)\mathbb{Q}_1^{(s)}(A_{2u})}{4}$$

$$\boxed{\text{z315}} \quad \mathbb{Q}_{5,1}^{(c)}(E_u, 1) = -\frac{\sqrt{6}\mathbb{Q}_{6,2}^{(a)}(E_g, 1)\mathbb{Q}_1^{(s)}(A_{2u})}{8} + \frac{3\sqrt{11}\mathbb{Q}_{6,2}^{(a)}(E_g, 2)\mathbb{Q}_1^{(s)}(A_{2u})}{16} + \frac{\sqrt{5}\mathbb{Q}_{6,2}^{(a)}(E_g, 3)\mathbb{Q}_1^{(s)}(A_{2u})}{16}$$

$$\boxed{\text{z316}} \quad \mathbb{Q}_{5,2}^{(c)}(E_u, 1) = -\frac{\sqrt{6}\mathbb{Q}_{6,1}^{(a)}(E_g, 1)\mathbb{Q}_1^{(s)}(A_{2u})}{8} + \frac{3\sqrt{11}\mathbb{Q}_{6,1}^{(a)}(E_g, 2)\mathbb{Q}_1^{(s)}(A_{2u})}{16} + \frac{\sqrt{5}\mathbb{Q}_{6,1}^{(a)}(E_g, 3)\mathbb{Q}_1^{(s)}(A_{2u})}{16}$$

$$\boxed{\text{z317}} \quad \mathbb{Q}_{5,1}^{(c)}(E_u, 2) = \frac{7\sqrt{290}\mathbb{Q}_{6,2}^{(a)}(E_g, 1)\mathbb{Q}_1^{(s)}(A_{2u})}{232} + \frac{\sqrt{4785}\mathbb{Q}_{6,2}^{(a)}(E_g, 2)\mathbb{Q}_1^{(s)}(A_{2u})}{464} + \frac{23\sqrt{87}\mathbb{Q}_{6,2}^{(a)}(E_g, 3)\mathbb{Q}_1^{(s)}(A_{2u})}{464}$$

$$\boxed{\text{z318}} \quad \mathbb{Q}_{5,2}^{(c)}(E_u, 2) = \frac{7\sqrt{290}\mathbb{Q}_{6,1}^{(a)}(E_g, 1)\mathbb{Q}_1^{(s)}(A_{2u})}{232} + \frac{\sqrt{4785}\mathbb{Q}_{6,1}^{(a)}(E_g, 2)\mathbb{Q}_1^{(s)}(A_{2u})}{464} + \frac{23\sqrt{87}\mathbb{Q}_{6,1}^{(a)}(E_g, 3)\mathbb{Q}_1^{(s)}(A_{2u})}{464}$$

$$\boxed{\text{z319}} \quad \mathbb{Q}_{5,1}^{(c)}(E_u, 3) = \frac{\sqrt{1914}\mathbb{Q}_{6,2}^{(a)}(E_g, 1)\mathbb{Q}_1^{(s)}(A_{2u})}{116} + \frac{13\sqrt{29}\mathbb{Q}_{6,2}^{(a)}(E_g, 2)\mathbb{Q}_1^{(s)}(A_{2u})}{232} - \frac{3\sqrt{1595}\mathbb{Q}_{6,2}^{(a)}(E_g, 3)\mathbb{Q}_1^{(s)}(A_{2u})}{232}$$

$$\boxed{\text{z320}} \quad \mathbb{Q}_{5,2}^{(c)}(E_u, 3) = \frac{\sqrt{1914}\mathbb{Q}_{6,1}^{(a)}(E_g, 1)\mathbb{Q}_1^{(s)}(A_{2u})}{116} + \frac{13\sqrt{29}\mathbb{Q}_{6,1}^{(a)}(E_g, 2)\mathbb{Q}_1^{(s)}(A_{2u})}{232} - \frac{3\sqrt{1595}\mathbb{Q}_{6,1}^{(a)}(E_g, 3)\mathbb{Q}_1^{(s)}(A_{2u})}{232}$$

• 'Pt1'-'Si2' bond-cluster

* 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**

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

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

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

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

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

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

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

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

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

$$\boxed{\text{z40}} \quad \mathbb{Q}_4^{(c)}(A_{2g}, a) = \frac{\sqrt{5}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_{1,2}^{(b)}(E_u)}{4} - \frac{\sqrt{3}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{1,2}^{(b)}(E_u)}{4} - \frac{\sqrt{5}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_{1,1}^{(b)}(E_u)}{4} + \frac{\sqrt{3}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{1,1}^{(b)}(E_u)}{4}$$

$$\boxed{\text{z41}} \quad \mathbb{Q}_4^{(c)}(A_{2g}, b) = \mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_3^{(b)}(B_{2u})$$

$$\boxed{\text{z42}} \quad \mathbb{Q}_4^{(c)}(A_{2g}, c) = -\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_3^{(b)}(B_{2u})$$

$$\boxed{\text{z43}} \quad \mathbb{Q}_1^{(c)}(A_{2u}, a) = \mathbb{Q}_1^{(a)}(A_{2u})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z44}} \quad \mathbb{Q}_1^{(c)}(A_{2u}, b) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2} + \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z45}} \quad \mathbb{Q}_1^{(c)}(A_{2u}, c) = -\frac{\sqrt{7}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_{2,2}^{(b)}(E_g)}{7} - \frac{\sqrt{105}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{2,2}^{(b)}(E_g)}{21} - \frac{\sqrt{7}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_{2,1}^{(b)}(E_g)}{7} - \frac{\sqrt{105}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{2,1}^{(b)}(E_g)}{21} + \frac{\sqrt{105}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_2^{(b)}(B_{1g})}{21}$$

$$\boxed{\text{z63}} \quad \mathbb{Q}_1^{(c)}(A_{2u}, d) = -\frac{\sqrt{6}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{6} - \frac{\sqrt{6}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{6} - \frac{\sqrt{6}\mathbb{G}_2^{(a)}(B_{2u})\mathbb{Q}_2^{(b)}(B_{1g})}{3}$$

$$\boxed{\text{z64}} \quad \mathbb{Q}_3^{(c)}(A_{2u}, a) = \mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z65}} \quad \mathbb{Q}_3^{(c)}(A_{2u}, b) = -\frac{\sqrt{35}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_{2,2}^{(b)}(E_g)}{28} - \frac{5\sqrt{21}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{2,2}^{(b)}(E_g)}{84} - \frac{\sqrt{35}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_{2,1}^{(b)}(E_g)}{28} - \frac{5\sqrt{21}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{2,1}^{(b)}(E_g)}{84} - \frac{4\sqrt{21}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_2^{(b)}(B_{1g})}{21}$$

$$\boxed{\text{z66}} \quad \mathbb{Q}_3^{(c)}(A_{2u}, c) = -\frac{\sqrt{3}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{3} - \frac{\sqrt{3}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{3} + \frac{\sqrt{3}\mathbb{G}_2^{(a)}(B_{2u})\mathbb{Q}_2^{(b)}(B_{1g})}{3}$$

$$\boxed{\text{z67}} \quad \mathbb{Q}_5^{(c)}(A_{2u}, 2) = \frac{\sqrt{5}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_{2,2}^{(b)}(E_g)}{4} - \frac{\sqrt{3}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{2,2}^{(b)}(E_g)}{4} + \frac{\sqrt{5}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_{2,1}^{(b)}(E_g)}{4} - \frac{\sqrt{3}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{2,1}^{(b)}(E_g)}{4}$$

$$\boxed{\text{z68}} \quad \mathbb{Q}_2^{(c)}(B_{1g}, a) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_{1,1}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_{1,2}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z69}} \quad \mathbb{Q}_2^{(c)}(B_{1g}, b) = \mathbb{Q}_1^{(a)}(A_{2u})\mathbb{Q}_3^{(b)}(B_{2u})$$

$$\boxed{\text{z70}} \quad \mathbb{Q}_2^{(c)}(B_{1g}, c) = \frac{3\sqrt{7}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_{1,1}^{(b)}(E_u)}{14} - \frac{\sqrt{105}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{1,1}^{(b)}(E_u)}{42} - \frac{3\sqrt{7}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_{1,2}^{(b)}(E_u)}{14} + \frac{\sqrt{105}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{1,2}^{(b)}(E_u)}{42} + \frac{\sqrt{105}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_1^{(b)}(A_{2u})}{21}$$

$$\boxed{\text{z89}} \quad \mathbb{Q}_2^{(c)}(B_{1g}, d) = -\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_3^{(b)}(B_{2u})$$

$$\boxed{\text{z90}} \quad \mathbb{Q}_2^{(c)}(B_{1g}, e) = -\frac{\sqrt{6}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_{1,1}^{(b)}(E_u)}{6} + \frac{\sqrt{6}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_{1,2}^{(b)}(E_u)}{6} + \frac{\sqrt{6}\mathbb{G}_2^{(a)}(B_{2u})\mathbb{Q}_1^{(b)}(A_{2u})}{3}$$

$$\boxed{\text{z91}} \quad \mathbb{Q}_4^{(c)}(B_{1g}) = \frac{\sqrt{35}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_{1,1}^{(b)}(E_u)}{14} + \frac{\sqrt{21}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{1,1}^{(b)}(E_u)}{14} - \frac{\sqrt{35}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_{1,2}^{(b)}(E_u)}{14} - \frac{\sqrt{21}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{1,2}^{(b)}(E_u)}{14} - \frac{\sqrt{21}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_1^{(b)}(A_{2u})}{7}$$

$$\boxed{\text{z92}} \quad \mathbb{Q}_3^{(c)}(B_{1u}, a) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} + \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z93}} \quad \mathbb{Q}_3^{(c)}(B_{1u}, b) = \mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_0^{(b)}(A_{1g})$$

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

$$\boxed{\text{z95}} \quad \mathbb{Q}_3^{(c)}(B_{1u}, d) = \mathbb{G}_2^{(a)}(A_{1u})\mathbb{Q}_2^{(b)}(B_{1g})$$

$$\boxed{\text{z131}} \quad \mathbb{Q}_5^{(c)}(B_{1u}) = \frac{\sqrt{2}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} + \frac{\sqrt{2}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z132}} \quad \mathbb{Q}_2^{(c)}(B_{2g}, a) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_{1,2}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_{1,1}^{(b)}(E_u)}{2}$$

