

# Model for “0h1”

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## General Condition

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

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## Group and Unit Cell

- Group: SG No. 221  $O_h^1 Pm\bar{3}m$  [ cubic ]
- Associated point group: PG No. 221  $O_h m\bar{3}m$  [ cubic ]
- Unit cell:
  - $a = 1.00000$ ,  $b = 1.00000$ ,  $c = 1.00000$ ,  $\alpha = 90.0$ ,  $\beta = 90.0$ ,  $\gamma = 90.0$
- Lattice vectors (conventional cell):
  - $\mathbf{a}_1 = [ 1.00000, 0.00000, 0.00000 ]$
  - $\mathbf{a}_2 = [ 0.00000, 1.00000, 0.00000 ]$
  - $\mathbf{a}_3 = [ 0.00000, 0.00000, 1.00000 ]$

Table 1: Symmetry operation

#	SO	#	SO	#	SO	#	SO	#	SO
1	$\{1 0\}$	2	$\{2_{001} 0\}$	3	$\{2_{010} 0\}$	4	$\{2_{100} 0\}$	5	$\{3^+_{111} 0\}$
6	$\{3^+_{-11-1} 0\}$	7	$\{3^+_{1-1-1} 0\}$	8	$\{3^+_{-1-11} 0\}$	9	$\{3^-_{111} 0\}$	10	$\{3^-_{1-1-1} 0\}$
11	$\{3^-_{-1-11} 0\}$	12	$\{3^-_{-11-1} 0\}$	13	$\{2_{110} 0\}$	14	$\{2_{1-10} 0\}$	15	$\{4^-_{001} 0\}$
16	$\{4^+_{001} 0\}$	17	$\{4^-_{100} 0\}$	18	$\{2_{011} 0\}$	19	$\{2_{01-1} 0\}$	20	$\{4^+_{100} 0\}$
21	$\{4^+_{010} 0\}$	22	$\{2_{101} 0\}$	23	$\{4^-_{010} 0\}$	24	$\{2_{-101} 0\}$	25	$\{-1 0\}$
26	$\{m_{001} 0\}$	27	$\{m_{010} 0\}$	28	$\{m_{100} 0\}$	29	$\{-3^+_{111} 0\}$	30	$\{-3^+_{-11-1} 0\}$
31	$\{-3^+_{1-1-1} 0\}$	32	$\{-3^+_{-1-11} 0\}$	33	$\{-3^-_{111} 0\}$	34	$\{-3^-_{1-1-1} 0\}$	35	$\{-3^-_{-1-11} 0\}$
36	$\{-3^-_{-11-1} 0\}$	37	$\{m_{110} 0\}$	38	$\{m_{1-10} 0\}$	39	$\{-4^-_{001} 0\}$	40	$\{-4^+_{001} 0\}$
41	$\{-4^-_{100} 0\}$	42	$\{m_{011} 0\}$	43	$\{m_{01-1} 0\}$	44	$\{-4^+_{100} 0\}$	45	$\{-4^+_{010} 0\}$
46	$\{m_{101} 0\}$	47	$\{-4^-_{010} 0\}$	48	$\{m_{-101} 0\}$				

Table 2: Harmonics

#	symbol	irrep.	rank	X	multiplicity	component	symmetry
1	$\mathbb{Q}_0(A_{1g})$	$A_{1g}$	0	$Q, T$	-	-	1
2	$\mathbb{Q}_4(A_{1g})$	$A_{1g}$	4	$Q, T$	-	-	$\frac{\sqrt{21}(x^4-3x^2y^2-3x^2z^2+y^4-3y^2z^2+z^4)}{6}$
3	$\mathbb{G}_0(A_{1u})$	$A_{1u}$	0	$G, M$	-	-	1
4	$\mathbb{G}_4(A_{1u})$	$A_{1u}$	4	$G, M$	-	-	$\frac{\sqrt{21}(x^4-3x^2y^2-3x^2z^2+y^4-3y^2z^2+z^4)}{6}$
5	$\mathbb{G}_3(A_{2g})$	$A_{2g}$	3	$G, M$	-	-	$\sqrt{15}xyz$
6	$\mathbb{Q}_3(A_{2u})$	$A_{2u}$	3	$Q, T$	-	-	$\sqrt{15}xyz$
7	$\mathbb{Q}_{2,1}(E_g)$	$E_g$	2	$Q, T$	-	1	$-\frac{x^2}{2} - \frac{y^2}{2} + z^2$
8	$\mathbb{Q}_{2,2}(E_g)$					2	$\frac{\sqrt{3}(x-y)(x+y)}{2}$
9	$\mathbb{Q}_{4,1}(E_g)$	$E_g$	4	$Q, T$	-	1	$-\frac{\sqrt{15}(x^4-12x^2y^2+6x^2z^2+y^4+6y^2z^2-2z^4)}{12}$
10	$\mathbb{Q}_{4,2}(E_g)$					2	$\frac{\sqrt{5}(x-y)(x+y)(x^2+y^2-6z^2)}{4}$
11	$\mathbb{G}_{2,1}(E_u)$	$E_u$	2	$G, M$	-	1	$-\frac{x^2}{2} - \frac{y^2}{2} + z^2$
12	$\mathbb{G}_{2,2}(E_u)$					2	$\frac{\sqrt{3}(x-y)(x+y)}{2}$
13	$\mathbb{G}_{4,1}(E_u)$	$E_u$	4	$G, M$	-	1	$-\frac{\sqrt{15}(x^4-12x^2y^2+6x^2z^2+y^4+6y^2z^2-2z^4)}{12}$
14	$\mathbb{G}_{4,2}(E_u)$					2	$\frac{\sqrt{5}(x-y)(x+y)(x^2+y^2-6z^2)}{4}$
15	$\mathbb{Q}_{5,1}(E_u)$	$E_u$	5	$Q, T$	-	1	$\frac{3\sqrt{35}xyz(x-y)(x+y)}{2}$
16	$\mathbb{Q}_{5,2}(E_u)$					2	$\frac{\sqrt{105}xyz(x^2+y^2-2z^2)}{2}$
17	$\mathbb{G}_{1,1}(T_{1g})$	$T_{1g}$	1	$G, M$	-	1	$x$
18	$\mathbb{G}_{1,2}(T_{1g})$					2	$y$
19	$\mathbb{G}_{1,3}(T_{1g})$					3	$z$
20	$\mathbb{G}_{3,1}(T_{1g})$	$T_{1g}$	3	$G, M$	-	1	$\frac{x(2x^2-3y^2-3z^2)}{2}$

continued ...

Table 2

#	symbol	irrep.	rank	X	multiplicity	component	symmetry
21	$\mathbb{G}_{3,2}(T_{1g})$					2	$-\frac{y(3x^2-2y^2+3z^2)}{2}$
22	$\mathbb{G}_{3,3}(T_{1g})$					3	$-\frac{z(3x^2+3y^2-2z^2)}{2}$
23	$\mathbb{Q}_{4,1}(T_{1g})$	$T_{1g}$	4	$Q, T$	-	1	$\frac{\sqrt{35}yz(y-z)(y+z)}{2}$
24	$\mathbb{Q}_{4,2}(T_{1g})$					2	$-\frac{\sqrt{35}xz(x-z)(x+z)}{2}$
25	$\mathbb{Q}_{4,3}(T_{1g})$					3	$\frac{\sqrt{35}xy(x-y)(x+y)}{2}$
26	$\mathbb{Q}_{1,1}(T_{1u})$	$T_{1u}$	1	$Q, T$	-	1	$x$
27	$\mathbb{Q}_{1,2}(T_{1u})$					2	$y$
28	$\mathbb{Q}_{1,3}(T_{1u})$					3	$z$
29	$\mathbb{Q}_{3,1}(T_{1u})$	$T_{1u}$	3	$Q, T$	-	1	$\frac{x(2x^2-3y^2-3z^2)}{2}$
30	$\mathbb{Q}_{3,2}(T_{1u})$					2	$-\frac{y(3x^2-2y^2+3z^2)}{2}$
31	$\mathbb{Q}_{3,3}(T_{1u})$					3	$-\frac{z(3x^2+3y^2-2z^2)}{2}$
32	$\mathbb{G}_{4,1}(T_{1u})$	$T_{1u}$	4	$G, M$	-	1	$\frac{\sqrt{35}yz(y-z)(y+z)}{2}$
33	$\mathbb{G}_{4,2}(T_{1u})$					2	$-\frac{\sqrt{35}xz(x-z)(x+z)}{2}$
34	$\mathbb{G}_{4,3}(T_{1u})$					3	$\frac{\sqrt{35}xy(x-y)(x+y)}{2}$
35	$\mathbb{Q}_{5,1}(T_{1u}, 2)$	$T_{1u}$	5	$Q, T$	2	1	$\frac{3\sqrt{35}x(y^2-2yz-z^2)(y^2+2yz-z^2)}{8}$
36	$\mathbb{Q}_{5,2}(T_{1u}, 2)$					2	$\frac{3\sqrt{35}y(x^2-2xz-z^2)(x^2+2xz-z^2)}{8}$
37	$\mathbb{Q}_{5,3}(T_{1u}, 2)$					3	$\frac{3\sqrt{35}z(x^2-2xy-y^2)(x^2+2xy-y^2)}{8}$
38	$\mathbb{Q}_{2,1}(T_{2g})$	$T_{2g}$	2	$Q, T$	-	1	$\sqrt{3}yz$
39	$\mathbb{Q}_{2,2}(T_{2g})$					2	$\sqrt{3}xz$
40	$\mathbb{Q}_{2,3}(T_{2g})$					3	$\sqrt{3}xy$
41	$\mathbb{G}_{3,1}(T_{2g})$	$T_{2g}$	3	$G, M$	-	1	$\frac{\sqrt{15}x(y-z)(y+z)}{2}$

continued ...