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

$$\boxed{\text{z134}} \quad \mathbb{Q}_2^{(c)}(B_{2g}, c) = -\frac{\sqrt{6}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_{1,2}^{(b)}(E_u)}{6} - \frac{\sqrt{6}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_{1,1}^{(b)}(E_u)}{6} - \frac{\sqrt{6}\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_1^{(b)}(A_{2u})}{3}$$

$$\boxed{\text{z135}} \quad \mathbb{Q}_2^{(c)}(B_{2g}, d) = \mathbb{G}_2^{(a)}(A_{1u})\mathbb{Q}_3^{(b)}(B_{2u})$$

$$\boxed{\text{z136}} \quad \mathbb{Q}_4^{(c)}(B_{2g}) = -\frac{\sqrt{35}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_{1,2}^{(b)}(E_u)}{28} - \frac{3\sqrt{21}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{1,2}^{(b)}(E_u)}{28} - \frac{\sqrt{35}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_{1,1}^{(b)}(E_u)}{28} - \frac{3\sqrt{21}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{1,1}^{(b)}(E_u)}{28} + \frac{\sqrt{21}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_1^{(b)}(A_{2u})}{7}$$

$$\boxed{\text{z137}} \quad \mathbb{Q}_3^{(c)}(B_{2u}, a) = \frac{\sqrt{3}\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{3} - \frac{\sqrt{3}\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{3} + \frac{\sqrt{3}\mathbb{Q}_1^{(a)}(A_{2u})\mathbb{Q}_2^{(b)}(B_{1g})}{3}$$

$$\boxed{\text{z138}} \quad \mathbb{Q}_3^{(c)}(B_{2u}, b) = \mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z139}} \quad \mathbb{Q}_3^{(c)}(B_{2u}, c) = \frac{\sqrt{3}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_{2,2}^{(b)}(E_g)}{12} - \frac{\sqrt{5}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{2,2}^{(b)}(E_g)}{4} - \frac{\sqrt{3}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_{2,1}^{(b)}(E_g)}{12} + \frac{\sqrt{5}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{2,1}^{(b)}(E_g)}{4} - \frac{\sqrt{3}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_2^{(b)}(B_{1g})}{3}$$

$$\boxed{\text{z140}} \quad \mathbb{Q}_5^{(c)}(B_{2u}) = -\frac{\sqrt{105}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_{2,2}^{(b)}(E_g)}{21} - \frac{\sqrt{7}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{2,2}^{(b)}(E_g)}{7} + \frac{\sqrt{105}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_{2,1}^{(b)}(E_g)}{21} + \frac{\sqrt{7}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{2,1}^{(b)}(E_g)}{7} + \frac{\sqrt{105}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_2^{(b)}(B_{1g})}{21}$$

$$\boxed{\text{z141}} \quad \mathbb{Q}_{2,1}^{(c)}(E_g, a) = \frac{\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_1^{(b)}(A_{2u})}{2} + \frac{\mathbb{Q}_1^{(a)}(A_{2u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z142}} \quad \mathbb{Q}_{2,2}^{(c)}(E_g, a) = \frac{\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_1^{(b)}(A_{2u})}{2} + \frac{\mathbb{Q}_1^{(a)}(A_{2u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z143}} \quad \mathbb{Q}_{2,1}^{(c)}(E_g, b) = -\frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_3^{(b)}(B_{2u})}{2}$$

$$\boxed{\text{z144}} \quad \mathbb{Q}_{2,2}^{(c)}(E_g, b) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_3^{(b)}(B_{2u})}{2}$$

$$\boxed{\text{z145}} \quad \mathbb{Q}_{2,1}^{(c)}(E_g, c) = -\frac{\sqrt{14}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_1^{(b)}(A_{2u})}{14} - \frac{\sqrt{210}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_1^{(b)}(A_{2u})}{42} - \frac{\sqrt{14}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{14} + \frac{\sqrt{210}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{42} - \frac{\sqrt{210}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{42}$$

$$\boxed{\text{z146}} \quad \mathbb{Q}_{2,2}^{(c)}(E_g, c) = -\frac{\sqrt{14}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_1^{(b)}(A_{2u})}{14} - \frac{\sqrt{210}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_1^{(b)}(A_{2u})}{42} - \frac{\sqrt{14}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{14} + \frac{\sqrt{210}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{42} + \frac{\sqrt{210}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{42}$$

$$\boxed{\text{z147}} \quad \mathbb{Q}_{2,1}^{(c)}(E_g, d) = -\frac{\sqrt{2}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_3^{(b)}(B_{2u})}{8} + \frac{\sqrt{30}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_3^{(b)}(B_{2u})}{8}$$

$$\boxed{\text{z148}} \quad \mathbb{Q}_{2,2}^{(c)}(E_g, d) = \frac{\sqrt{2}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_3^{(b)}(B_{2u})}{8} - \frac{\sqrt{30}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_3^{(b)}(B_{2u})}{8}$$

$$\boxed{\text{z149}} \quad \mathbb{Q}_{2,1}^{(c)}(E_g, e) = \frac{\sqrt{3}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_1^{(b)}(A_{2u})}{6} + \frac{\mathbb{G}_2^{(a)}(A_{1u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{2} + \frac{\sqrt{3}\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{6} + \frac{\sqrt{3}\mathbb{G}_2^{(a)}(B_{2u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{6}$$

$$\boxed{\text{z150}} \quad \mathbb{Q}_{2,2}^{(c)}(E_g, e) = \frac{\sqrt{3}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_1^{(b)}(A_{2u})}{6} - \frac{\mathbb{G}_2^{(a)}(A_{1u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{2} + \frac{\sqrt{3}\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{6} - \frac{\sqrt{3}\mathbb{G}_2^{(a)}(B_{2u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{6}$$

$$\boxed{\text{z151}} \quad \mathbb{Q}_{4,1}^{(c)}(E_g, 1a) = \frac{\sqrt{10}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_1^{(b)}(A_{2u})}{8} + \frac{\sqrt{6}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_1^{(b)}(A_{2u})}{8} - \frac{\sqrt{10}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{8} - \frac{\sqrt{6}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{8}$$

$$\boxed{\text{z152}} \quad \mathbb{Q}_{4,2}^{(c)}(E_g, 1a) = \frac{\sqrt{10}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_1^{(b)}(A_{2u})}{8} + \frac{\sqrt{6}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_1^{(b)}(A_{2u})}{8} - \frac{\sqrt{10}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{8} + \frac{\sqrt{6}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{8}$$

$$\boxed{\text{z153}} \quad \mathbb{Q}_{4,1}^{(c)}(E_g, 1b) = -\frac{\sqrt{30}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_3^{(b)}(B_{2u})}{8} - \frac{\sqrt{2}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_3^{(b)}(B_{2u})}{8}$$

$$\boxed{\text{z154}} \quad \mathbb{Q}_{4,2}^{(c)}(E_g, 1b) = \frac{\sqrt{30}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_3^{(b)}(B_{2u})}{8} + \frac{\sqrt{2}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_3^{(b)}(B_{2u})}{8}$$

$$\boxed{\text{z155}} \quad \mathbb{Q}_{4,1}^{(c)}(E_g, 1c) = -\frac{\sqrt{2}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_3^{(b)}(B_{2u})}{2}$$

$$\boxed{\text{z156}} \quad \mathbb{Q}_{4,2}^{(c)}(E_g, 1c) = \frac{\sqrt{2}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_3^{(b)}(B_{2u})}{2}$$

$$\boxed{\text{z157}} \quad \mathbb{Q}_{4,1}^{(c)}(E_g, 2) = -\frac{\sqrt{70}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_1^{(b)}(A_{2u})}{56} + \frac{3\sqrt{42}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_1^{(b)}(A_{2u})}{56} - \frac{\sqrt{70}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{56} + \frac{\sqrt{42}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{14} + \frac{3\sqrt{42}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{56}$$

$$\boxed{\text{z158}} \quad \mathbb{Q}_{4,2}^{(c)}(E_g, 2) = -\frac{\sqrt{70}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_1^{(b)}(A_{2u})}{56} + \frac{3\sqrt{42}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_1^{(b)}(A_{2u})}{56} - \frac{\sqrt{70}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{56} + \frac{\sqrt{42}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{14} - \frac{3\sqrt{42}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{56}$$

$$\boxed{\text{z159}} \quad \mathbb{Q}_{1,1}^{(c)}(E_u, a) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z160}} \quad \mathbb{Q}_{1,2}^{(c)}(E_u, a) = \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z197}} \quad \mathbb{Q}_{1,1}^{(c)}(E_u, b) = \frac{\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_2^{(b)}(B_{1g})}{2} + \frac{\mathbb{Q}_1^{(a)}(A_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z198}} \quad \mathbb{Q}_{1,2}^{(c)}(E_u, b) = -\frac{\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_2^{(b)}(B_{1g})}{2} + \frac{\mathbb{Q}_1^{(a)}(A_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z199}} \quad \mathbb{Q}_{1,1}^{(c)}(E_u, c) = \frac{3\sqrt{14}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_2^{(b)}(B_{1g})}{28} - \frac{\sqrt{210}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_2^{(b)}(B_{1g})}{84} - \frac{\sqrt{14}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{14} + \frac{\sqrt{210}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{42} + \frac{\sqrt{210}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{42}$$

$$\boxed{\text{z200}} \quad \mathbb{Q}_{1,2}^{(c)}(E_u, c) = -\frac{3\sqrt{14}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_2^{(b)}(B_{1g})}{28} + \frac{\sqrt{210}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_2^{(b)}(B_{1g})}{84} - \frac{\sqrt{14}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{14} + \frac{\sqrt{210}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{42} - \frac{\sqrt{210}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{42}$$

$$\boxed{\text{z201}} \quad \mathbb{Q}_{1,1}^{(c)}(E_u, d) = \frac{\sqrt{3}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_2^{(b)}(B_{1g})}{6} - \frac{\mathbb{G}_2^{(a)}(A_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} - \frac{\sqrt{3}\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{6} + \frac{\sqrt{3}\mathbb{G}_2^{(a)}(B_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{6}$$

$$\boxed{\text{z202}} \quad \mathbb{Q}_{1,2}^{(c)}(E_u, d) = -\frac{\sqrt{3}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_2^{(b)}(B_{1g})}{6} + \frac{\mathbb{G}_2^{(a)}(A_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2} - \frac{\sqrt{3}\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{6} - \frac{\sqrt{3}\mathbb{G}_2^{(a)}(B_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{6}$$

$$\boxed{\text{z203}} \quad \mathbb{Q}_{3,1}^{(c)}(E_u, 1a) = \frac{\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_2^{(b)}(B_{1g})}{2} - \frac{\mathbb{Q}_1^{(a)}(A_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z226}} \quad \mathbb{Q}_{3,2}^{(c)}(E_u, 1a) = -\frac{\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_2^{(b)}(B_{1g})}{2} - \frac{\mathbb{Q}_1^{(a)}(A_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z227}} \quad \mathbb{Q}_{3,1}^{(c)}(E_u, 1b) = \frac{\sqrt{2}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z228}} \quad \mathbb{Q}_{3,2}^{(c)}(E_u, 1b) = \frac{\sqrt{2}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z229}} \quad \mathbb{Q}_{3,1}^{(c)}(E_u, 1c) = \frac{33\sqrt{1834}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_2^{(b)}(B_{1g})}{3668} + \frac{17\sqrt{27510}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_2^{(b)}(B_{1g})}{11004} - \frac{2\sqrt{1834}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{917} - \frac{17\sqrt{27510}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{5502} + \frac{2\sqrt{27510}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2751}$$

$$\begin{aligned}
\boxed{\text{z230}} \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{z231}} \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{z232}} \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{z233}} \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{z250}} \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{z251}} \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{z252}} \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{z253}} \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{z254}} \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{z255}} \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{z256}} \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{z277}} \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{z278}} \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{z279}} \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}
\end{aligned}$$

$$\boxed{\text{z280}} \quad \mathbb{G}_2^{(c)}(A_{1u}, a) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} - \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z281}} \quad \mathbb{G}_2^{(c)}(A_{1u}, b) = -\frac{\sqrt{7}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_{2,1}^{(b)}(E_g)}{28} - \frac{5\sqrt{105}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{2,1}^{(b)}(E_g)}{84} + \frac{\sqrt{7}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_{2,2}^{(b)}(E_g)}{28} + \frac{5\sqrt{105}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{2,2}^{(b)}(E_g)}{84} - \frac{\sqrt{105}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_2^{(b)}(B_{1g})}{21}$$

$$\boxed{\text{z282}} \quad \mathbb{G}_2^{(c)}(A_{1u}, c) = \mathbb{G}_2^{(a)}(A_{1u})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z283}} \quad \mathbb{G}_2^{(c)}(A_{1u}, d) = \frac{\sqrt{6}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{6} - \frac{\sqrt{6}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{6} - \frac{\sqrt{6}\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_2^{(b)}(B_{1g})}{3}$$

$$\boxed{\text{z284}} \quad \mathbb{G}_4^{(c)}(A_{1u}, 1) = -\frac{\sqrt{5}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_{2,1}^{(b)}(E_g)}{4} - \frac{\sqrt{3}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{2,1}^{(b)}(E_g)}{12} + \frac{\sqrt{5}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_{2,2}^{(b)}(E_g)}{4} + \frac{\sqrt{3}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{2,2}^{(b)}(E_g)}{12} + \frac{\sqrt{3}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_2^{(b)}(B_{1g})}{3}$$

$$\boxed{\text{z321}} \quad \mathbb{G}_1^{(c)}(A_{2g}, a) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_{1,2}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_{1,1}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z322}} \quad \mathbb{G}_1^{(c)}(A_{2g}, b) = \frac{\sqrt{30}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_{1,2}^{(b)}(E_u)}{10} - \frac{\sqrt{30}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_{1,1}^{(b)}(E_u)}{10} + \frac{\sqrt{10}\mathbb{G}_2^{(a)}(A_{1u})\mathbb{Q}_1^{(b)}(A_{2u})}{5}$$

$$\boxed{\text{z323}} \quad \mathbb{G}_3^{(c)}(A_{2g}, a) = -\frac{\sqrt{3}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_{1,2}^{(b)}(E_u)}{4} - \frac{\sqrt{5}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{1,2}^{(b)}(E_u)}{4} + \frac{\sqrt{3}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_{1,1}^{(b)}(E_u)}{4} + \frac{\sqrt{5}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{1,1}^{(b)}(E_u)}{4}$$

$$\boxed{\text{z324}} \quad \mathbb{G}_3^{(c)}(A_{2g}, b) = -\frac{\sqrt{5}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_{1,2}^{(b)}(E_u)}{5} + \frac{\sqrt{5}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_{1,1}^{(b)}(E_u)}{5} + \frac{\sqrt{15}\mathbb{G}_2^{(a)}(A_{1u})\mathbb{Q}_1^{(b)}(A_{2u})}{5}$$

$$\boxed{\text{z325}} \quad \mathbb{G}_3^{(c)}(B_{1g}, a) = -\frac{\sqrt{3}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{1,1}^{(b)}(E_u)}{3} + \frac{\sqrt{3}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{1,2}^{(b)}(E_u)}{3} - \frac{\sqrt{3}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_1^{(b)}(A_{2u})}{3}$$

$$\boxed{\text{z326}} \quad \mathbb{G}_3^{(c)}(B_{1g}, b) = \frac{\sqrt{3}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_{1,1}^{(b)}(E_u)}{3} - \frac{\sqrt{3}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_{1,2}^{(b)}(E_u)}{3} + \frac{\sqrt{3}\mathbb{G}_2^{(a)}(B_{2u})\mathbb{Q}_1^{(b)}(A_{2u})}{3}$$

$$\boxed{\text{z327}} \quad \mathbb{G}_2^{(c)}(B_{1u}, a) = \mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_0^{(b)}(A_{1g})$$

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

$$\boxed{\text{z329}} \quad \mathbb{G}_3^{(c)}(B_{2g}, a) = \frac{\sqrt{5}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_{1,2}^{(b)}(E_u)}{4} + \frac{\sqrt{3}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{1,2}^{(b)}(E_u)}{12} + \frac{\sqrt{5}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_{1,1}^{(b)}(E_u)}{4} + \frac{\sqrt{3}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{1,1}^{(b)}(E_u)}{12} + \frac{\sqrt{3}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_1^{(b)}(A_{2u})}{3}$$

$$\boxed{\text{z330}} \quad \mathbb{G}_3^{(c)}(B_{2g}, b) = -\frac{\sqrt{3}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_{1,2}^{(b)}(E_u)}{3} - \frac{\sqrt{3}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_{1,1}^{(b)}(E_u)}{3} + \frac{\sqrt{3}\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_1^{(b)}(A_{2u})}{3}$$

$$\boxed{\text{z331}} \quad \mathbb{G}_2^{(c)}(B_{2u}, a) = -\frac{\sqrt{6}\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{6} + \frac{\sqrt{6}\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{6} + \frac{\sqrt{6}\mathbb{Q}_1^{(a)}(A_{2u})\mathbb{Q}_2^{(b)}(B_{1g})}{3}$$

$$\boxed{\text{z332}} \quad \mathbb{G}_2^{(c)}(B_{2u}, b) = -\frac{3\sqrt{21}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_{2,2}^{(b)}(E_g)}{28} + \frac{\sqrt{35}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{2,2}^{(b)}(E_g)}{28} + \frac{3\sqrt{21}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_{2,1}^{(b)}(E_g)}{28} - \frac{\sqrt{35}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{2,1}^{(b)}(E_g)}{28} - \frac{\sqrt{21}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_2^{(b)}(B_{1g})}{7}$$

$$\boxed{\text{z333}} \quad \mathbb{G}_2^{(c)}(B_{2u}, c) = \mathbb{G}_2^{(a)}(B_{2u})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z334}} \quad \mathbb{G}_2^{(c)}(B_{2u}, d) = \frac{\sqrt{2}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2} - \frac{\sqrt{2}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z335}} \quad \mathbb{G}_{1,1}^{(c)}(E_g, a) = \frac{\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_1^{(b)}(A_{2u})}{2} - \frac{\mathbb{Q}_1^{(a)}(A_{2u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z336}} \quad \mathbb{G}_{1,2}^{(c)}(E_g, a) = \frac{\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_1^{(b)}(A_{2u})}{2} - \frac{\mathbb{Q}_1^{(a)}(A_{2u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z337}} \quad \mathbb{G}_{1,1}^{(c)}(E_g, b) = -\frac{\sqrt{15}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_1^{(b)}(A_{2u})}{10} - \frac{\sqrt{5}\mathbb{G}_2^{(a)}(A_{1u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{10} + \frac{\sqrt{15}\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{10} + \frac{\sqrt{15}\mathbb{G}_2^{(a)}(B_{2u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{10}$$

$$\boxed{\text{z338}} \quad \mathbb{G}_{1,2}^{(c)}(E_g, b) = -\frac{\sqrt{15}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_1^{(b)}(A_{2u})}{10} + \frac{\sqrt{5}\mathbb{G}_2^{(a)}(A_{1u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{10} + \frac{\sqrt{15}\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{10} - \frac{\sqrt{15}\mathbb{G}_2^{(a)}(B_{2u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{10}$$

$$\boxed{\text{z339}} \quad \mathbb{G}_{3,1}^{(c)}(E_g, 1a) = -\frac{\sqrt{6}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_1^{(b)}(A_{2u})}{8} + \frac{\sqrt{10}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_1^{(b)}(A_{2u})}{8} + \frac{\sqrt{6}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{8} - \frac{\sqrt{10}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{8}$$

$$\boxed{\text{z340}} \quad \mathbb{G}_{3,2}^{(c)}(E_g, 1a) = -\frac{\sqrt{6}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_1^{(b)}(A_{2u})}{8} + \frac{\sqrt{10}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_1^{(b)}(A_{2u})}{8} + \frac{\sqrt{6}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{8} + \frac{\sqrt{10}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{8}$$

$$\boxed{\text{z341}} \quad \mathbb{G}_{3,1}^{(c)}(E_g, 1b) = \frac{\sqrt{10}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_1^{(b)}(A_{2u})}{10} - \frac{\sqrt{30}\mathbb{G}_2^{(a)}(A_{1u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{20} + \frac{3\sqrt{10}\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{20} - \frac{\sqrt{10}\mathbb{G}_2^{(a)}(B_{2u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{10}$$

$$\boxed{\text{z342}} \quad \mathbb{G}_{3,2}^{(c)}(E_g, 1b) = \frac{\sqrt{10}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_1^{(b)}(A_{2u})}{10} + \frac{\sqrt{30}\mathbb{G}_2^{(a)}(A_{1u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{20} + \frac{3\sqrt{10}\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{20} + \frac{\sqrt{10}\mathbb{G}_2^{(a)}(B_{2u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{10}$$