Table 2

#	symbol	irrep.	rank	X	multiplicity	component	symmetry
42	$\mathbb{G}_{3,2}(T_{2g})$					2	$-\frac{\sqrt{15}y(x-z)(x+z)}{2}$
43	$\mathbb{G}_{3,3}(T_{2g})$					3	$\frac{\sqrt{15}z(x-y)(x+y)}{2}$
44	$\mathbb{Q}_{4,1}(T_{2g})$	$T_{2g}$	4	$Q, T$	-	1	$\frac{\sqrt{5}yz(6x^2-y^2-z^2)}{2}$
45	$\mathbb{Q}_{4,2}(T_{2g})$					2	$-\frac{\sqrt{5}xz(x^2-6y^2+z^2)}{2}$
46	$\mathbb{Q}_{4,3}(T_{2g})$					3	$-\frac{\sqrt{5}xy(x^2+y^2-6z^2)}{2}$
47	$\mathbb{G}_{2,1}(T_{2u})$	$T_{2u}$	2	$G, M$	-	1	$\sqrt{3}yz$
48	$\mathbb{G}_{2,2}(T_{2u})$					2	$\sqrt{3}xz$
49	$\mathbb{G}_{2,3}(T_{2u})$					3	$\sqrt{3}xy$
50	$\mathbb{Q}_{3,1}(T_{2u})$	$T_{2u}$	3	$Q, T$	-	1	$\frac{\sqrt{15}x(y-z)(y+z)}{2}$
51	$\mathbb{Q}_{3,2}(T_{2u})$					2	$-\frac{\sqrt{15}y(x-z)(x+z)}{2}$
52	$\mathbb{Q}_{3,3}(T_{2u})$					3	$\frac{\sqrt{15}z(x-y)(x+y)}{2}$
53	$\mathbb{G}_{4,1}(T_{2u})$	$T_{2u}$	4	$G, M$	-	1	$\frac{\sqrt{5}yz(6x^2-y^2-z^2)}{2}$
54	$\mathbb{G}_{4,2}(T_{2u})$					2	$-\frac{\sqrt{5}xz(x^2-6y^2+z^2)}{2}$
55	$\mathbb{G}_{4,3}(T_{2u})$					3	$-\frac{\sqrt{5}xy(x^2+y^2-6z^2)}{2}$
56	$\mathbb{Q}_{5,1}(T_{2u})$	$T_{2u}$	5	$Q, T$	-	1	$\frac{\sqrt{105}x(y-z)(y+z)(2x^2-y^2-z^2)}{4}$
57	$\mathbb{Q}_{5,2}(T_{2u})$					2	$\frac{\sqrt{105}y(x-z)(x+z)(x^2-2y^2+z^2)}{4}$
58	$\mathbb{Q}_{5,3}(T_{2u})$					3	$-\frac{\sqrt{105}z(x-y)(x+y)(x^2+y^2-2z^2)}{4}$

— Basis in full matrix —

Table 3: dimension = 8

#	orbital@atom(SL)	#	orbital@atom(SL)	#	orbital@atom(SL)	#	orbital@atom(SL)	#	orbital@atom(SL)
0	$ s, \uparrow\rangle @A(1)$	1	$ s, \downarrow\rangle @A(1)$	2	$ p_x, \uparrow\rangle @A(1)$	3	$ p_x, \downarrow\rangle @A(1)$	4	$ p_y, \uparrow\rangle @A(1)$
5	$ p_y, \downarrow\rangle @A(1)$	6	$ p_z, \uparrow\rangle @A(1)$	7	$ p_z, \downarrow\rangle @A(1)$				

Table 4: Atomic basis (orbital part only)

orbital	definition
$ s\rangle$	1
$ p_x\rangle$	$x$
$ p_y\rangle$	$y$
$ p_z\rangle$	$z$

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**SAMB**


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604 (all 604) SAMBs

- 'A' site-cluster : **A**
  - \* bra:  $\langle s, \uparrow|, \langle s, \downarrow|$
  - \* ket:  $|s, \uparrow\rangle, |s, \downarrow\rangle$
  - \* wyckoff: **1a**

z1

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

- 'A' site-cluster : A

\* bra:  $\langle s, \uparrow |, \langle s, \downarrow |$

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

\* wyckoff: **1a**

$$\boxed{\text{z269}} \quad \mathbb{G}_0^{(1,1;c)}(A_{1u}) = \mathbb{G}_0^{(1,1;a)}(A_{1u})\mathbb{Q}_0^{(s)}(A_{1g})$$

$$\boxed{\text{z300}} \quad \mathbb{G}_{2,1}^{(1,-1;c)}(E_u) = \frac{\sqrt{2}\mathbb{G}_{2,1}^{(1,-1;a)}(E_u)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

$$\boxed{\text{z301}} \quad \mathbb{G}_{2,2}^{(1,-1;c)}(E_u) = \frac{\sqrt{2}\mathbb{G}_{2,2}^{(1,-1;a)}(E_u)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

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

$$\boxed{\text{z363}} \quad \mathbb{Q}_{1,2}^{(c)}(T_{1u}) = \frac{\sqrt{3}\mathbb{Q}_{1,2}^{(a)}(T_{1u})\mathbb{Q}_0^{(s)}(A_{1g})}{3}$$

$$\boxed{\text{z364}} \quad \mathbb{Q}_{1,3}^{(c)}(T_{1u}) = \frac{\sqrt{3}\mathbb{Q}_{1,3}^{(a)}(T_{1u})\mathbb{Q}_0^{(s)}(A_{1g})}{3}$$

$$\boxed{\text{z365}} \quad \mathbb{Q}_{1,1}^{(1,0;c)}(T_{1u}) = \frac{\sqrt{3}\mathbb{Q}_{1,1}^{(1,0;a)}(T_{1u})\mathbb{Q}_0^{(s)}(A_{1g})}{3}$$

$$\boxed{\text{z366}} \quad \mathbb{Q}_{1,2}^{(1,0;c)}(T_{1u}) = \frac{\sqrt{3}\mathbb{Q}_{1,2}^{(1,0;a)}(T_{1u})\mathbb{Q}_0^{(s)}(A_{1g})}{3}$$

$$\boxed{\text{z367}} \quad \mathbb{Q}_{1,3}^{(1,0;c)}(T_{1u}) = \frac{\sqrt{3}\mathbb{Q}_{1,3}^{(1,0;a)}(T_{1u})\mathbb{Q}_0^{(s)}(A_{1g})}{3}$$

$$\boxed{\text{z485}} \quad \mathbb{G}_{2,1}^{(1,-1;c)}(T_{2u}) = \frac{\sqrt{3}\mathbb{G}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{Q}_0^{(s)}(A_{1g})}{3}$$

$$\boxed{\text{z486}} \quad \mathbb{G}_{2,2}^{(1,-1;c)}(T_{2u}) = \frac{\sqrt{3}\mathbb{G}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{Q}_0^{(s)}(A_{1g})}{3}$$

$$\boxed{\text{z487}} \quad \mathbb{G}_{2,3}^{(1,-1;c)}(T_{2u}) = \frac{\sqrt{3}\mathbb{G}_{2,3}^{(1,-1;a)}(T_{2u})\mathbb{Q}_0^{(s)}(A_{1g})}{3}$$

• 'A' site-cluster : **A**

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

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

\* wyckoff: **1a**

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

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

$$\boxed{\text{z30}} \quad \mathbb{Q}_{2,1}^{(c)}(E_g) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

$$\boxed{\text{z31}} \quad \mathbb{Q}_{2,2}^{(c)}(E_g) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

$$\boxed{\text{z32}} \quad \mathbb{Q}_{2,1}^{(1,-1;c)}(E_g) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

$$\boxed{\text{z33}} \quad \mathbb{Q}_{2,2}^{(1,-1;c)}(E_g) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

$$\boxed{\text{z86}} \quad \mathbb{G}_{1,1}^{(1,0;c)}(T_{1g}) = \frac{\sqrt{3}\mathbb{G}_{1,1}^{(1,0;a)}(T_{1g})\mathbb{Q}_0^{(s)}(A_{1g})}{3}$$

$$\boxed{\text{z87}} \quad \mathbb{G}_{1,2}^{(1,0;c)}(T_{1g}) = \frac{\sqrt{3}\mathbb{G}_{1,2}^{(1,0;a)}(T_{1g})\mathbb{Q}_0^{(s)}(A_{1g})}{3}$$

$$\boxed{\text{z88}} \quad \mathbb{G}_{1,3}^{(1,0;c)}(T_{1g}) = \frac{\sqrt{3}\mathbb{G}_{1,3}^{(1,0;a)}(T_{1g})\mathbb{Q}_0^{(s)}(A_{1g})}{3}$$

$$\boxed{\text{z170}} \quad \mathbb{Q}_{2,1}^{(c)}(T_{2g}) = \frac{\sqrt{3}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_0^{(s)}(A_{1g})}{3}$$

$$\boxed{\text{z171}} \quad \mathbb{Q}_{2,2}^{(c)}(T_{2g}) = \frac{\sqrt{3}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_0^{(s)}(A_{1g})}{3}$$

$$\boxed{\text{z172}} \quad \mathbb{Q}_{2,3}^{(c)}(T_{2g}) = \frac{\sqrt{3}\mathbb{Q}_{2,3}^{(a)}(T_{2g})\mathbb{Q}_0^{(s)}(A_{1g})}{3}$$

$$\boxed{\text{z173}} \quad \mathbb{Q}_{2,1}^{(1,-1;c)}(T_{2g}) = \frac{\sqrt{3}\mathbb{Q}_{2,1}^{(1,-1;a)}(T_{2g})\mathbb{Q}_0^{(s)}(A_{1g})}{3}$$



$$\boxed{\text{z174}} \quad \mathbb{Q}_{2,2}^{(1,-1;c)}(T_{2g}) = \frac{\sqrt{3}\mathbb{Q}_{2,2}^{(1,-1;a)}(T_{2g})\mathbb{Q}_0^{(s)}(A_{1g})}{3}$$

$$\boxed{\text{z175}} \quad \mathbb{Q}_{2,3}^{(1,-1;c)}(T_{2g}) = \frac{\sqrt{3}\mathbb{Q}_{2,3}^{(1,-1;a)}(T_{2g})\mathbb{Q}_0^{(s)}(A_{1g})}{3}$$

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

\* bra:  $\langle s, \uparrow |, \langle s, \downarrow |$

\* ket:  $|s, \uparrow\rangle, |s, \downarrow\rangle$

\* wyckoff: **3a@3d**

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

$$\boxed{\text{z34}} \quad \mathbb{G}_0^{(1,-1;c)}(A_{1u}) = \frac{\sqrt{3}\mathbb{M}_{1,1}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{3} + \frac{\sqrt{3}\mathbb{M}_{1,2}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{3} + \frac{\sqrt{3}\mathbb{M}_{1,3}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3}$$

$$\boxed{\text{z35}} \quad \mathbb{Q}_{2,1}^{(c)}(E_g) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$$

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

$$\boxed{\text{z302}} \quad \mathbb{G}_{2,1}^{(1,-1;c)}(E_u) = -\frac{\sqrt{3}\mathbb{M}_{1,1}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} - \frac{\sqrt{3}\mathbb{M}_{1,2}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} + \frac{\sqrt{3}\mathbb{M}_{1,3}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3}$$

$$\boxed{\text{z303}} \quad \mathbb{G}_{2,2}^{(1,-1;c)}(E_u) = \frac{\mathbb{M}_{1,1}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{2} - \frac{\mathbb{M}_{1,2}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{2}$$

$$\boxed{\text{z368}} \quad \mathbb{Q}_{1,1}^{(1,-1;c)}(T_{1u}) = \frac{\sqrt{6}\mathbb{M}_{1,2}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{6} - \frac{\sqrt{6}\mathbb{M}_{1,3}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6}$$

$$\boxed{\text{z369}} \quad \mathbb{Q}_{1,2}^{(1,-1;c)}(T_{1u}) = -\frac{\sqrt{6}\mathbb{M}_{1,1}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{6} + \frac{\sqrt{6}\mathbb{M}_{1,3}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6}$$

$$\boxed{\text{z370}} \quad \mathbb{Q}_{1,3}^{(1,-1;c)}(T_{1u}) = \frac{\sqrt{6}\mathbb{M}_{1,1}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} - \frac{\sqrt{6}\mathbb{M}_{1,2}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6}$$

$$\boxed{\text{z488}} \quad \mathbb{G}_{2,1}^{(1,-1;c)}(T_{2u}) = \frac{\sqrt{6}\mathbb{M}_{1,2}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{6} + \frac{\sqrt{6}\mathbb{M}_{1,3}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6}$$

$$\boxed{\text{z489}} \quad \mathbb{G}_{2,2}^{(1,-1;c)}(T_{2u}) = \frac{\sqrt{6}\mathbb{M}_{1,1}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{6} + \frac{\sqrt{6}\mathbb{M}_{1,3}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6}$$

$$\boxed{\text{z490}} \quad \mathbb{G}_{2,3}^{(1,-1;c)}(T_{2u}) = \frac{\sqrt{6}\mathbb{M}_{1,1}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} + \frac{\sqrt{6}\mathbb{M}_{1,2}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6}$$