$$\boxed{\text{z343}} \quad \mathbb{G}_{3,1}^{(c)}(E_g, 2a) = \frac{\sqrt{10}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_1^{(b)}(A_{2u})}{8} - \frac{\sqrt{6}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_1^{(b)}(A_{2u})}{24} + \frac{\sqrt{10}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{8} + \frac{\sqrt{6}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{6} - \frac{\sqrt{6}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{24}$$

$$\boxed{\text{z344}} \quad \mathbb{G}_{3,2}^{(c)}(E_g, 2a) = \frac{\sqrt{10}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_1^{(b)}(A_{2u})}{8} - \frac{\sqrt{6}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_1^{(b)}(A_{2u})}{24} + \frac{\sqrt{10}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{8} + \frac{\sqrt{6}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{6} + \frac{\sqrt{6}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{24}$$

$$\boxed{\text{z345}} \quad \mathbb{G}_{3,1}^{(c)}(E_g, 2b) = \frac{\sqrt{6}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_1^{(b)}(A_{2u})}{6} - \frac{\sqrt{2}\mathbb{G}_2^{(a)}(A_{1u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{4} - \frac{\sqrt{6}\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{12} + \frac{\sqrt{6}\mathbb{G}_2^{(a)}(B_{2u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{6}$$

$$\boxed{\text{z346}} \quad \mathbb{G}_{3,2}^{(c)}(E_g, 2b) = \frac{\sqrt{6}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_1^{(b)}(A_{2u})}{6} + \frac{\sqrt{2}\mathbb{G}_2^{(a)}(A_{1u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{4} - \frac{\sqrt{6}\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{12} - \frac{\sqrt{6}\mathbb{G}_2^{(a)}(B_{2u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{6}$$

$$\boxed{\text{z347}} \quad \mathbb{G}_{2,1}^{(c)}(E_u, a) = \frac{\sqrt{2}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z348}} \quad \mathbb{G}_{2,2}^{(c)}(E_u, a) = \frac{\sqrt{2}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z349}} \quad \mathbb{G}_{2,1}^{(c)}(E_u, b) = -\frac{\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_2^{(b)}(B_{1g})}{2} - \frac{\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z350}} \quad \mathbb{G}_{2,2}^{(c)}(E_u, b) = \frac{\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_2^{(b)}(B_{1g})}{2} - \frac{\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$$

- 'Pt2'-'Si1' bond-cluster

* 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

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

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

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

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

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

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

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

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

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

$$\boxed{\text{z47}} \quad \mathbb{Q}_4^{(c)}(A_{2g}, a) = \frac{\sqrt{5}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_{1,2}^{(b)}(E_u)}{4} - \frac{\sqrt{3}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{1,2}^{(b)}(E_u)}{4} - \frac{\sqrt{5}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_{1,1}^{(b)}(E_u)}{4} + \frac{\sqrt{3}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{1,1}^{(b)}(E_u)}{4}$$

$$\boxed{\text{z48}} \quad \mathbb{Q}_4^{(c)}(A_{2g}, b) = \mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_3^{(b)}(B_{2u})$$

$$\boxed{\text{z49}} \quad \mathbb{Q}_4^{(c)}(A_{2g}, c) = -\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_3^{(b)}(B_{2u})$$

$$\boxed{\text{z50}} \quad \mathbb{Q}_1^{(c)}(A_{2u}, a) = \mathbb{Q}_1^{(a)}(A_{2u})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z51}} \quad \mathbb{Q}_1^{(c)}(A_{2u}, b) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2} + \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z52}} \quad \mathbb{Q}_1^{(c)}(A_{2u}, c) = -\frac{\sqrt{7}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_{2,2}^{(b)}(E_g)}{7} - \frac{\sqrt{105}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{2,2}^{(b)}(E_g)}{21} - \frac{\sqrt{7}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_{2,1}^{(b)}(E_g)}{7} - \frac{\sqrt{105}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{2,1}^{(b)}(E_g)}{21} + \frac{\sqrt{105}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_2^{(b)}(B_{1g})}{21}$$

$$\boxed{\text{z71}} \quad \mathbb{Q}_1^{(c)}(A_{2u}, d) = -\frac{\sqrt{6}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{6} - \frac{\sqrt{6}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{6} - \frac{\sqrt{6}\mathbb{G}_2^{(a)}(B_{2u})\mathbb{Q}_2^{(b)}(B_{1g})}{3}$$

$$\boxed{\text{z72}} \quad \mathbb{Q}_3^{(c)}(A_{2u}, a) = \mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z73}} \quad \mathbb{Q}_3^{(c)}(A_{2u}, b) = -\frac{\sqrt{35}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_{2,2}^{(b)}(E_g)}{28} - \frac{5\sqrt{21}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{2,2}^{(b)}(E_g)}{84} - \frac{\sqrt{35}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_{2,1}^{(b)}(E_g)}{28} - \frac{5\sqrt{21}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{2,1}^{(b)}(E_g)}{84} - \frac{4\sqrt{21}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_2^{(b)}(B_{1g})}{21}$$

$$\boxed{\text{z74}} \quad \mathbb{Q}_3^{(c)}(A_{2u}, c) = -\frac{\sqrt{3}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{3} - \frac{\sqrt{3}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{3} + \frac{\sqrt{3}\mathbb{G}_2^{(a)}(B_{2u})\mathbb{Q}_2^{(b)}(B_{1g})}{3}$$

$$\boxed{\text{z75}} \quad \mathbb{Q}_5^{(c)}(A_{2u}, 2) = \frac{\sqrt{5}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_{2,2}^{(b)}(E_g)}{4} - \frac{\sqrt{3}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{2,2}^{(b)}(E_g)}{4} + \frac{\sqrt{5}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_{2,1}^{(b)}(E_g)}{4} - \frac{\sqrt{3}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{2,1}^{(b)}(E_g)}{4}$$

$$\boxed{z76} \quad \mathbb{Q}_2^{(c)}(B_{1g}, a) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_{1,1}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_{1,2}^{(b)}(E_u)}{2}$$

$$\boxed{z77} \quad \mathbb{Q}_2^{(c)}(B_{1g}, b) = \mathbb{Q}_1^{(a)}(A_{2u})\mathbb{Q}_3^{(b)}(B_{2u})$$

$$\boxed{z78} \quad \mathbb{Q}_2^{(c)}(B_{1g}, c) = \frac{3\sqrt{7}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_{1,1}^{(b)}(E_u)}{14} - \frac{\sqrt{105}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{1,1}^{(b)}(E_u)}{42} - \frac{3\sqrt{7}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_{1,2}^{(b)}(E_u)}{14} + \frac{\sqrt{105}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{1,2}^{(b)}(E_u)}{42} + \frac{\sqrt{105}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_1^{(b)}(A_{2u})}{21}$$

$$\boxed{z96} \quad \mathbb{Q}_2^{(c)}(B_{1g}, d) = -\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_3^{(b)}(B_{2u})$$

$$\boxed{z97} \quad \mathbb{Q}_2^{(c)}(B_{1g}, e) = -\frac{\sqrt{6}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_{1,1}^{(b)}(E_u)}{6} + \frac{\sqrt{6}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_{1,2}^{(b)}(E_u)}{6} + \frac{\sqrt{6}\mathbb{G}_2^{(a)}(B_{2u})\mathbb{Q}_1^{(b)}(A_{2u})}{3}$$

$$\boxed{z98} \quad \mathbb{Q}_4^{(c)}(B_{1g}) = \frac{\sqrt{35}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_{1,1}^{(b)}(E_u)}{14} + \frac{\sqrt{21}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{1,1}^{(b)}(E_u)}{14} - \frac{\sqrt{35}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_{1,2}^{(b)}(E_u)}{14} - \frac{\sqrt{21}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{1,2}^{(b)}(E_u)}{14} - \frac{\sqrt{21}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_1^{(b)}(A_{2u})}{7}$$

$$\boxed{z99} \quad \mathbb{Q}_3^{(c)}(B_{1u}, a) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} + \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$$

$$\boxed{z100} \quad \mathbb{Q}_3^{(c)}(B_{1u}, b) = \mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{z101} \quad \mathbb{Q}_3^{(c)}(B_{1u}, c) = -\frac{\sqrt{2}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} - \frac{\sqrt{2}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$$

$$\boxed{z102} \quad \mathbb{Q}_3^{(c)}(B_{1u}, d) = \mathbb{G}_2^{(a)}(A_{1u})\mathbb{Q}_2^{(b)}(B_{1g})$$

$$\boxed{z161} \quad \mathbb{Q}_5^{(c)}(B_{1u}) = \frac{\sqrt{2}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} + \frac{\sqrt{2}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$$

$$\boxed{z162} \quad \mathbb{Q}_2^{(c)}(B_{2g}, a) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_{1,2}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_{1,1}^{(b)}(E_u)}{2}$$

$$\boxed{z163} \quad \mathbb{Q}_2^{(c)}(B_{2g}, b) = -\frac{\sqrt{7}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_{1,2}^{(b)}(E_u)}{7} + \frac{\sqrt{105}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{1,2}^{(b)}(E_u)}{21} - \frac{\sqrt{7}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_{1,1}^{(b)}(E_u)}{7} + \frac{\sqrt{105}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{1,1}^{(b)}(E_u)}{21} + \frac{\sqrt{105}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_1^{(b)}(A_{2u})}{21}$$

$$\boxed{z164} \quad \mathbb{Q}_2^{(c)}(B_{2g}, c) = -\frac{\sqrt{6}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_{1,2}^{(b)}(E_u)}{6} - \frac{\sqrt{6}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_{1,1}^{(b)}(E_u)}{6} - \frac{\sqrt{6}\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_1^{(b)}(A_{2u})}{3}$$

$$\boxed{z165} \quad \mathbb{Q}_2^{(c)}(B_{2g}, d) = \mathbb{G}_2^{(a)}(A_{1u})\mathbb{Q}_3^{(b)}(B_{2u})$$

$$\boxed{\text{z166}} \quad \mathbb{Q}_4^{(c)}(B_{2g}) = -\frac{\sqrt{35}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_{1,2}^{(b)}(E_u)}{28} - \frac{3\sqrt{21}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{1,2}^{(b)}(E_u)}{28} - \frac{\sqrt{35}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_{1,1}^{(b)}(E_u)}{28} - \frac{3\sqrt{21}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{1,1}^{(b)}(E_u)}{28} + \frac{\sqrt{21}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_1^{(b)}(A_{2u})}{7}$$