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

\* bra:  $\langle s, \uparrow |, \langle s, \downarrow |$

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

\* wyckoff: **3a@3d**

$$\boxed{\text{z5}} \quad \mathbb{Q}_0^{(c)}(A_{1g}) = \frac{\sqrt{3}\mathbb{T}_{1,1}^{(a)}(T_{1u})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{3} + \frac{\sqrt{3}\mathbb{T}_{1,2}^{(a)}(T_{1u})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{3} + \frac{\sqrt{3}\mathbb{T}_{1,3}^{(a)}(T_{1u})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3}$$

$$\boxed{\text{z6}} \quad \mathbb{Q}_0^{(1,0;c)}(A_{1g}) = \frac{\sqrt{3}\mathbb{T}_{1,1}^{(1,0;a)}(T_{1u})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{3} + \frac{\sqrt{3}\mathbb{T}_{1,2}^{(1,0;a)}(T_{1u})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{3} + \frac{\sqrt{3}\mathbb{T}_{1,3}^{(1,0;a)}(T_{1u})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3}$$

$$\boxed{\text{z21}} \quad \mathbb{G}_0^{(1,-1;c)}(A_{1u}) = \frac{\sqrt{2}\mathbb{G}_{2,1}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} + \frac{\sqrt{2}\mathbb{G}_{2,2}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z36}} \quad \mathbb{G}_0^{(1,1;c)}(A_{1u}) = \mathbb{G}_0^{(1,1;a)}(A_{1u})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z37}} \quad \mathbb{G}_3^{(1,-1;c)}(A_{2g}) = \frac{\sqrt{3}\mathbb{M}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{3} + \frac{\sqrt{3}\mathbb{M}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{3} + \frac{\sqrt{3}\mathbb{M}_{2,3}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3}$$

$$\boxed{\text{z38}} \quad \mathbb{Q}_3^{(1,-1;c)}(A_{2u}) = \frac{\sqrt{2}\mathbb{G}_{2,1}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2} - \frac{\sqrt{2}\mathbb{G}_{2,2}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z39}} \quad \mathbb{Q}_{2,1}^{(c)}(E_g) = -\frac{\sqrt{3}\mathbb{T}_{1,1}^{(a)}(T_{1u})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} - \frac{\sqrt{3}\mathbb{T}_{1,2}^{(a)}(T_{1u})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} + \frac{\sqrt{3}\mathbb{T}_{1,3}^{(a)}(T_{1u})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3}$$

$$\boxed{\text{z40}} \quad \mathbb{Q}_{2,2}^{(c)}(E_g) = \frac{\mathbb{T}_{1,1}^{(a)}(T_{1u})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{2} - \frac{\mathbb{T}_{1,2}^{(a)}(T_{1u})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{2}$$

$$\boxed{\text{z41}} \quad \mathbb{Q}_{2,1}^{(1,-1;c)}(E_g) = -\frac{\mathbb{M}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{2} + \frac{\mathbb{M}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{2}$$

$$\boxed{\text{z89}} \quad \mathbb{Q}_{2,2}^{(1,-1;c)}(E_g) = -\frac{\sqrt{3}\mathbb{M}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} - \frac{\sqrt{3}\mathbb{M}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} + \frac{\sqrt{3}\mathbb{M}_{2,3}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3}$$

$$\boxed{\text{z90}} \quad \mathbb{Q}_{2,1}^{(1,0;c)}(E_g) = -\frac{\sqrt{3}\mathbb{T}_{1,1}^{(1,0;a)}(T_{1u})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} - \frac{\sqrt{3}\mathbb{T}_{1,2}^{(1,0;a)}(T_{1u})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} + \frac{\sqrt{3}\mathbb{T}_{1,3}^{(1,0;a)}(T_{1u})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3}$$

$$\boxed{\text{z91}} \quad \mathbb{Q}_{2,2}^{(1,0;c)}(E_g) = \frac{\mathbb{T}_{1,1}^{(1,0;a)}(T_{1u})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{2} - \frac{\mathbb{T}_{1,2}^{(1,0;a)}(T_{1u})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{2}$$

$$\boxed{\text{z92}} \quad \mathbb{G}_{2,1}^{(1,-1;c)}(E_u, a) = \frac{\sqrt{2}\mathbb{G}_{2,1}^{(1,-1;a)}(E_u)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z93}} \quad \mathbb{G}_{2,2}^{(1,-1;c)}(E_u, a) = \frac{\sqrt{2}\mathbb{G}_{2,2}^{(1,-1;a)}(E_u)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z94}} \quad \mathbb{G}_{2,1}^{(1,-1;c)}(E_u, b) = \frac{\mathbb{G}_{2,1}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} - \frac{\mathbb{G}_{2,2}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z95}} \quad \mathbb{G}_{2,2}^{(1,-1;c)}(E_u, b) = -\frac{\mathbb{G}_{2,1}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2} - \frac{\mathbb{G}_{2,2}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z96}} \quad \mathbb{G}_{2,1}^{(1,1;c)}(E_u) = \frac{\sqrt{2}\mathbb{G}_0^{(1,1;a)}(A_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z97}} \quad \mathbb{G}_{2,2}^{(1,1;c)}(E_u) = \frac{\sqrt{2}\mathbb{G}_0^{(1,1;a)}(A_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z98}} \quad \mathbb{G}_{1,1}^{(c)}(T_{1g}) = \frac{\sqrt{6}\mathbb{T}_{1,2}^{(a)}(T_{1u})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{6} - \frac{\sqrt{6}\mathbb{T}_{1,3}^{(a)}(T_{1u})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6}$$

$$\boxed{\text{z99}} \quad \mathbb{G}_{1,2}^{(c)}(T_{1g}) = -\frac{\sqrt{6}\mathbb{T}_{1,1}^{(a)}(T_{1u})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{6} + \frac{\sqrt{6}\mathbb{T}_{1,3}^{(a)}(T_{1u})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6}$$

$$\boxed{\text{z100}} \quad \mathbb{G}_{1,3}^{(c)}(T_{1g}) = \frac{\sqrt{6}\mathbb{T}_{1,1}^{(a)}(T_{1u})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} - \frac{\sqrt{6}\mathbb{T}_{1,2}^{(a)}(T_{1u})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6}$$

$$\boxed{\text{z101}} \quad \mathbb{G}_{1,1}^{(1,-1;c)}(T_{1g}) = -\frac{\sqrt{30}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{T}_{1,1}^{(b)}(T_{1u})}{30} + \frac{\sqrt{10}\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{T}_{1,1}^{(b)}(T_{1u})}{10} + \frac{\sqrt{10}\mathbb{M}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{10} + \frac{\sqrt{10}\mathbb{M}_{2,3}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{10}$$

$$\boxed{\text{z102}} \quad \mathbb{G}_{1,2}^{(1,-1;c)}(T_{1g}) = -\frac{\sqrt{30}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{T}_{1,2}^{(b)}(T_{1u})}{30} + \frac{\sqrt{10}\mathbb{M}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{10} - \frac{\sqrt{10}\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{T}_{1,2}^{(b)}(T_{1u})}{10} + \frac{\sqrt{10}\mathbb{M}_{2,3}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{10}$$

$$\boxed{\text{z103}} \quad \mathbb{G}_{1,3}^{(1,-1;c)}(T_{1g}) = \frac{\sqrt{30}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{T}_{1,3}^{(b)}(T_{1u})}{15} + \frac{\sqrt{10}\mathbb{M}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{10} + \frac{\sqrt{10}\mathbb{M}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{10}$$

$$\begin{aligned}
\text{z176} \quad \mathbb{G}_{3,1}^{(1,-1;c)}(T_{1g}) &= -\frac{\sqrt{5}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{T}_{1,1}^{(b)}(T_{1u})}{10} + \frac{\sqrt{15}\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{T}_{1,1}^{(b)}(T_{1u})}{10} - \frac{\sqrt{15}\mathbb{M}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{15} - \frac{\sqrt{15}\mathbb{M}_{2,3}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{15} \\
\text{z177} \quad \mathbb{G}_{3,2}^{(1,-1;c)}(T_{1g}) &= -\frac{\sqrt{5}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{T}_{1,2}^{(b)}(T_{1u})}{10} - \frac{\sqrt{15}\mathbb{M}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{15} - \frac{\sqrt{15}\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{T}_{1,2}^{(b)}(T_{1u})}{10} - \frac{\sqrt{15}\mathbb{M}_{2,3}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{15} \\
\text{z178} \quad \mathbb{G}_{3,3}^{(1,-1;c)}(T_{1g}) &= \frac{\sqrt{5}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{T}_{1,3}^{(b)}(T_{1u})}{5} - \frac{\sqrt{15}\mathbb{M}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{15} - \frac{\sqrt{15}\mathbb{M}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{15} \\
\text{z179} \quad \mathbb{G}_{1,1}^{(1,0;c)}(T_{1g}) &= \frac{\sqrt{6}\mathbb{T}_{1,2}^{(1,0;a)}(T_{1u})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{6} - \frac{\sqrt{6}\mathbb{T}_{1,3}^{(1,0;a)}(T_{1u})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} \\
\text{z180} \quad \mathbb{G}_{1,2}^{(1,0;c)}(T_{1g}) &= -\frac{\sqrt{6}\mathbb{T}_{1,1}^{(1,0;a)}(T_{1u})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{6} + \frac{\sqrt{6}\mathbb{T}_{1,3}^{(1,0;a)}(T_{1u})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} \\
\text{z181} \quad \mathbb{G}_{1,3}^{(1,0;c)}(T_{1g}) &= \frac{\sqrt{6}\mathbb{T}_{1,1}^{(1,0;a)}(T_{1u})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} - \frac{\sqrt{6}\mathbb{T}_{1,2}^{(1,0;a)}(T_{1u})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} \\
\text{z182} \quad \mathbb{G}_{1,1}^{(1,1;c)}(T_{1g}) &= \frac{\sqrt{3}\mathbb{M}_0^{(1,1;a)}(A_{1u})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{3} \\
\text{z183} \quad \mathbb{G}_{1,2}^{(1,1;c)}(T_{1g}) &= \frac{\sqrt{3}\mathbb{M}_0^{(1,1;a)}(A_{1u})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{3} \\
\text{z184} \quad \mathbb{G}_{1,3}^{(1,1;c)}(T_{1g}) &= \frac{\sqrt{3}\mathbb{M}_0^{(1,1;a)}(A_{1u})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3} \\
\text{z185} \quad \mathbb{Q}_{1,1}^{(c)}(T_{1u}, a) &= \frac{\sqrt{3}\mathbb{Q}_{1,1}^{(a)}(T_{1u})\mathbb{Q}_0^{(b)}(A_{1g})}{3} \\
\text{z186} \quad \mathbb{Q}_{1,2}^{(c)}(T_{1u}, a) &= \frac{\sqrt{3}\mathbb{Q}_{1,2}^{(a)}(T_{1u})\mathbb{Q}_0^{(b)}(A_{1g})}{3} \\
\text{z187} \quad \mathbb{Q}_{1,3}^{(c)}(T_{1u}, a) &= \frac{\sqrt{3}\mathbb{Q}_{1,3}^{(a)}(T_{1u})\mathbb{Q}_0^{(b)}(A_{1g})}{3} \\
\text{z271} \quad \mathbb{Q}_{1,1}^{(c)}(T_{1u}, b) &= -\frac{\sqrt{3}\mathbb{Q}_{1,1}^{(a)}(T_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{6} + \frac{\mathbb{Q}_{1,1}^{(a)}(T_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2} \\
\text{z272} \quad \mathbb{Q}_{1,2}^{(c)}(T_{1u}, b) &= -\frac{\sqrt{3}\mathbb{Q}_{1,2}^{(a)}(T_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{6} - \frac{\mathbb{Q}_{1,2}^{(a)}(T_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}
\end{aligned}$$

$$\begin{aligned}
\boxed{\text{z287}} \quad \mathbb{Q}_{1,3}^{(c)}(T_{1u}, b) &= \frac{\sqrt{3}\mathbb{Q}_{1,3}^{(a)}(T_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{3} \\
\boxed{\text{z304}} \quad \mathbb{Q}_{1,1}^{(1,-1;c)}(T_{1u}) &= \frac{\mathbb{G}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} + \frac{\sqrt{3}\mathbb{G}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{6} \\
\boxed{\text{z305}} \quad \mathbb{Q}_{1,2}^{(1,-1;c)}(T_{1u}) &= -\frac{\mathbb{G}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} + \frac{\sqrt{3}\mathbb{G}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{6} \\
\boxed{\text{z306}} \quad \mathbb{Q}_{1,3}^{(1,-1;c)}(T_{1u}) &= -\frac{\sqrt{3}\mathbb{G}_{2,3}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{3} \\
\boxed{\text{z307}} \quad \mathbb{Q}_{1,1}^{(1,0;c)}(T_{1u}, a) &= \frac{\sqrt{3}\mathbb{Q}_{1,1}^{(1,0;a)}(T_{1u})\mathbb{Q}_0^{(b)}(A_{1g})}{3} \\
\boxed{\text{z308}} \quad \mathbb{Q}_{1,2}^{(1,0;c)}(T_{1u}, a) &= \frac{\sqrt{3}\mathbb{Q}_{1,2}^{(1,0;a)}(T_{1u})\mathbb{Q}_0^{(b)}(A_{1g})}{3} \\
\boxed{\text{z309}} \quad \mathbb{Q}_{1,3}^{(1,0;c)}(T_{1u}, a) &= \frac{\sqrt{3}\mathbb{Q}_{1,3}^{(1,0;a)}(T_{1u})\mathbb{Q}_0^{(b)}(A_{1g})}{3} \\
\boxed{\text{z371}} \quad \mathbb{Q}_{1,1}^{(1,0;c)}(T_{1u}, b) &= -\frac{\sqrt{3}\mathbb{Q}_{1,1}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{6} + \frac{\mathbb{Q}_{1,1}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2} \\
\boxed{\text{z372}} \quad \mathbb{Q}_{1,2}^{(1,0;c)}(T_{1u}, b) &= -\frac{\sqrt{3}\mathbb{Q}_{1,2}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{6} - \frac{\mathbb{Q}_{1,2}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2} \\
\boxed{\text{z373}} \quad \mathbb{Q}_{1,3}^{(1,0;c)}(T_{1u}, b) &= \frac{\sqrt{3}\mathbb{Q}_{1,3}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{3} \\
\boxed{\text{z374}} \quad \mathbb{Q}_{2,1}^{(c)}(T_{2g}) &= \frac{\sqrt{6}\mathbb{T}_{1,2}^{(a)}(T_{1u})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{6} + \frac{\sqrt{6}\mathbb{T}_{1,3}^{(a)}(T_{1u})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} \\
\boxed{\text{z375}} \quad \mathbb{Q}_{2,2}^{(c)}(T_{2g}) &= \frac{\sqrt{6}\mathbb{T}_{1,1}^{(a)}(T_{1u})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{6} + \frac{\sqrt{6}\mathbb{T}_{1,3}^{(a)}(T_{1u})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} \\
\boxed{\text{z376}} \quad \mathbb{Q}_{2,3}^{(c)}(T_{2g}) &= \frac{\sqrt{6}\mathbb{T}_{1,1}^{(a)}(T_{1u})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} + \frac{\sqrt{6}\mathbb{T}_{1,2}^{(a)}(T_{1u})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} \\
\boxed{\text{z377}} \quad \mathbb{Q}_{2,1}^{(1,-1;c)}(T_{2g}) &= \frac{\sqrt{6}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} + \frac{\sqrt{2}\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} - \frac{\sqrt{2}\mathbb{M}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{6} + \frac{\sqrt{2}\mathbb{M}_{2,3}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6}
\end{aligned}$$

$$\begin{aligned}
\text{z378} \quad \mathbb{Q}_{2,2}^{(1,-1;c)}(T_{2g}) &= -\frac{\sqrt{6}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} + \frac{\sqrt{2}\mathbb{M}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{6} + \frac{\sqrt{2}\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} - \frac{\sqrt{2}\mathbb{M}_{2,3}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} \\
\text{z379} \quad \mathbb{Q}_{2,3}^{(1,-1;c)}(T_{2g}) &= -\frac{\sqrt{2}\mathbb{M}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} - \frac{\sqrt{2}\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3} + \frac{\sqrt{2}\mathbb{M}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} \\
\text{z380} \quad \mathbb{Q}_{2,1}^{(1,0;c)}(T_{2g}) &= \frac{\sqrt{6}\mathbb{T}_{1,2}^{(1,0;a)}(T_{1u})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{6} + \frac{\sqrt{6}\mathbb{T}_{1,3}^{(1,0;a)}(T_{1u})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} \\
\text{z381} \quad \mathbb{Q}_{2,2}^{(1,0;c)}(T_{2g}) &= \frac{\sqrt{6}\mathbb{T}_{1,1}^{(1,0;a)}(T_{1u})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{6} + \frac{\sqrt{6}\mathbb{T}_{1,3}^{(1,0;a)}(T_{1u})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} \\
\text{z382} \quad \mathbb{Q}_{2,3}^{(1,0;c)}(T_{2g}) &= \frac{\sqrt{6}\mathbb{T}_{1,1}^{(1,0;a)}(T_{1u})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} + \frac{\sqrt{6}\mathbb{T}_{1,2}^{(1,0;a)}(T_{1u})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} \\
\text{z383} \quad \mathbb{G}_{3,1}^{(1,-1;c)}(T_{2g}) &= -\frac{\sqrt{3}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} - \frac{\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} - \frac{\mathbb{M}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3} + \frac{\mathbb{M}_{2,3}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{3} \\
\text{z384} \quad \mathbb{G}_{3,2}^{(1,-1;c)}(T_{2g}) &= \frac{\sqrt{3}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} + \frac{\mathbb{M}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3} - \frac{\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} - \frac{\mathbb{M}_{2,3}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{3} \\
\text{z385} \quad \mathbb{G}_{3,3}^{(1,-1;c)}(T_{2g}) &= -\frac{\mathbb{M}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{3} + \frac{\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3} + \frac{\mathbb{M}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{3} \\
\text{z491} \quad \mathbb{Q}_{3,1}^{(c)}(T_{2u}) &= -\frac{\mathbb{Q}_{1,1}^{(a)}(T_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} - \frac{\sqrt{3}\mathbb{Q}_{1,1}^{(a)}(T_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{6} \\
\text{z492} \quad \mathbb{Q}_{3,2}^{(c)}(T_{2u}) &= \frac{\mathbb{Q}_{1,2}^{(a)}(T_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} - \frac{\sqrt{3}\mathbb{Q}_{1,2}^{(a)}(T_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{6} \\
\text{z493} \quad \mathbb{Q}_{3,3}^{(c)}(T_{2u}) &= \frac{\sqrt{3}\mathbb{Q}_{1,3}^{(a)}(T_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{3} \\
\text{z494} \quad \mathbb{Q}_{3,1}^{(1,-1;c)}(T_{2u}) &= -\frac{\sqrt{3}\mathbb{G}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{6} + \frac{\mathbb{G}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2} \\
\text{z495} \quad \mathbb{Q}_{3,2}^{(1,-1;c)}(T_{2u}) &= -\frac{\sqrt{3}\mathbb{G}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{6} - \frac{\mathbb{G}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2} \\
\text{z496} \quad \mathbb{Q}_{3,3}^{(1,-1;c)}(T_{2u}) &= \frac{\sqrt{3}\mathbb{G}_{2,3}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{3}
\end{aligned}$$

$$\boxed{\text{z497}} \quad \mathbb{Q}_{3,1}^{(1,0;c)}(T_{2u}) = -\frac{\mathbb{Q}_{1,1}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} - \frac{\sqrt{3}\mathbb{Q}_{1,1}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{6}$$

$$\boxed{\text{z498}} \quad \mathbb{Q}_{3,2}^{(1,0;c)}(T_{2u}) = \frac{\mathbb{Q}_{1,2}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} - \frac{\sqrt{3}\mathbb{Q}_{1,2}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{6}$$

$$\boxed{\text{z499}} \quad \mathbb{Q}_{3,3}^{(1,0;c)}(T_{2u}) = \frac{\sqrt{3}\mathbb{Q}_{1,3}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{3}$$

$$\boxed{\text{z500}} \quad \mathbb{G}_{2,1}^{(1,-1;c)}(T_{2u}) = \frac{\sqrt{3}\mathbb{G}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{Q}_0^{(b)}(A_{1g})}{3}$$

$$\boxed{\text{z501}} \quad \mathbb{G}_{2,2}^{(1,-1;c)}(T_{2u}) = \frac{\sqrt{3}\mathbb{G}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{Q}_0^{(b)}(A_{1g})}{3}$$

$$\boxed{\text{z502}} \quad \mathbb{G}_{2,3}^{(1,-1;c)}(T_{2u}) = \frac{\sqrt{3}\mathbb{G}_{2,3}^{(1,-1;a)}(T_{2u})\mathbb{Q}_0^{(b)}(A_{1g})}{3}$$

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

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

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

\* wyckoff: **3aQ3d**

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

$$\boxed{\text{z8}} \quad \mathbb{Q}_0^{(c)}(A_{1g}, b) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} + \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z9}} \quad \mathbb{Q}_0^{(1,-1;c)}(A_{1g}) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} + \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$$