$$\boxed{\text{z167}} \quad \mathbb{Q}_3^{(c)}(B_{2u}, a) = \frac{\sqrt{3}\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{3} - \frac{\sqrt{3}\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{3} + \frac{\sqrt{3}\mathbb{Q}_1^{(a)}(A_{2u})\mathbb{Q}_2^{(b)}(B_{1g})}{3}$$

$$\boxed{\text{z168}} \quad \mathbb{Q}_3^{(c)}(B_{2u}, b) = \mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z169}} \quad \mathbb{Q}_3^{(c)}(B_{2u}, c) = \frac{\sqrt{3}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_{2,2}^{(b)}(E_g)}{12} - \frac{\sqrt{5}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{2,2}^{(b)}(E_g)}{4} - \frac{\sqrt{3}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_{2,1}^{(b)}(E_g)}{12} + \frac{\sqrt{5}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{2,1}^{(b)}(E_g)}{4} - \frac{\sqrt{3}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_2^{(b)}(B_{1g})}{3}$$

$$\boxed{\text{z170}} \quad \mathbb{Q}_5^{(c)}(B_{2u}) = -\frac{\sqrt{105}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_{2,2}^{(b)}(E_g)}{21} - \frac{\sqrt{7}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{2,2}^{(b)}(E_g)}{7} + \frac{\sqrt{105}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_{2,1}^{(b)}(E_g)}{21} + \frac{\sqrt{7}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{2,1}^{(b)}(E_g)}{7} + \frac{\sqrt{105}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_2^{(b)}(B_{1g})}{21}$$

$$\boxed{\text{z171}} \quad \mathbb{Q}_{2,1}^{(c)}(E_g, a) = \frac{\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_1^{(b)}(A_{2u})}{2} + \frac{\mathbb{Q}_1^{(a)}(A_{2u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z172}} \quad \mathbb{Q}_{2,2}^{(c)}(E_g, a) = \frac{\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_1^{(b)}(A_{2u})}{2} + \frac{\mathbb{Q}_1^{(a)}(A_{2u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z173}} \quad \mathbb{Q}_{2,1}^{(c)}(E_g, b) = -\frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_3^{(b)}(B_{2u})}{2}$$

$$\boxed{\text{z174}} \quad \mathbb{Q}_{2,2}^{(c)}(E_g, b) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_3^{(b)}(B_{2u})}{2}$$

$$\boxed{\text{z175}} \quad \mathbb{Q}_{2,1}^{(c)}(E_g, c) = -\frac{\sqrt{14}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_1^{(b)}(A_{2u})}{14} - \frac{\sqrt{210}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_1^{(b)}(A_{2u})}{42} - \frac{\sqrt{14}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{14} + \frac{\sqrt{210}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{42} - \frac{\sqrt{210}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{42}$$

$$\boxed{\text{z176}} \quad \mathbb{Q}_{2,2}^{(c)}(E_g, c) = -\frac{\sqrt{14}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_1^{(b)}(A_{2u})}{14} - \frac{\sqrt{210}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_1^{(b)}(A_{2u})}{42} - \frac{\sqrt{14}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{14} + \frac{\sqrt{210}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{42} + \frac{\sqrt{210}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{42}$$

$$\boxed{\text{z177}} \quad \mathbb{Q}_{2,1}^{(c)}(E_g, d) = -\frac{\sqrt{2}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_3^{(b)}(B_{2u})}{8} + \frac{\sqrt{30}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_3^{(b)}(B_{2u})}{8}$$

$$\boxed{\text{z178}} \quad \mathbb{Q}_{2,2}^{(c)}(E_g, d) = \frac{\sqrt{2}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_3^{(b)}(B_{2u})}{8} - \frac{\sqrt{30}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_3^{(b)}(B_{2u})}{8}$$

$$\boxed{\text{z179}} \quad \mathbb{Q}_{2,1}^{(c)}(E_g, e) = \frac{\sqrt{3}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_1^{(b)}(A_{2u})}{6} + \frac{\mathbb{G}_2^{(a)}(A_{1u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{2} + \frac{\sqrt{3}\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{6} + \frac{\sqrt{3}\mathbb{G}_2^{(a)}(B_{2u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{6}$$

$$\boxed{\text{z180}} \quad \mathbb{Q}_{2,2}^{(c)}(E_g, e) = \frac{\sqrt{3}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_1^{(b)}(A_{2u})}{6} - \frac{\mathbb{G}_2^{(a)}(A_{1u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{2} + \frac{\sqrt{3}\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{6} - \frac{\sqrt{3}\mathbb{G}_2^{(a)}(B_{2u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{6}$$

$$\boxed{\text{z181}} \quad \mathbb{Q}_{4,1}^{(c)}(E_g, 1a) = \frac{\sqrt{10}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_1^{(b)}(A_{2u})}{8} + \frac{\sqrt{6}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_1^{(b)}(A_{2u})}{8} - \frac{\sqrt{10}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{8} - \frac{\sqrt{6}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{8}$$

$$\boxed{\text{z182}} \quad \mathbb{Q}_{4,2}^{(c)}(E_g, 1a) = \frac{\sqrt{10}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_1^{(b)}(A_{2u})}{8} + \frac{\sqrt{6}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_1^{(b)}(A_{2u})}{8} - \frac{\sqrt{10}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{8} + \frac{\sqrt{6}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{8}$$

$$\boxed{\text{z183}} \quad \mathbb{Q}_{4,1}^{(c)}(E_g, 1b) = -\frac{\sqrt{30}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_3^{(b)}(B_{2u})}{8} - \frac{\sqrt{2}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_3^{(b)}(B_{2u})}{8}$$

$$\boxed{\text{z184}} \quad \mathbb{Q}_{4,2}^{(c)}(E_g, 1b) = \frac{\sqrt{30}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_3^{(b)}(B_{2u})}{8} + \frac{\sqrt{2}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_3^{(b)}(B_{2u})}{8}$$

$$\boxed{\text{z185}} \quad \mathbb{Q}_{4,1}^{(c)}(E_g, 1c) = -\frac{\sqrt{2}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_3^{(b)}(B_{2u})}{2}$$

$$\boxed{\text{z186}} \quad \mathbb{Q}_{4,2}^{(c)}(E_g, 1c) = \frac{\sqrt{2}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_3^{(b)}(B_{2u})}{2}$$

$$\boxed{\text{z187}} \quad \mathbb{Q}_{4,1}^{(c)}(E_g, 2) = -\frac{\sqrt{70}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_1^{(b)}(A_{2u})}{56} + \frac{3\sqrt{42}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_1^{(b)}(A_{2u})}{56} - \frac{\sqrt{70}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{56} + \frac{\sqrt{42}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{14} + \frac{3\sqrt{42}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{56}$$

$$\boxed{\text{z188}} \quad \mathbb{Q}_{4,2}^{(c)}(E_g, 2) = -\frac{\sqrt{70}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_1^{(b)}(A_{2u})}{56} + \frac{3\sqrt{42}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_1^{(b)}(A_{2u})}{56} - \frac{\sqrt{70}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{56} + \frac{\sqrt{42}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{14} - \frac{3\sqrt{42}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{56}$$

$$\boxed{\text{z189}} \quad \mathbb{Q}_{1,1}^{(c)}(E_u, a) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z190}} \quad \mathbb{Q}_{1,2}^{(c)}(E_u, a) = \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z204}} \quad \mathbb{Q}_{1,1}^{(c)}(E_u, b) = \frac{\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_2^{(b)}(B_{1g})}{2} + \frac{\mathbb{Q}_1^{(a)}(A_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z205}} \quad \mathbb{Q}_{1,2}^{(c)}(E_u, b) = -\frac{\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_2^{(b)}(B_{1g})}{2} + \frac{\mathbb{Q}_1^{(a)}(A_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z206}} \quad \mathbb{Q}_{1,1}^{(c)}(E_u, c) = \frac{3\sqrt{14}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_2^{(b)}(B_{1g})}{28} - \frac{\sqrt{210}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_2^{(b)}(B_{1g})}{84} - \frac{\sqrt{14}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{14} + \frac{\sqrt{210}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{42} + \frac{\sqrt{210}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{42}$$

$$\boxed{\text{z207}} \quad \mathbb{Q}_{1,2}^{(c)}(E_u, c) = -\frac{3\sqrt{14}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_2^{(b)}(B_{1g})}{28} + \frac{\sqrt{210}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_2^{(b)}(B_{1g})}{84} - \frac{\sqrt{14}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{14} + \frac{\sqrt{210}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{42} - \frac{\sqrt{210}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{42}$$

$$\boxed{\text{z208}} \quad \mathbb{Q}_{1,1}^{(c)}(E_u, d) = \frac{\sqrt{3}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_2^{(b)}(B_{1g})}{6} - \frac{\mathbb{G}_2^{(a)}(A_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} - \frac{\sqrt{3}\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{6} + \frac{\sqrt{3}\mathbb{G}_2^{(a)}(B_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{6}$$

$$\boxed{\text{z209}} \quad \mathbb{Q}_{1,2}^{(c)}(E_u, d) = -\frac{\sqrt{3}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_2^{(b)}(B_{1g})}{6} + \frac{\mathbb{G}_2^{(a)}(A_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2} - \frac{\sqrt{3}\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{6} - \frac{\sqrt{3}\mathbb{G}_2^{(a)}(B_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{6}$$

$$\boxed{\text{z210}} \quad \mathbb{Q}_{3,1}^{(c)}(E_u, 1a) = \frac{\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_2^{(b)}(B_{1g})}{2} - \frac{\mathbb{Q}_1^{(a)}(A_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z234}} \quad \mathbb{Q}_{3,2}^{(c)}(E_u, 1a) = -\frac{\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_2^{(b)}(B_{1g})}{2} - \frac{\mathbb{Q}_1^{(a)}(A_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z235}} \quad \mathbb{Q}_{3,1}^{(c)}(E_u, 1b) = \frac{\sqrt{2}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z236}} \quad \mathbb{Q}_{3,2}^{(c)}(E_u, 1b) = \frac{\sqrt{2}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z237}} \quad \mathbb{Q}_{3,1}^{(c)}(E_u, 1c) = \frac{33\sqrt{1834}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_2^{(b)}(B_{1g})}{3668} + \frac{17\sqrt{27510}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_2^{(b)}(B_{1g})}{11004} - \frac{2\sqrt{1834}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{917} - \frac{17\sqrt{27510}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{5502} + \frac{2\sqrt{27510}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2751}$$