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

$$\boxed{\text{z22}} \quad \mathbb{G}_0^{(c)}(A_{1u}) = \frac{\sqrt{3}\mathbb{M}_{1,1}^{(a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{3} + \frac{\sqrt{3}\mathbb{M}_{1,2}^{(a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{3} + \frac{\sqrt{3}\mathbb{M}_{1,3}^{(a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3}$$

$$\boxed{\text{z23}} \quad \mathbb{G}_0^{(1,-1;c)}(A_{1u}) = \frac{\sqrt{3}\mathbb{M}_{1,1}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{3} + \frac{\sqrt{3}\mathbb{M}_{1,2}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{3} + \frac{\sqrt{3}\mathbb{M}_{1,3}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3}$$

$$\boxed{\text{z42}} \quad \mathbb{G}_4^{(1,-1;c)}(A_{1u}) = \frac{\sqrt{3}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{3} + \frac{\sqrt{3}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{3} + \frac{\sqrt{3}\mathbb{M}_{3,3}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3}$$

$$\boxed{\text{z43}} \quad \mathbb{G}_0^{(1,1;c)}(A_{1u}) = \frac{\sqrt{3}\mathbb{M}_{1,1}^{(1,1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{3} + \frac{\sqrt{3}\mathbb{M}_{1,2}^{(1,1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{3} + \frac{\sqrt{3}\mathbb{M}_{1,3}^{(1,1;a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3}$$

$$\boxed{\text{z44}} \quad \mathbb{G}_3^{(c)}(A_{2g}) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2} - \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z45}} \quad \mathbb{G}_3^{(1,-1;c)}(A_{2g}) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2} - \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z46}} \quad \mathbb{Q}_3^{(1,-1;c)}(A_{2u}) = -\frac{\sqrt{3}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{3} - \frac{\sqrt{3}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{3} - \frac{\sqrt{3}\mathbb{M}_{3,3}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3}$$

$$\boxed{\text{z47}} \quad \mathbb{Q}_3^{(1,0;c)}(A_{2u}) = \frac{\sqrt{3}\mathbb{T}_{2,1}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{3} + \frac{\sqrt{3}\mathbb{T}_{2,2}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{3} + \frac{\sqrt{3}\mathbb{T}_{2,3}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3}$$

$$\boxed{\text{z48}} \quad \mathbb{Q}_{2,1}^{(c)}(E_g, a) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z49}} \quad \mathbb{Q}_{2,2}^{(c)}(E_g, a) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z50}} \quad \mathbb{Q}_{2,1}^{(c)}(E_g, b) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z51}} \quad \mathbb{Q}_{2,2}^{(c)}(E_g, b) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z52}} \quad \mathbb{Q}_{2,1}^{(c)}(E_g, c) = \frac{\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} - \frac{\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z53}} \quad \mathbb{Q}_{2,2}^{(c)}(E_g, c) = -\frac{\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2} - \frac{\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z104}} \quad \mathbb{Q}_{2,1}^{(1,-1;c)}(E_g, a) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z105}} \quad \mathbb{Q}_{2,2}^{(1,-1;c)}(E_g, a) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$



$$\begin{aligned}
\text{z106} \quad \mathbb{Q}_{2,1}^{(1,-1;c)}(E_g, b) &= \frac{\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} - \frac{\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2} \\
\text{z107} \quad \mathbb{Q}_{2,2}^{(1,-1;c)}(E_g, b) &= -\frac{\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2} - \frac{\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} \\
\text{z108} \quad \mathbb{Q}_{2,1}^{(1,1;c)}(E_g) &= \frac{\sqrt{2}\mathbb{Q}_0^{(1,1;a)}(A_{1g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} \\
\text{z109} \quad \mathbb{Q}_{2,2}^{(1,1;c)}(E_g) &= \frac{\sqrt{2}\mathbb{Q}_0^{(1,1;a)}(A_{1g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2} \\
\text{z110} \quad \mathbb{G}_{2,1}^{(c)}(E_u) &= -\frac{\sqrt{3}\mathbb{M}_{1,1}^{(a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} - \frac{\sqrt{3}\mathbb{M}_{1,2}^{(a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} + \frac{\sqrt{3}\mathbb{M}_{1,3}^{(a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3} \\
\text{z111} \quad \mathbb{G}_{2,2}^{(c)}(E_u) &= \frac{\mathbb{M}_{1,1}^{(a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{2} - \frac{\mathbb{M}_{1,2}^{(a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{2} \\
\text{z112} \quad \mathbb{G}_{2,1}^{(1,-1;c)}(E_u, a) &= -\frac{\sqrt{42}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{28} - \frac{\sqrt{70}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{28} - \frac{\sqrt{42}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{28} + \frac{\sqrt{70}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{28} + \frac{\sqrt{42}\mathbb{M}_{3,3}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{14} \\
\text{z113} \quad \mathbb{G}_{2,2}^{(1,-1;c)}(E_u, a) &= \frac{3\sqrt{14}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{28} - \frac{\sqrt{210}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{84} - \frac{3\sqrt{14}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{28} - \frac{\sqrt{210}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{84} + \frac{\sqrt{210}\mathbb{M}_{3,3}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{42} \\
\text{z114} \quad \mathbb{G}_{2,1}^{(1,-1;c)}(E_u, b) &= -\frac{\sqrt{3}\mathbb{M}_{1,1}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} - \frac{\sqrt{3}\mathbb{M}_{1,2}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} + \frac{\sqrt{3}\mathbb{M}_{1,3}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3} \\
\text{z115} \quad \mathbb{G}_{2,2}^{(1,-1;c)}(E_u, b) &= \frac{\mathbb{M}_{1,1}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{2} - \frac{\mathbb{M}_{1,2}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{2} \\
\text{z188} \quad \mathbb{G}_{4,1}^{(1,-1;c)}(E_u) &= -\frac{\sqrt{210}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{84} + \frac{3\sqrt{14}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{28} - \frac{\sqrt{210}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{84} - \frac{3\sqrt{14}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{28} + \frac{\sqrt{210}\mathbb{M}_{3,3}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{42} \\
\text{z189} \quad \mathbb{G}_{4,2}^{(1,-1;c)}(E_u) &= \frac{\sqrt{70}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{28} + \frac{\sqrt{42}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{28} - \frac{\sqrt{70}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{28} + \frac{\sqrt{42}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{28} - \frac{\sqrt{42}\mathbb{M}_{3,3}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{14} \\
\text{z190} \quad \mathbb{G}_{2,1}^{(1,0;c)}(E_u) &= -\frac{\mathbb{T}_{2,1}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{2} + \frac{\mathbb{T}_{2,2}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{2} \\
\text{z191} \quad \mathbb{G}_{2,2}^{(1,0;c)}(E_u) &= -\frac{\sqrt{3}\mathbb{T}_{2,1}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} - \frac{\sqrt{3}\mathbb{T}_{2,2}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} + \frac{\sqrt{3}\mathbb{T}_{2,3}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3}
\end{aligned}$$

$$\boxed{\text{z192}} \quad \mathbb{G}_{2,1}^{(1,1;c)}(E_u) = -\frac{\sqrt{3}\mathbb{M}_{1,1}^{(1,1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} - \frac{\sqrt{3}\mathbb{M}_{1,2}^{(1,1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} + \frac{\sqrt{3}\mathbb{M}_{1,3}^{(1,1;a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3}$$

$$\boxed{\text{z193}} \quad \mathbb{G}_{2,2}^{(1,1;c)}(E_u) = \frac{\mathbb{M}_{1,1}^{(1,1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{2} - \frac{\mathbb{M}_{1,2}^{(1,1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{2}$$

$$\boxed{\text{z194}} \quad \mathbb{Q}_{4,1}^{(c)}(T_{1g}) = -\frac{\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} - \frac{\sqrt{3}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{6}$$

$$\boxed{\text{z195}} \quad \mathbb{Q}_{4,2}^{(c)}(T_{1g}) = \frac{\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} - \frac{\sqrt{3}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{6}$$

$$\boxed{\text{z196}} \quad \mathbb{Q}_{4,3}^{(c)}(T_{1g}) = \frac{\sqrt{3}\mathbb{Q}_{2,3}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{3}$$

$$\boxed{\text{z197}} \quad \mathbb{Q}_{4,1}^{(1,-1;c)}(T_{1g}) = -\frac{\mathbb{Q}_{2,1}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} - \frac{\sqrt{3}\mathbb{Q}_{2,1}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{6}$$

$$\boxed{\text{z198}} \quad \mathbb{Q}_{4,2}^{(1,-1;c)}(T_{1g}) = \frac{\mathbb{Q}_{2,2}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} - \frac{\sqrt{3}\mathbb{Q}_{2,2}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{6}$$

$$\boxed{\text{z199}} \quad \mathbb{Q}_{4,3}^{(1,-1;c)}(T_{1g}) = \frac{\sqrt{3}\mathbb{Q}_{2,3}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{3}$$

$$\boxed{\text{z200}} \quad \mathbb{G}_{1,1}^{(1,0;c)}(T_{1g}, a) = \frac{\sqrt{3}\mathbb{G}_{1,1}^{(1,0;a)}(T_{1g})\mathbb{Q}_0^{(b)}(A_{1g})}{3}$$

$$\boxed{\text{z201}} \quad \mathbb{G}_{1,2}^{(1,0;c)}(T_{1g}, a) = \frac{\sqrt{3}\mathbb{G}_{1,2}^{(1,0;a)}(T_{1g})\mathbb{Q}_0^{(b)}(A_{1g})}{3}$$

$$\boxed{\text{z202}} \quad \mathbb{G}_{1,3}^{(1,0;c)}(T_{1g}, a) = \frac{\sqrt{3}\mathbb{G}_{1,3}^{(1,0;a)}(T_{1g})\mathbb{Q}_0^{(b)}(A_{1g})}{3}$$

$$\boxed{\text{z273}} \quad \mathbb{G}_{1,1}^{(1,0;c)}(T_{1g}, b) = -\frac{\sqrt{3}\mathbb{G}_{1,1}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{6} + \frac{\mathbb{G}_{1,1}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z274}} \quad \mathbb{G}_{1,2}^{(1,0;c)}(T_{1g}, b) = -\frac{\sqrt{3}\mathbb{G}_{1,2}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{6} - \frac{\mathbb{G}_{1,2}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z275}} \quad \mathbb{G}_{1,3}^{(1,0;c)}(T_{1g}, b) = \frac{\sqrt{3}\mathbb{G}_{1,3}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{3}$$