$$\boxed{\text{z238}} \quad \mathbb{Q}_{3,2}^{(c)}(E_u, 1c) = -\frac{33\sqrt{1834}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_2^{(b)}(B_{1g})}{3668} - \frac{17\sqrt{27510}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_2^{(b)}(B_{1g})}{11004} - \frac{2\sqrt{1834}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{917} - \frac{17\sqrt{27510}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{5502} - \frac{2\sqrt{27510}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2751}$$

$$\boxed{\text{z239}} \quad \mathbb{Q}_{3,1}^{(c)}(E_u, 1d) = -\frac{\sqrt{15}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_2^{(b)}(B_{1g})}{30} + \frac{\sqrt{5}\mathbb{G}_2^{(a)}(A_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{10} + \frac{\sqrt{15}\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{30} + \frac{\sqrt{15}\mathbb{G}_2^{(a)}(B_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{6}$$

$$\boxed{\text{z240}} \quad \mathbb{Q}_{3,2}^{(c)}(E_u, 1d) = \frac{\sqrt{15}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_2^{(b)}(B_{1g})}{30} - \frac{\sqrt{5}\mathbb{G}_2^{(a)}(A_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{10} + \frac{\sqrt{15}\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{30} - \frac{\sqrt{15}\mathbb{G}_2^{(a)}(B_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{6}$$

$$\boxed{\text{z241}} \quad \mathbb{Q}_{3,1}^{(c)}(E_u, 2a) = \frac{\sqrt{2}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z257}} \quad \mathbb{Q}_{3,2}^{(c)}(E_u, 2a) = \frac{\sqrt{2}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z258}} \quad \mathbb{Q}_{3,1}^{(c)}(E_u, 2b) = \frac{25\sqrt{655}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_2^{(b)}(B_{1g})}{2096} - \frac{5\sqrt{393}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_2^{(b)}(B_{1g})}{2096} - \frac{7\sqrt{655}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{1048} + \frac{5\sqrt{393}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{1048} - \frac{4\sqrt{393}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{131}$$

$$\boxed{\text{z259}} \quad \mathbb{Q}_{3,2}^{(c)}(E_u, 2b) = -\frac{25\sqrt{655}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_2^{(b)}(B_{1g})}{2096} + \frac{5\sqrt{393}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_2^{(b)}(B_{1g})}{2096} - \frac{7\sqrt{655}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{1048} + \frac{5\sqrt{393}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{1048} + \frac{4\sqrt{393}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{131}$$

$$\boxed{\text{z260}} \quad \mathbb{Q}_{3,1}^{(c)}(E_u, 2c) = \frac{\sqrt{15}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_2^{(b)}(B_{1g})}{10} + \frac{\sqrt{5}\mathbb{G}_2^{(a)}(A_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{5} - \frac{\sqrt{15}\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{10}$$

$$\boxed{\text{z261}} \quad \mathbb{Q}_{3,2}^{(c)}(E_u, 2c) = -\frac{\sqrt{15}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_2^{(b)}(B_{1g})}{10} - \frac{\sqrt{5}\mathbb{G}_2^{(a)}(A_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{5} - \frac{\sqrt{15}\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{10}$$

$$\boxed{\text{z262}} \quad \mathbb{Q}_{5,1}^{(c)}(E_u, 1) = \frac{5\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_2^{(b)}(B_{1g})}{16} - \frac{\sqrt{15}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_2^{(b)}(B_{1g})}{80} + \frac{5\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{8} + \frac{\sqrt{15}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{40}$$

$$\boxed{\text{z263}} \quad \mathbb{Q}_{5,2}^{(c)}(E_u, 1) = -\frac{5\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_2^{(b)}(B_{1g})}{16} + \frac{\sqrt{15}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_2^{(b)}(B_{1g})}{80} + \frac{5\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{8} + \frac{\sqrt{15}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{40}$$

$$\boxed{\text{z285}} \quad \mathbb{Q}_{5,1}^{(c)}(E_u, 2) = -\frac{\sqrt{10}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_2^{(b)}(B_{1g})}{5} - \frac{\sqrt{10}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{10}$$

$$\boxed{\text{z286}} \quad \mathbb{Q}_{5,2}^{(c)}(E_u, 2) = \frac{\sqrt{10}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_2^{(b)}(B_{1g})}{5} - \frac{\sqrt{10}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{10}$$

$$\boxed{\text{z287}} \quad \mathbb{G}_0^{(c)}(A_{1u}) = \frac{\sqrt{3}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{3} - \frac{\sqrt{3}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{3} + \frac{\sqrt{3}\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_2^{(b)}(B_{1g})}{3}$$

$$\boxed{\text{z288}} \quad \mathbb{G}_2^{(c)}(A_{1u}, a) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} - \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z289}} \quad \mathbb{G}_2^{(c)}(A_{1u}, b) = -\frac{\sqrt{7}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_{2,1}^{(b)}(E_g)}{28} - \frac{5\sqrt{105}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{2,1}^{(b)}(E_g)}{84} + \frac{\sqrt{7}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_{2,2}^{(b)}(E_g)}{28} + \frac{5\sqrt{105}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{2,2}^{(b)}(E_g)}{84} - \frac{\sqrt{105}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_2^{(b)}(B_{1g})}{21}$$

$$\boxed{\text{z290}} \quad \mathbb{G}_2^{(c)}(A_{1u}, c) = \mathbb{G}_2^{(a)}(A_{1u})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z291}} \quad \mathbb{G}_2^{(c)}(A_{1u}, d) = \frac{\sqrt{6}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{6} - \frac{\sqrt{6}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{6} - \frac{\sqrt{6}\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_2^{(b)}(B_{1g})}{3}$$

$$\boxed{\text{z292}} \quad \mathbb{G}_4^{(c)}(A_{1u}, 1) = -\frac{\sqrt{5}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_{2,1}^{(b)}(E_g)}{4} - \frac{\sqrt{3}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{2,1}^{(b)}(E_g)}{12} + \frac{\sqrt{5}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_{2,2}^{(b)}(E_g)}{4} + \frac{\sqrt{3}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{2,2}^{(b)}(E_g)}{12} + \frac{\sqrt{3}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_2^{(b)}(B_{1g})}{3}$$

$$\boxed{\text{z351}} \quad \mathbb{G}_1^{(c)}(A_{2g}, a) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_{1,2}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_{1,1}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z352}} \quad \mathbb{G}_1^{(c)}(A_{2g}, b) = \frac{\sqrt{30}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_{1,2}^{(b)}(E_u)}{10} - \frac{\sqrt{30}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_{1,1}^{(b)}(E_u)}{10} + \frac{\sqrt{10}\mathbb{G}_2^{(a)}(A_{1u})\mathbb{Q}_1^{(b)}(A_{2u})}{5}$$

$$\boxed{\text{z353}} \quad \mathbb{G}_3^{(c)}(A_{2g}, a) = -\frac{\sqrt{3}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_{1,2}^{(b)}(E_u)}{4} - \frac{\sqrt{5}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{1,2}^{(b)}(E_u)}{4} + \frac{\sqrt{3}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_{1,1}^{(b)}(E_u)}{4} + \frac{\sqrt{5}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{1,1}^{(b)}(E_u)}{4}$$

$$\boxed{\text{z354}} \quad \mathbb{G}_3^{(c)}(A_{2g}, b) = -\frac{\sqrt{5}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_{1,2}^{(b)}(E_u)}{5} + \frac{\sqrt{5}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_{1,1}^{(b)}(E_u)}{5} + \frac{\sqrt{15}\mathbb{G}_2^{(a)}(A_{1u})\mathbb{Q}_1^{(b)}(A_{2u})}{5}$$

$$\boxed{\text{z355}} \quad \mathbb{G}_3^{(c)}(B_{1g}, a) = -\frac{\sqrt{3}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{1,1}^{(b)}(E_u)}{3} + \frac{\sqrt{3}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{1,2}^{(b)}(E_u)}{3} - \frac{\sqrt{3}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_1^{(b)}(A_{2u})}{3}$$

$$\boxed{\text{z356}} \quad \mathbb{G}_3^{(c)}(B_{1g}, b) = \frac{\sqrt{3}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_{1,1}^{(b)}(E_u)}{3} - \frac{\sqrt{3}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_{1,2}^{(b)}(E_u)}{3} + \frac{\sqrt{3}\mathbb{G}_2^{(a)}(B_{2u})\mathbb{Q}_1^{(b)}(A_{2u})}{3}$$

$$\boxed{\text{z357}} \quad \mathbb{G}_2^{(c)}(B_{1u}, a) = \mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z358}} \quad \mathbb{G}_2^{(c)}(B_{1u}, b) = -\frac{\sqrt{2}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} - \frac{\sqrt{2}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z359}} \quad \mathbb{G}_3^{(c)}(B_{2g}, a) = \frac{\sqrt{5}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_{1,2}^{(b)}(E_u)}{4} + \frac{\sqrt{3}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{1,2}^{(b)}(E_u)}{12} + \frac{\sqrt{5}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_{1,1}^{(b)}(E_u)}{4} + \frac{\sqrt{3}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{1,1}^{(b)}(E_u)}{12} + \frac{\sqrt{3}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_1^{(b)}(A_{2u})}{3}$$

$$\boxed{\text{z360}} \quad \mathbb{G}_3^{(c)}(B_{2g}, b) = -\frac{\sqrt{3}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_{1,2}^{(b)}(E_u)}{3} - \frac{\sqrt{3}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_{1,1}^{(b)}(E_u)}{3} + \frac{\sqrt{3}\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_1^{(b)}(A_{2u})}{3}$$

$$\boxed{\text{z361}} \quad \mathbb{G}_2^{(c)}(B_{2u}, a) = -\frac{\sqrt{6}\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{6} + \frac{\sqrt{6}\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{6} + \frac{\sqrt{6}\mathbb{Q}_1^{(a)}(A_{2u})\mathbb{Q}_2^{(b)}(B_{1g})}{3}$$

$$\boxed{\text{z362}} \quad \mathbb{G}_2^{(c)}(B_{2u}, b) = -\frac{3\sqrt{21}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_{2,2}^{(b)}(E_g)}{28} + \frac{\sqrt{35}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{2,2}^{(b)}(E_g)}{28} + \frac{3\sqrt{21}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_{2,1}^{(b)}(E_g)}{28} - \frac{\sqrt{35}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{2,1}^{(b)}(E_g)}{28} - \frac{\sqrt{21}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_2^{(b)}(B_{1g})}{7}$$