$$\begin{aligned}
\text{z276} \quad \mathbb{Q}_{1,1}^{(c)}(T_{1u}) &= \frac{\sqrt{6}\mathbb{M}_{1,2}^{(a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{6} - \frac{\sqrt{6}\mathbb{M}_{1,3}^{(a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} \\
\text{z288} \quad \mathbb{Q}_{1,2}^{(c)}(T_{1u}) &= -\frac{\sqrt{6}\mathbb{M}_{1,1}^{(a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{6} + \frac{\sqrt{6}\mathbb{M}_{1,3}^{(a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} \\
\text{z289} \quad \mathbb{Q}_{1,3}^{(c)}(T_{1u}) &= \frac{\sqrt{6}\mathbb{M}_{1,1}^{(a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} - \frac{\sqrt{6}\mathbb{M}_{1,2}^{(a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} \\
\text{z310} \quad \mathbb{Q}_{1,1}^{(1,-1;c)}(T_{1u}) &= \frac{\sqrt{6}\mathbb{M}_{1,2}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{6} - \frac{\sqrt{6}\mathbb{M}_{1,3}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} \\
\text{z311} \quad \mathbb{Q}_{1,2}^{(1,-1;c)}(T_{1u}) &= -\frac{\sqrt{6}\mathbb{M}_{1,1}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{6} + \frac{\sqrt{6}\mathbb{M}_{1,3}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} \\
\text{z312} \quad \mathbb{Q}_{1,3}^{(1,-1;c)}(T_{1u}) &= \frac{\sqrt{6}\mathbb{M}_{1,1}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} - \frac{\sqrt{6}\mathbb{M}_{1,2}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} \\
\text{z313} \quad \mathbb{Q}_{3,1}^{(1,-1;c)}(T_{1u}) &= -\frac{\mathbb{M}_{3,2}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{4} - \frac{\sqrt{15}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{12} + \frac{\mathbb{M}_{3,3}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{4} - \frac{\sqrt{15}\mathbb{M}_{3,3}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{12} \\
\text{z314} \quad \mathbb{Q}_{3,2}^{(1,-1;c)}(T_{1u}) &= \frac{\mathbb{M}_{3,1}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{4} - \frac{\sqrt{15}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{12} - \frac{\mathbb{M}_{3,3}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{4} - \frac{\sqrt{15}\mathbb{M}_{3,3}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{12} \\
\text{z315} \quad \mathbb{Q}_{3,3}^{(1,-1;c)}(T_{1u}) &= -\frac{\mathbb{M}_{3,1}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{4} - \frac{\sqrt{15}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{12} + \frac{\mathbb{M}_{3,2}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{4} - \frac{\sqrt{15}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{12} \\
\text{z316} \quad \mathbb{Q}_{1,1}^{(1,0;c)}(T_{1u}) &= -\frac{\sqrt{30}\mathbb{T}_{2,1}^{(1,0;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(T_{1u})}{30} + \frac{\sqrt{10}\mathbb{T}_{2,2}^{(1,0;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(T_{1u})}{10} + \frac{\sqrt{10}\mathbb{T}_{2,2}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{10} + \frac{\sqrt{10}\mathbb{T}_{2,3}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{10} \\
\text{z317} \quad \mathbb{Q}_{1,2}^{(1,0;c)}(T_{1u}) &= -\frac{\sqrt{30}\mathbb{T}_{2,1}^{(1,0;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(T_{1u})}{30} + \frac{\sqrt{10}\mathbb{T}_{2,1}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{10} - \frac{\sqrt{10}\mathbb{T}_{2,2}^{(1,0;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(T_{1u})}{10} + \frac{\sqrt{10}\mathbb{T}_{2,3}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{10} \\
\text{z318} \quad \mathbb{Q}_{1,3}^{(1,0;c)}(T_{1u}) &= \frac{\sqrt{30}\mathbb{T}_{2,1}^{(1,0;a)}(E_g)\mathbb{T}_{1,3}^{(b)}(T_{1u})}{15} + \frac{\sqrt{10}\mathbb{T}_{2,1}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{10} + \frac{\sqrt{10}\mathbb{T}_{2,2}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{10} \\
\text{z319} \quad \mathbb{Q}_{3,1}^{(1,0;c)}(T_{1u}) &= -\frac{\sqrt{5}\mathbb{T}_{2,1}^{(1,0;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(T_{1u})}{10} + \frac{\sqrt{15}\mathbb{T}_{2,2}^{(1,0;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(T_{1u})}{10} - \frac{\sqrt{15}\mathbb{T}_{2,2}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{15} - \frac{\sqrt{15}\mathbb{T}_{2,3}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{15} \\
\text{z320} \quad \mathbb{Q}_{3,2}^{(1,0;c)}(T_{1u}) &= -\frac{\sqrt{5}\mathbb{T}_{2,1}^{(1,0;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(T_{1u})}{10} - \frac{\sqrt{15}\mathbb{T}_{2,1}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{15} - \frac{\sqrt{15}\mathbb{T}_{2,2}^{(1,0;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(T_{1u})}{10} - \frac{\sqrt{15}\mathbb{T}_{2,3}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{15}
\end{aligned}$$

$$\begin{aligned}
\boxed{\text{z321}} \quad \mathbb{Q}_{3,3}^{(1,0;c)}(T_{1u}) &= \frac{\sqrt{5}\mathbb{T}_{2,1}^{(1,0;a)}(E_g)\mathbb{T}_{1,3}^{(b)}(T_{1u})}{5} - \frac{\sqrt{15}\mathbb{T}_{2,1}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{15} - \frac{\sqrt{15}\mathbb{T}_{2,2}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{15} \\
\boxed{\text{z386}} \quad \mathbb{Q}_{1,1}^{(1,1;c)}(T_{1u}) &= \frac{\sqrt{6}\mathbb{M}_{1,2}^{(1,1;a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{6} - \frac{\sqrt{6}\mathbb{M}_{1,3}^{(1,1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} \\
\boxed{\text{z387}} \quad \mathbb{Q}_{1,2}^{(1,1;c)}(T_{1u}) &= -\frac{\sqrt{6}\mathbb{M}_{1,1}^{(1,1;a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{6} + \frac{\sqrt{6}\mathbb{M}_{1,3}^{(1,1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} \\
\boxed{\text{z388}} \quad \mathbb{Q}_{1,3}^{(1,1;c)}(T_{1u}) &= \frac{\sqrt{6}\mathbb{M}_{1,1}^{(1,1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} - \frac{\sqrt{6}\mathbb{M}_{1,2}^{(1,1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} \\
\boxed{\text{z389}} \quad \mathbb{G}_{4,1}^{(1,-1;c)}(T_{1u}) &= \frac{\sqrt{15}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{12} - \frac{\mathbb{M}_{3,2}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{4} - \frac{\sqrt{15}\mathbb{M}_{3,3}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{12} - \frac{\mathbb{M}_{3,3}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{4} \\
\boxed{\text{z390}} \quad \mathbb{G}_{4,2}^{(1,-1;c)}(T_{1u}) &= -\frac{\sqrt{15}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{12} - \frac{\mathbb{M}_{3,1}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{4} + \frac{\sqrt{15}\mathbb{M}_{3,3}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{12} - \frac{\mathbb{M}_{3,3}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{4} \\
\boxed{\text{z391}} \quad \mathbb{G}_{4,3}^{(1,-1;c)}(T_{1u}) &= \frac{\sqrt{15}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{12} - \frac{\mathbb{M}_{3,1}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{4} - \frac{\sqrt{15}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{12} - \frac{\mathbb{M}_{3,2}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{4} \\
\boxed{\text{z392}} \quad \mathbb{Q}_{2,1}^{(c)}(T_{2g}, a) &= \frac{\sqrt{3}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_0^{(b)}(A_{1g})}{3} \\
\boxed{\text{z393}} \quad \mathbb{Q}_{2,2}^{(c)}(T_{2g}, a) &= \frac{\sqrt{3}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_0^{(b)}(A_{1g})}{3} \\
\boxed{\text{z394}} \quad \mathbb{Q}_{2,3}^{(c)}(T_{2g}, a) &= \frac{\sqrt{3}\mathbb{Q}_{2,3}^{(a)}(T_{2g})\mathbb{Q}_0^{(b)}(A_{1g})}{3} \\
\boxed{\text{z395}} \quad \mathbb{Q}_{2,1}^{(c)}(T_{2g}, b) &= \frac{\sqrt{3}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{6} - \frac{\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2} \\
\boxed{\text{z396}} \quad \mathbb{Q}_{2,2}^{(c)}(T_{2g}, b) &= \frac{\sqrt{3}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{6} + \frac{\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2} \\
\boxed{\text{z397}} \quad \mathbb{Q}_{2,3}^{(c)}(T_{2g}, b) &= -\frac{\sqrt{3}\mathbb{Q}_{2,3}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{3} \\
\boxed{\text{z398}} \quad \mathbb{Q}_{2,1}^{(1,-1;c)}(T_{2g}, a) &= \frac{\sqrt{3}\mathbb{Q}_{2,1}^{(1,-1;a)}(T_{2g})\mathbb{Q}_0^{(b)}(A_{1g})}{3}
\end{aligned}$$

$$\begin{aligned}
\boxed{\text{z399}} \quad \mathbb{Q}_{2,2}^{(1,-1;c)}(T_{2g}, a) &= \frac{\sqrt{3}\mathbb{Q}_{2,2}^{(1,-1;a)}(T_{2g})\mathbb{Q}_0^{(b)}(A_{1g})}{3} \\
\boxed{\text{z400}} \quad \mathbb{Q}_{2,3}^{(1,-1;c)}(T_{2g}, a) &= \frac{\sqrt{3}\mathbb{Q}_{2,3}^{(1,-1;a)}(T_{2g})\mathbb{Q}_0^{(b)}(A_{1g})}{3} \\
\boxed{\text{z401}} \quad \mathbb{Q}_{2,1}^{(1,-1;c)}(T_{2g}, b) &= \frac{\sqrt{3}\mathbb{Q}_{2,1}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{6} - \frac{\mathbb{Q}_{2,1}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2} \\
\boxed{\text{z402}} \quad \mathbb{Q}_{2,2}^{(1,-1;c)}(T_{2g}, b) &= \frac{\sqrt{3}\mathbb{Q}_{2,2}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{6} + \frac{\mathbb{Q}_{2,2}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2} \\
\boxed{\text{z403}} \quad \mathbb{Q}_{2,3}^{(1,-1;c)}(T_{2g}, b) &= -\frac{\sqrt{3}\mathbb{Q}_{2,3}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{3} \\
\boxed{\text{z404}} \quad \mathbb{Q}_{2,1}^{(1,0;c)}(T_{2g}) &= -\frac{\mathbb{G}_{1,1}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} - \frac{\sqrt{3}\mathbb{G}_{1,1}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{6} \\
\boxed{\text{z405}} \quad \mathbb{Q}_{2,2}^{(1,0;c)}(T_{2g}) &= \frac{\mathbb{G}_{1,2}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} - \frac{\sqrt{3}\mathbb{G}_{1,2}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{6} \\
\boxed{\text{z406}} \quad \mathbb{Q}_{2,3}^{(1,0;c)}(T_{2g}) &= \frac{\sqrt{3}\mathbb{G}_{1,3}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{3} \\
\boxed{\text{z503}} \quad \mathbb{Q}_{3,1}^{(1,-1;c)}(T_{2u}) &= \frac{\sqrt{15}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{12} + \frac{\mathbb{M}_{3,2}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{12} + \frac{\sqrt{15}\mathbb{M}_{3,3}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{12} - \frac{\mathbb{M}_{3,3}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{12} + \frac{\mathbb{M}_3^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{3} \\
\boxed{\text{z504}} \quad \mathbb{Q}_{3,2}^{(1,-1;c)}(T_{2u}) &= \frac{\sqrt{15}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{12} - \frac{\mathbb{M}_{3,1}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{12} + \frac{\sqrt{15}\mathbb{M}_{3,3}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{12} + \frac{\mathbb{M}_{3,3}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{12} + \frac{\mathbb{M}_3^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{3} \\
\boxed{\text{z505}} \quad \mathbb{Q}_{3,3}^{(1,-1;c)}(T_{2u}) &= \frac{\sqrt{15}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{12} + \frac{\mathbb{M}_{3,1}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{12} + \frac{\sqrt{15}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{12} - \frac{\mathbb{M}_{3,2}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{12} + \frac{\mathbb{M}_3^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3} \\
\boxed{\text{z506}} \quad \mathbb{Q}_{3,1}^{(1,0;c)}(T_{2u}) &= -\frac{\sqrt{3}\mathbb{T}_{2,1}^{(1,0;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} - \frac{\mathbb{T}_{2,2}^{(1,0;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} - \frac{\mathbb{T}_{2,2}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3} + \frac{\mathbb{T}_{2,3}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{3} \\
\boxed{\text{z507}} \quad \mathbb{Q}_{3,2}^{(1,0;c)}(T_{2u}) &= \frac{\sqrt{3}\mathbb{T}_{2,1}^{(1,0;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} + \frac{\mathbb{T}_{2,1}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3} - \frac{\mathbb{T}_{2,2}^{(1,0;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} - \frac{\mathbb{T}_{2,3}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{3} \\
\boxed{\text{z508}} \quad \mathbb{Q}_{3,3}^{(1,0;c)}(T_{2u}) &= -\frac{\mathbb{T}_{2,1}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{3} + \frac{\mathbb{T}_{2,2}^{(1,0;a)}(E_g)\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3} + \frac{\mathbb{T}_{2,2}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{3}
\end{aligned}$$