$$\boxed{\text{z363}} \quad \mathbb{G}_2^{(c)}(B_{2u}, c) = \mathbb{G}_2^{(a)}(B_{2u})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z364}} \quad \mathbb{G}_2^{(c)}(B_{2u}, d) = \frac{\sqrt{2}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2} - \frac{\sqrt{2}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z365}} \quad \mathbb{G}_{1,1}^{(c)}(E_g, a) = \frac{\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_1^{(b)}(A_{2u})}{2} - \frac{\mathbb{Q}_1^{(a)}(A_{2u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z366}} \quad \mathbb{G}_{1,2}^{(c)}(E_g, a) = \frac{\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_1^{(b)}(A_{2u})}{2} - \frac{\mathbb{Q}_1^{(a)}(A_{2u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z367}} \quad \mathbb{G}_{1,1}^{(c)}(E_g, b) = -\frac{\sqrt{15}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_1^{(b)}(A_{2u})}{10} - \frac{\sqrt{5}\mathbb{G}_2^{(a)}(A_{1u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{10} + \frac{\sqrt{15}\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{10} + \frac{\sqrt{15}\mathbb{G}_2^{(a)}(B_{2u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{10}$$

$$\boxed{\text{z368}} \quad \mathbb{G}_{1,2}^{(c)}(E_g, b) = -\frac{\sqrt{15}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_1^{(b)}(A_{2u})}{10} + \frac{\sqrt{5}\mathbb{G}_2^{(a)}(A_{1u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{10} + \frac{\sqrt{15}\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{10} - \frac{\sqrt{15}\mathbb{G}_2^{(a)}(B_{2u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{10}$$

$$\boxed{\text{z369}} \quad \mathbb{G}_{3,1}^{(c)}(E_g, 1a) = -\frac{\sqrt{6}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_1^{(b)}(A_{2u})}{8} + \frac{\sqrt{10}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_1^{(b)}(A_{2u})}{8} + \frac{\sqrt{6}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{8} - \frac{\sqrt{10}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{8}$$

$$\boxed{\text{z370}} \quad \mathbb{G}_{3,2}^{(c)}(E_g, 1a) = -\frac{\sqrt{6}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_1^{(b)}(A_{2u})}{8} + \frac{\sqrt{10}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_1^{(b)}(A_{2u})}{8} + \frac{\sqrt{6}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{8} + \frac{\sqrt{10}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{8}$$

$$\boxed{\text{z371}} \quad \mathbb{G}_{3,1}^{(c)}(E_g, 1b) = \frac{\sqrt{10}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_1^{(b)}(A_{2u})}{10} - \frac{\sqrt{30}\mathbb{G}_2^{(a)}(A_{1u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{20} + \frac{3\sqrt{10}\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{20} - \frac{\sqrt{10}\mathbb{G}_2^{(a)}(B_{2u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{10}$$

$$\boxed{\text{z372}} \quad \mathbb{G}_{3,2}^{(c)}(E_g, 1b) = \frac{\sqrt{10}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_1^{(b)}(A_{2u})}{10} + \frac{\sqrt{30}\mathbb{G}_2^{(a)}(A_{1u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{20} + \frac{3\sqrt{10}\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{20} + \frac{\sqrt{10}\mathbb{G}_2^{(a)}(B_{2u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{10}$$

$$\boxed{\text{z373}} \quad \mathbb{G}_{3,1}^{(c)}(E_g, 2a) = \frac{\sqrt{10}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_1^{(b)}(A_{2u})}{8} - \frac{\sqrt{6}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_1^{(b)}(A_{2u})}{24} + \frac{\sqrt{10}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{8} + \frac{\sqrt{6}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{6} - \frac{\sqrt{6}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{24}$$

$$\boxed{\text{z374}} \quad \mathbb{G}_{3,2}^{(c)}(E_g, 2a) = \frac{\sqrt{10}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_1^{(b)}(A_{2u})}{8} - \frac{\sqrt{6}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_1^{(b)}(A_{2u})}{24} + \frac{\sqrt{10}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{8} + \frac{\sqrt{6}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{6} + \frac{\sqrt{6}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{24}$$

$$\boxed{\text{z375}} \quad \mathbb{G}_{3,1}^{(c)}(E_g, 2b) = \frac{\sqrt{6}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_1^{(b)}(A_{2u})}{6} - \frac{\sqrt{2}\mathbb{G}_2^{(a)}(A_{1u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{4} - \frac{\sqrt{6}\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{12} + \frac{\sqrt{6}\mathbb{G}_2^{(a)}(B_{2u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{6}$$

$$\boxed{\text{z376}} \quad \mathbb{G}_{3,2}^{(c)}(E_g, 2b) = \frac{\sqrt{6}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_1^{(b)}(A_{2u})}{6} + \frac{\sqrt{2}\mathbb{G}_2^{(a)}(A_{1u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{4} - \frac{\sqrt{6}\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{12} - \frac{\sqrt{6}\mathbb{G}_2^{(a)}(B_{2u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{6}$$

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

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

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

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

Atomic SAMB

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

$$\boxed{x84} \quad \mathbb{Q}_1^{(a)}(A_{2u}) = \begin{bmatrix} 0 & 0 & \frac{\sqrt{5}}{5} \\ 0 & 0 & 0 \\ 0 & \frac{\sqrt{15}}{10} & 0 \\ \frac{\sqrt{15}}{10} & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{x85} \quad \mathbb{Q}_3^{(a)}(A_{2u}) = \begin{bmatrix} 0 & 0 & \frac{\sqrt{30}}{10} \\ 0 & 0 & 0 \\ 0 & -\frac{\sqrt{10}}{10} & 0 \\ -\frac{\sqrt{10}}{10} & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{x86} \quad \mathbb{Q}_3^{(a)}(B_{1u}) = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ \frac{\sqrt{6}}{6} & 0 & 0 \\ 0 & \frac{\sqrt{6}}{6} & 0 \\ 0 & 0 & \frac{\sqrt{6}}{6} \end{bmatrix}$$

$$\boxed{x87} \quad \mathbb{Q}_3^{(a)}(B_{2u}) = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{6}}{6} \\ 0 & -\frac{\sqrt{6}}{6} & 0 \\ \frac{\sqrt{6}}{6} & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{x88} \quad \mathbb{Q}_{1,1}^{(a)}(E_u) = \begin{bmatrix} -\frac{\sqrt{5}}{10} & 0 & 0 \\ \frac{\sqrt{15}}{10} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{15}}{10} \\ 0 & \frac{\sqrt{15}}{10} & 0 \end{bmatrix}$$

$$\boxed{x89} \quad \mathbb{Q}_{1,2}^{(a)}(E_u) = \begin{bmatrix} 0 & -\frac{\sqrt{5}}{10} & 0 \\ 0 & -\frac{\sqrt{15}}{10} & 0 \\ 0 & 0 & \frac{\sqrt{15}}{10} \\ 0 & 0 & 0 \\ \frac{\sqrt{15}}{10} & 0 & 0 \end{bmatrix}$$

$$\boxed{x90} \quad \mathbb{Q}_{3,1}^{(a)}(E_u, 1) = \begin{bmatrix} -\frac{\sqrt{30}}{20} & 0 & 0 \\ \frac{3\sqrt{10}}{20} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{10}}{10} \\ 0 & -\frac{\sqrt{10}}{10} & 0 \end{bmatrix}$$

$$\boxed{x91} \quad \mathbb{Q}_{3,2}^{(a)}(E_u, 1) = \begin{bmatrix} 0 & -\frac{\sqrt{30}}{20} & 0 \\ 0 & -\frac{3\sqrt{10}}{20} & 0 \\ 0 & 0 & -\frac{\sqrt{10}}{10} \\ 0 & 0 & 0 \\ -\frac{\sqrt{10}}{10} & 0 & 0 \end{bmatrix}$$

$$\boxed{x92} \quad \mathbb{Q}_{3,1}^{(a)}(E_u, 2) = \begin{bmatrix} -\frac{\sqrt{2}}{4} & 0 & 0 \\ -\frac{\sqrt{6}}{12} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{6}}{6} \\ 0 & \frac{\sqrt{6}}{6} & 0 \end{bmatrix}$$

$$\boxed{x93} \quad \mathbb{Q}_{3,2}^{(a)}(E_u, 2) = \begin{bmatrix} 0 & -\frac{\sqrt{2}}{4} & 0 \\ 0 & \frac{\sqrt{6}}{12} & 0 \\ 0 & 0 & -\frac{\sqrt{6}}{6} \\ 0 & 0 & 0 \\ \frac{\sqrt{6}}{6} & 0 & 0 \end{bmatrix}$$

$$\boxed{x94} \quad \mathbb{G}_2^{(a)}(A_{1u}) = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ \frac{1}{2} & 0 & 0 \\ 0 & -\frac{1}{2} & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{x95} \quad \mathbb{G}_2^{(a)}(B_{1u}) = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ \frac{\sqrt{3}}{6} & 0 & 0 \\ 0 & \frac{\sqrt{3}}{6} & 0 \\ 0 & 0 & -\frac{\sqrt{3}}{3} \end{bmatrix}$$

$$\boxed{x96} \quad \mathbb{G}_2^{(a)}(B_{2u}) = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{3}}{3} \\ 0 & \frac{\sqrt{3}}{6} & 0 \\ -\frac{\sqrt{3}}{6} & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x97}} \quad \mathbb{G}_{2,1}^{(a)}(E_u) = \begin{bmatrix} -\frac{1}{2} & 0 & 0 \\ -\frac{\sqrt{3}}{6} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{3}}{6} \\ 0 & -\frac{\sqrt{3}}{6} & 0 \end{bmatrix}$$

$$\boxed{\text{x98}} \quad \mathbb{G}_{2,2}^{(a)}(E_u) = \begin{bmatrix} 0 & -\frac{1}{2} & 0 \\ 0 & \frac{\sqrt{3}}{6} & 0 \\ 0 & 0 & \frac{\sqrt{3}}{6} \\ 0 & 0 & 0 \\ -\frac{\sqrt{3}}{6} & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x99}} \quad \mathbb{M}_2^{(a)}(A_{1u}) = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ \frac{i}{2} & 0 & 0 \\ 0 & -\frac{i}{2} & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x100}} \quad \mathbb{M}_2^{(a)}(B_{1u}) = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ \frac{\sqrt{3}i}{6} & 0 & 0 \\ 0 & \frac{\sqrt{3}i}{6} & 0 \\ 0 & 0 & -\frac{\sqrt{3}i}{3} \end{bmatrix}$$

$$\boxed{\text{x101}} \quad \mathbb{M}_2^{(a)}(B_{2u}) = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{3}i}{3} \\ 0 & \frac{\sqrt{3}i}{6} & 0 \\ -\frac{\sqrt{3}i}{6} & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x102}} \quad \mathbb{M}_{2,1}^{(a)}(E_u) = \begin{bmatrix} -\frac{i}{2} & 0 & 0 \\ -\frac{\sqrt{3}i}{6} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{3}i}{6} \\ 0 & -\frac{\sqrt{3}i}{6} & 0 \end{bmatrix}$$

$$\boxed{\text{x103}} \quad \mathbb{M}_{2,2}^{(a)}(E_u) = \begin{bmatrix} 0 & -\frac{i}{2} & 0 \\ 0 & \frac{\sqrt{3}i}{6} & 0 \\ 0 & 0 & \frac{\sqrt{3}i}{6} \\ 0 & 0 & 0 \\ -\frac{\sqrt{3}i}{6} & 0 & 0 \end{bmatrix}$$

$$\boxed{x104} \quad \mathbb{T}_1^{(a)}(A_{2u}) = \begin{bmatrix} 0 & 0 & -\frac{\sqrt{5}i}{5} \\ 0 & 0 & 0 \\ 0 & -\frac{\sqrt{15}i}{10} & 0 \\ -\frac{\sqrt{15}i}{10} & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{x105} \quad \mathbb{T}_3^{(a)}(A_{2u}) = \begin{bmatrix} 0 & 0 & -\frac{\sqrt{30}i}{10} \\ 0 & 0 & 0 \\ 0 & \frac{\sqrt{10}i}{10} & 0 \\ \frac{\sqrt{10}i}{10} & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{x106} \quad \mathbb{T}_3^{(a)}(B_{1u}) = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ -\frac{\sqrt{6}i}{6} & 0 & 0 \\ 0 & -\frac{\sqrt{6}i}{6} & 0 \\ 0 & 0 & -\frac{\sqrt{6}i}{6} \end{bmatrix}$$

$$\boxed{x107} \quad \mathbb{T}_3^{(a)}(B_{2u}) = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{6}i}{6} \\ 0 & \frac{\sqrt{6}i}{6} & 0 \\ -\frac{\sqrt{6}i}{6} & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{x108} \quad \mathbb{T}_{1,1}^{(a)}(E_u) = \begin{bmatrix} \frac{\sqrt{5}i}{10} & 0 & 0 \\ -\frac{\sqrt{15}i}{10} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{15}i}{10} \\ 0 & -\frac{\sqrt{15}i}{10} & 0 \end{bmatrix}$$

$$\boxed{x109} \quad \mathbb{T}_{1,2}^{(a)}(E_u) = \begin{bmatrix} 0 & \frac{\sqrt{5}i}{10} & 0 \\ 0 & \frac{\sqrt{15}i}{10} & 0 \\ 0 & 0 & -\frac{\sqrt{15}i}{10} \\ 0 & 0 & 0 \\ -\frac{\sqrt{15}i}{10} & 0 & 0 \end{bmatrix}$$

$$\boxed{x110} \quad \mathbb{T}_{3,1}^{(a)}(E_u, 1) = \begin{bmatrix} \frac{\sqrt{30}i}{20} & 0 & 0 \\ -\frac{3\sqrt{10}i}{20} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{10}i}{10} \\ 0 & \frac{\sqrt{10}i}{10} & 0 \end{bmatrix}$$

$$\boxed{x111} \quad \mathbb{T}_{3,2}^{(a)}(E_u, 1) = \begin{bmatrix} 0 & \frac{\sqrt{30}i}{20} & 0 \\ 0 & \frac{3\sqrt{10}i}{20} & 0 \\ 0 & 0 & \frac{\sqrt{10}i}{10} \\ 0 & 0 & 0 \\ \frac{\sqrt{10}i}{10} & 0 & 0 \end{bmatrix}$$

$$\boxed{x112} \quad \mathbb{T}_{3,1}^{(a)}(E_u, 2) = \begin{bmatrix} \frac{\sqrt{2}i}{4} & 0 & 0 \\ \frac{\sqrt{6}i}{12} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{6}i}{6} \\ 0 & -\frac{\sqrt{6}i}{6} & 0 \end{bmatrix}$$

$$\boxed{x113} \quad \mathbb{T}_{3,2}^{(a)}(E_u, 2) = \begin{bmatrix} 0 & \frac{\sqrt{2}i}{4} & 0 \\ 0 & -\frac{\sqrt{6}i}{12} & 0 \\ 0 & 0 & \frac{\sqrt{6}i}{6} \\ 0 & 0 & 0 \\ -\frac{\sqrt{6}i}{6} & 0 & 0 \end{bmatrix}$$

— Cluster SAMB —

- Site cluster

** Wyckoff: 2c

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

$$\boxed{y2} \quad \mathbb{Q}_1^{(s)}(A_{2u}) = \left[\frac{\sqrt{2}}{2}, -\frac{\sqrt{2}}{2} \right]$$

** Wyckoff: 2b

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

$$\boxed{y4} \quad \mathbb{Q}_3^{(s)}(B_{2u}) = \left[\frac{\sqrt{2}}{2}, -\frac{\sqrt{2}}{2} \right]$$

** Wyckoff: 2a

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

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

• Bond cluster

** Wyckoff: 8a@8i

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

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

$$\boxed{y9} \quad \mathbb{Q}_1^{(s)}(A_{2u}) = \left[\frac{\sqrt{2}}{4}, \frac{\sqrt{2}}{4}, \frac{\sqrt{2}}{4}, \frac{\sqrt{2}}{4}, -\frac{\sqrt{2}}{4}, -\frac{\sqrt{2}}{4}, -\frac{\sqrt{2}}{4}, -\frac{\sqrt{2}}{4} \right]$$

$$\boxed{y10} \quad \mathbb{T}_1^{(s)}(A_{2u}) = \left[\frac{\sqrt{2}i}{4}, \frac{\sqrt{2}i}{4}, \frac{\sqrt{2}i}{4}, \frac{\sqrt{2}i}{4}, -\frac{\sqrt{2}i}{4}, -\frac{\sqrt{2}i}{4}, -\frac{\sqrt{2}i}{4}, -\frac{\sqrt{2}i}{4} \right]$$

$$\boxed{y11} \quad \mathbb{Q}_2^{(s)}(B_{1g}) = \left[\frac{\sqrt{2}}{4}, \frac{\sqrt{2}}{4}, -\frac{\sqrt{2}}{4}, -\frac{\sqrt{2}}{4}, \frac{\sqrt{2}}{4}, \frac{\sqrt{2}}{4}, -\frac{\sqrt{2}}{4}, -\frac{\sqrt{2}}{4} \right]$$

$$\boxed{y12} \quad \mathbb{T}_2^{(s)}(B_{1g}) = \left[\frac{\sqrt{2}i}{4}, \frac{\sqrt{2}i}{4}, -\frac{\sqrt{2}i}{4}, -\frac{\sqrt{2}i}{4}, \frac{\sqrt{2}i}{4}, \frac{\sqrt{2}i}{4}, -\frac{\sqrt{2}i}{4}, -\frac{\sqrt{2}i}{4} \right]$$

$$\boxed{y13} \quad \mathbb{M}_2^{(s)}(B_{2u}) = \left[\frac{\sqrt{2}i}{4}, \frac{\sqrt{2}i}{4}, -\frac{\sqrt{2}i}{4}, -\frac{\sqrt{2}i}{4}, -\frac{\sqrt{2}i}{4}, -\frac{\sqrt{2}i}{4}, \frac{\sqrt{2}i}{4}, \frac{\sqrt{2}i}{4} \right]$$

$$\boxed{y14} \quad \mathbb{Q}_3^{(s)}(B_{2u}) = \left[\frac{\sqrt{2}}{4}, \frac{\sqrt{2}}{4}, -\frac{\sqrt{2}}{4}, -\frac{\sqrt{2}}{4}, -\frac{\sqrt{2}}{4}, -\frac{\sqrt{2}}{4}, \frac{\sqrt{2}}{4}, \frac{\sqrt{2}}{4} \right]$$

$$\boxed{y15} \quad \mathbb{Q}_{2,1}^{(s)}(E_g) = \left[\frac{1}{2}, -\frac{1}{2}, 0, 0, -\frac{1}{2}, \frac{1}{2}, 0, 0 \right]$$

$$\boxed{\text{y16}} \quad \mathbb{Q}_{2,2}^{(s)}(E_g) = \left[0, 0, -\frac{1}{2}, \frac{1}{2}, 0, 0, -\frac{1}{2}, \frac{1}{2} \right]$$

$$\boxed{\text{y17}} \quad \mathbb{T}_{2,1}^{(s)}(E_g) = \left[\frac{i}{2}, -\frac{i}{2}, 0, 0, -\frac{i}{2}, \frac{i}{2}, 0, 0 \right]$$

$$\boxed{\text{y18}} \quad \mathbb{T}_{2,2}^{(s)}(E_g) = \left[0, 0, -\frac{i}{2}, \frac{i}{2}, 0, 0, -\frac{i}{2}, \frac{i}{2} \right]$$

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

$$\boxed{\text{y20}} \quad \mathbb{Q}_{1,2}^{(s)}(E_u) = \left[\frac{1}{2}, -\frac{1}{2}, 0, 0, \frac{1}{2}, -\frac{1}{2}, 0, 0 \right]$$

$$\boxed{\text{y21}} \quad \mathbb{T}_{1,1}^{(s)}(E_u) = \left[0, 0, -\frac{i}{2}, \frac{i}{2}, 0, 0, \frac{i}{2}, -\frac{i}{2} \right]$$

$$\boxed{\text{y22}} \quad \mathbb{T}_{1,2}^{(s)}(E_u) = \left[\frac{i}{2}, -\frac{i}{2}, 0, 0, \frac{i}{2}, -\frac{i}{2}, 0, 0 \right]$$

— Site and Bond —

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), -4m2

SL	position (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 (s)	mapping
1	[0.25000, 0.25000, 0.37850]	[1,2,3,4,13,14,15,16]

continued ...

Table 8

SL	position (s)	mapping
2	[0.75000, 0.75000, 0.62150]	[5,6,7,8,9,10,11,12]

Table 9: 'Si1' (#3) site cluster (2b), -4m2

SL	position (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 (8a@8i), D, $|\mathbf{v}|=2.46277$ (cartesian)

SL	vector (\mathbf{v})	center (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 (8a@8i), 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]
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]