$$\boxed{\text{z523}} \quad \mathbb{G}_{2,3}^{(1,0;c)}(T_{2u}) = -\frac{\sqrt{2}\mathbb{T}_{2,1}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} - \frac{\sqrt{2}\mathbb{T}_{2,2}^{(1,0;a)}(E_g)\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3} + \frac{\sqrt{2}\mathbb{T}_{2,2}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6}$$

$$\boxed{\text{z524}} \quad \mathbb{G}_{2,1}^{(1,1;c)}(T_{2u}) = \frac{\sqrt{6}\mathbb{M}_{1,2}^{(1,1;a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{6} + \frac{\sqrt{6}\mathbb{M}_{1,3}^{(1,1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6}$$

$$\boxed{\text{z525}} \quad \mathbb{G}_{2,2}^{(1,1;c)}(T_{2u}) = \frac{\sqrt{6}\mathbb{M}_{1,1}^{(1,1;a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{6} + \frac{\sqrt{6}\mathbb{M}_{1,3}^{(1,1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6}$$

$$\boxed{\text{z526}} \quad \mathbb{G}_{2,3}^{(1,1;c)}(T_{2u}) = \frac{\sqrt{6}\mathbb{M}_{1,1}^{(1,1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} + \frac{\sqrt{6}\mathbb{M}_{1,2}^{(1,1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6}$$

• 'A'-'A' bond-cluster : **A;A\_002\_1**

- \* bra:  $\langle s, \uparrow |, \langle s, \downarrow |$
- \* ket:  $|s, \uparrow \rangle, |s, \downarrow \rangle$
- \* wyckoff: **6b03c**

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

$$\boxed{\text{z54}} \quad \mathbb{G}_0^{(1,-1;c)}(A_{1u}) = \frac{\sqrt{3}\mathbb{M}_{1,1}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{3} + \frac{\sqrt{3}\mathbb{M}_{1,2}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{3} + \frac{\sqrt{3}\mathbb{M}_{1,3}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3}$$

$$\boxed{\text{z55}} \quad \mathbb{Q}_3^{(1,-1;c)}(A_{2u}) = \frac{\sqrt{3}\mathbb{M}_{1,1}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{3} + \frac{\sqrt{3}\mathbb{M}_{1,2}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{3} + \frac{\sqrt{3}\mathbb{M}_{1,3}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{3}$$

$$\boxed{\text{z203}} \quad \mathbb{Q}_{2,1}^{(c)}(E_g) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z204}} \quad \mathbb{Q}_{2,2}^{(c)}(E_g) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z205}} \quad \mathbb{G}_{2,1}^{(1,-1;c)}(E_u, a) = -\frac{\sqrt{3}\mathbb{M}_{1,1}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} - \frac{\sqrt{3}\mathbb{M}_{1,2}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} + \frac{\sqrt{3}\mathbb{M}_{1,3}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3}$$

$$\boxed{\text{z277}} \quad \mathbb{G}_{2,2}^{(1,-1;c)}(E_u, a) = \frac{\mathbb{M}_{1,1}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{2} - \frac{\mathbb{M}_{1,2}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{2}$$

$$\boxed{\text{z290}} \quad \mathbb{G}_{2,1}^{(1,-1;c)}(E_u, b) = \frac{\mathbb{M}_{1,1}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{2} - \frac{\mathbb{M}_{1,2}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{2}$$

$$\begin{aligned}
\text{z322} \quad \mathbb{G}_{2,2}^{(1,-1;c)}(E_u, b) &= \frac{\sqrt{3}\mathbb{M}_{1,1}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{6} + \frac{\sqrt{3}\mathbb{M}_{1,2}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{6} - \frac{\sqrt{3}\mathbb{M}_{1,3}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{3} \\
\text{z323} \quad \mathbb{Q}_{1,1}^{(1,-1;c)}(T_{1u}, a) &= \frac{\sqrt{6}\mathbb{M}_{1,2}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{6} - \frac{\sqrt{6}\mathbb{M}_{1,3}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} \\
\text{z324} \quad \mathbb{Q}_{1,2}^{(1,-1;c)}(T_{1u}, a) &= -\frac{\sqrt{6}\mathbb{M}_{1,1}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{6} + \frac{\sqrt{6}\mathbb{M}_{1,3}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} \\
\text{z325} \quad \mathbb{Q}_{1,3}^{(1,-1;c)}(T_{1u}, a) &= \frac{\sqrt{6}\mathbb{M}_{1,1}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} - \frac{\sqrt{6}\mathbb{M}_{1,2}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} \\
\text{z407} \quad \mathbb{Q}_{1,1}^{(1,-1;c)}(T_{1u}, b) &= \frac{\sqrt{6}\mathbb{M}_{1,2}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{6} + \frac{\sqrt{6}\mathbb{M}_{1,3}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{6} \\
\text{z408} \quad \mathbb{Q}_{1,2}^{(1,-1;c)}(T_{1u}, b) &= \frac{\sqrt{6}\mathbb{M}_{1,1}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{6} + \frac{\sqrt{6}\mathbb{M}_{1,3}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{6} \\
\text{z409} \quad \mathbb{Q}_{1,3}^{(1,-1;c)}(T_{1u}, b) &= \frac{\sqrt{6}\mathbb{M}_{1,1}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{6} + \frac{\sqrt{6}\mathbb{M}_{1,2}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{6} \\
\text{z410} \quad \mathbb{Q}_{2,1}^{(c)}(T_{2g}) &= \frac{\sqrt{3}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{3} \\
\text{z411} \quad \mathbb{Q}_{2,2}^{(c)}(T_{2g}) &= \frac{\sqrt{3}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{3} \\
\text{z412} \quad \mathbb{Q}_{2,3}^{(c)}(T_{2g}) &= \frac{\sqrt{3}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{3} \\
\text{z527} \quad \mathbb{Q}_{3,1}^{(1,-1;c)}(T_{2u}) &= \frac{\sqrt{6}\mathbb{M}_{1,2}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{6} - \frac{\sqrt{6}\mathbb{M}_{1,3}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{6} \\
\text{z528} \quad \mathbb{Q}_{3,2}^{(1,-1;c)}(T_{2u}) &= -\frac{\sqrt{6}\mathbb{M}_{1,1}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{6} + \frac{\sqrt{6}\mathbb{M}_{1,3}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{6} \\
\text{z529} \quad \mathbb{Q}_{3,3}^{(1,-1;c)}(T_{2u}) &= \frac{\sqrt{6}\mathbb{M}_{1,1}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{6} - \frac{\sqrt{6}\mathbb{M}_{1,2}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{6} \\
\text{z530} \quad \mathbb{G}_{2,1}^{(1,-1;c)}(T_{2u}) &= \frac{\sqrt{6}\mathbb{M}_{1,2}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{6} + \frac{\sqrt{6}\mathbb{M}_{1,3}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6}
\end{aligned}$$



$$\boxed{\text{z531}} \quad \mathbb{G}_{2,2}^{(1,-1;c)}(T_{2u}) = \frac{\sqrt{6}\mathbb{M}_{1,1}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{6} + \frac{\sqrt{6}\mathbb{M}_{1,3}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6}$$

$$\boxed{\text{z532}} \quad \mathbb{G}_{2,3}^{(1,-1;c)}(T_{2u}) = \frac{\sqrt{6}\mathbb{M}_{1,1}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} + \frac{\sqrt{6}\mathbb{M}_{1,2}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6}$$

• 'A'-'A' bond-cluster : **A;A\_002\_1**

\* bra:  $\langle s, \uparrow |, \langle s, \downarrow |$

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

\* wyckoff: **6b@3c**

$$\boxed{\text{z12}} \quad \mathbb{Q}_0^{(c)}(A_{1g}) = \frac{\sqrt{3}\mathbb{T}_{1,1}^{(a)}(T_{1u})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{3} + \frac{\sqrt{3}\mathbb{T}_{1,2}^{(a)}(T_{1u})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{3} + \frac{\sqrt{3}\mathbb{T}_{1,3}^{(a)}(T_{1u})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3}$$

$$\boxed{\text{z13}} \quad \mathbb{Q}_0^{(1,-1;c)}(A_{1g}) = \frac{\sqrt{3}\mathbb{M}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{3} + \frac{\sqrt{3}\mathbb{M}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{3} + \frac{\sqrt{3}\mathbb{M}_{2,3}^{(1,-1;a)}(T_{2u})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{3}$$

$$\boxed{\text{z14}} \quad \mathbb{Q}_0^{(1,0;c)}(A_{1g}) = \frac{\sqrt{3}\mathbb{T}_{1,1}^{(1,0;a)}(T_{1u})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{3} + \frac{\sqrt{3}\mathbb{T}_{1,2}^{(1,0;a)}(T_{1u})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{3} + \frac{\sqrt{3}\mathbb{T}_{1,3}^{(1,0;a)}(T_{1u})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3}$$

$$\boxed{\text{z24}} \quad \mathbb{G}_0^{(1,-1;c)}(A_{1u}) = \frac{\sqrt{5}\mathbb{G}_{2,1}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{5} + \frac{\sqrt{5}\mathbb{G}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{5} + \frac{\sqrt{5}\mathbb{G}_{2,2}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{5} + \frac{\sqrt{5}\mathbb{G}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{5} + \frac{\sqrt{5}\mathbb{G}_{2,3}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{5}$$

$$\boxed{\text{z25}} \quad \mathbb{G}_4^{(1,-1;c)}(A_{1u}) = \frac{\sqrt{30}\mathbb{G}_{2,1}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{10} - \frac{\sqrt{30}\mathbb{G}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{15} + \frac{\sqrt{30}\mathbb{G}_{2,2}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{10} - \frac{\sqrt{30}\mathbb{G}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{15} - \frac{\sqrt{30}\mathbb{G}_{2,3}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{15}$$

$$\boxed{\text{z26}} \quad \mathbb{G}_0^{(1,1;c)}(A_{1u}) = \mathbb{G}_0^{(1,1;a)}(A_{1u})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z56}} \quad \mathbb{G}_3^{(c)}(A_{2g}) = \frac{\sqrt{3}\mathbb{T}_{1,1}^{(a)}(T_{1u})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{3} + \frac{\sqrt{3}\mathbb{T}_{1,2}^{(a)}(T_{1u})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{3} + \frac{\sqrt{3}\mathbb{T}_{1,3}^{(a)}(T_{1u})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{3}$$

$$\boxed{\text{z57}} \quad \mathbb{G}_3^{(1,-1;c)}(A_{2g}) = \frac{\sqrt{3}\mathbb{M}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{3} + \frac{\sqrt{3}\mathbb{M}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{3} + \frac{\sqrt{3}\mathbb{M}_{2,3}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3}$$

$$\boxed{\text{z58}} \quad \mathbb{G}_3^{(1,0;c)}(A_{2g}) = \frac{\sqrt{3}\mathbb{T}_{1,1}^{(1,0;a)}(T_{1u})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{3} + \frac{\sqrt{3}\mathbb{T}_{1,2}^{(1,0;a)}(T_{1u})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{3} + \frac{\sqrt{3}\mathbb{T}_{1,3}^{(1,0;a)}(T_{1u})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{3}$$

$$\boxed{\text{z59}} \quad \mathbb{Q}_3^{(c)}(A_{2u}) = \frac{\sqrt{3}\mathbb{Q}_{1,1}^{(a)}(T_{1u})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{3} + \frac{\sqrt{3}\mathbb{Q}_{1,2}^{(a)}(T_{1u})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{3} + \frac{\sqrt{3}\mathbb{Q}_{1,3}^{(a)}(T_{1u})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{3}$$

$$\begin{aligned}
\text{z60} \quad \mathbb{Q}_3^{(1,-1;c)}(A_{2u}) &= \frac{\sqrt{2}\mathbb{G}_{2,1}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2} - \frac{\sqrt{2}\mathbb{G}_{2,2}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} \\
\text{z61} \quad \mathbb{Q}_3^{(1,0;c)}(A_{2u}) &= \frac{\sqrt{3}\mathbb{Q}_{1,1}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{3} + \frac{\sqrt{3}\mathbb{Q}_{1,2}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{3} + \frac{\sqrt{3}\mathbb{Q}_{1,3}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{3} \\
\text{z62} \quad \mathbb{Q}_{2,1}^{(c)}(E_g, a) &= -\frac{\sqrt{3}\mathbb{T}_{1,1}^{(a)}(T_{1u})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} - \frac{\sqrt{3}\mathbb{T}_{1,2}^{(a)}(T_{1u})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} + \frac{\sqrt{3}\mathbb{T}_{1,3}^{(a)}(T_{1u})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3} \\
\text{z63} \quad \mathbb{Q}_{2,2}^{(c)}(E_g, a) &= \frac{\mathbb{T}_{1,1}^{(a)}(T_{1u})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{2} - \frac{\mathbb{T}_{1,2}^{(a)}(T_{1u})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{2} \\
\text{z64} \quad \mathbb{Q}_{2,1}^{(c)}(E_g, b) &= \frac{\mathbb{T}_{1,1}^{(a)}(T_{1u})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{2} - \frac{\mathbb{T}_{1,2}^{(a)}(T_{1u})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{2} \\
\text{z65} \quad \mathbb{Q}_{2,2}^{(c)}(E_g, b) &= \frac{\sqrt{3}\mathbb{T}_{1,1}^{(a)}(T_{1u})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{6} + \frac{\sqrt{3}\mathbb{T}_{1,2}^{(a)}(T_{1u})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{6} - \frac{\sqrt{3}\mathbb{T}_{1,3}^{(a)}(T_{1u})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{3} \\
\text{z66} \quad \mathbb{Q}_{2,1}^{(1,-1;c)}(E_g, a) &= -\frac{\mathbb{M}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{2} + \frac{\mathbb{M}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{2} \\
\text{z67} \quad \mathbb{Q}_{2,2}^{(1,-1;c)}(E_g, a) &= -\frac{\sqrt{3}\mathbb{M}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} - \frac{\sqrt{3}\mathbb{M}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} + \frac{\sqrt{3}\mathbb{M}_{2,3}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3} \\
\text{z116} \quad \mathbb{Q}_{2,1}^{(1,-1;c)}(E_g, b) &= \frac{\sqrt{3}\mathbb{M}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{6} + \frac{\sqrt{3}\mathbb{M}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{6} - \frac{\sqrt{3}\mathbb{M}_{2,3}^{(1,-1;a)}(T_{2u})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{3} \\
\text{z117} \quad \mathbb{Q}_{2,2}^{(1,-1;c)}(E_g, b) &= -\frac{\mathbb{M}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{2} + \frac{\mathbb{M}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{2} \\
\text{z118} \quad \mathbb{Q}_{2,1}^{(1,0;c)}(E_g, a) &= -\frac{\sqrt{3}\mathbb{T}_{1,1}^{(1,0;a)}(T_{1u})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} - \frac{\sqrt{3}\mathbb{T}_{1,2}^{(1,0;a)}(T_{1u})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} + \frac{\sqrt{3}\mathbb{T}_{1,3}^{(1,0;a)}(T_{1u})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3} \\
\text{z119} \quad \mathbb{Q}_{2,2}^{(1,0;c)}(E_g, a) &= \frac{\mathbb{T}_{1,1}^{(1,0;a)}(T_{1u})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{2} - \frac{\mathbb{T}_{1,2}^{(1,0;a)}(T_{1u})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{2} \\
\text{z120} \quad \mathbb{Q}_{2,1}^{(1,0;c)}(E_g, b) &= \frac{\mathbb{T}_{1,1}^{(1,0;a)}(T_{1u})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{2} - \frac{\mathbb{T}_{1,2}^{(1,0;a)}(T_{1u})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{2} \\
\text{z121} \quad \mathbb{Q}_{2,2}^{(1,0;c)}(E_g, b) &= \frac{\sqrt{3}\mathbb{T}_{1,1}^{(1,0;a)}(T_{1u})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{6} + \frac{\sqrt{3}\mathbb{T}_{1,2}^{(1,0;a)}(T_{1u})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{6} - \frac{\sqrt{3}\mathbb{T}_{1,3}^{(1,0;a)}(T_{1u})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{3}
\end{aligned}$$

$$\begin{aligned}
\text{z122} \quad \mathbb{G}_{2,1}^{(c)}(E_u) &= \frac{\mathbb{Q}_{1,1}^{(a)}(T_{1u})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{2} - \frac{\mathbb{Q}_{1,2}^{(a)}(T_{1u})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{2} \\
\text{z123} \quad \mathbb{G}_{2,2}^{(c)}(E_u) &= \frac{\sqrt{3}\mathbb{Q}_{1,1}^{(a)}(T_{1u})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{6} + \frac{\sqrt{3}\mathbb{Q}_{1,2}^{(a)}(T_{1u})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{6} - \frac{\sqrt{3}\mathbb{Q}_{1,3}^{(a)}(T_{1u})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{3} \\
\text{z124} \quad \mathbb{G}_{2,1}^{(1,-1;c)}(E_u, a) &= \frac{\sqrt{2}\mathbb{G}_{2,1}^{(1,-1;a)}(E_u)\mathbb{Q}_0^{(b)}(A_{1g})}{2} \\
\text{z125} \quad \mathbb{G}_{2,2}^{(1,-1;c)}(E_u, a) &= \frac{\sqrt{2}\mathbb{G}_{2,2}^{(1,-1;a)}(E_u)\mathbb{Q}_0^{(b)}(A_{1g})}{2} \\
\text{z126} \quad \mathbb{G}_{2,1}^{(1,-1;c)}(E_u, b) &= \frac{\sqrt{7}\mathbb{G}_{2,1}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{7} + \frac{\sqrt{7}\mathbb{G}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{14} - \frac{\sqrt{7}\mathbb{G}_{2,2}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{7} + \frac{\sqrt{7}\mathbb{G}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{14} - \frac{\sqrt{7}\mathbb{G}_{2,3}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{7} \\
\text{z127} \quad \mathbb{G}_{2,2}^{(1,-1;c)}(E_u, b) &= -\frac{\sqrt{7}\mathbb{G}_{2,1}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{7} - \frac{\sqrt{21}\mathbb{G}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{14} - \frac{\sqrt{7}\mathbb{G}_{2,2}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{7} + \frac{\sqrt{21}\mathbb{G}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{14} \\
\text{z128} \quad \mathbb{G}_{4,1}^{(1,-1;c)}(E_u) &= \frac{\sqrt{21}\mathbb{G}_{2,1}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{14} - \frac{\sqrt{21}\mathbb{G}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{21} - \frac{\sqrt{21}\mathbb{G}_{2,2}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{14} - \frac{\sqrt{21}\mathbb{G}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{21} + \frac{2\sqrt{21}\mathbb{G}_{2,3}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{21} \\
\text{z129} \quad \mathbb{G}_{4,2}^{(1,-1;c)}(E_u) &= -\frac{\sqrt{21}\mathbb{G}_{2,1}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{14} + \frac{\sqrt{7}\mathbb{G}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{7} - \frac{\sqrt{21}\mathbb{G}_{2,2}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{14} - \frac{\sqrt{7}\mathbb{G}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{7} \\
\text{z130} \quad \mathbb{G}_{2,1}^{(1,0;c)}(E_u) &= \frac{\mathbb{Q}_{1,1}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{2} - \frac{\mathbb{Q}_{1,2}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{2} \\
\text{z131} \quad \mathbb{G}_{2,2}^{(1,0;c)}(E_u) &= \frac{\sqrt{3}\mathbb{Q}_{1,1}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{6} + \frac{\sqrt{3}\mathbb{Q}_{1,2}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{6} - \frac{\sqrt{3}\mathbb{Q}_{1,3}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{3} \\
\text{z132} \quad \mathbb{G}_{2,1}^{(1,1;c)}(E_u) &= \frac{\sqrt{2}\mathbb{G}_0^{(1,1;a)}(A_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} \\
\text{z133} \quad \mathbb{G}_{2,2}^{(1,1;c)}(E_u) &= \frac{\sqrt{2}\mathbb{G}_0^{(1,1;a)}(A_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2} \\
\text{z134} \quad \mathbb{Q}_{4,1}^{(1,-1;c)}(T_{1g}) &= -\frac{\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{M}_{2,1}^{(b)}(T_{2u})}{2} - \frac{\sqrt{3}\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{M}_{2,1}^{(b)}(T_{2u})}{6} \\
\text{z135} \quad \mathbb{Q}_{4,2}^{(1,-1;c)}(T_{1g}) &= \frac{\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{M}_{2,2}^{(b)}(T_{2u})}{2} - \frac{\sqrt{3}\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{M}_{2,2}^{(b)}(T_{2u})}{6}
\end{aligned}$$

$$\begin{aligned}
\boxed{\text{z136}} \quad \mathbb{Q}_{4,3}^{(1,-1;c)}(T_{1g}) &= \frac{\sqrt{3}\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{M}_{2,3}^{(b)}(T_{2u})}{3} \\
\boxed{\text{z137}} \quad \mathbb{G}_{1,1}^{(c)}(T_{1g}, a) &= \frac{\sqrt{6}\mathbb{T}_{1,2}^{(a)}(T_{1u})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{6} - \frac{\sqrt{6}\mathbb{T}_{1,3}^{(a)}(T_{1u})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} \\
\boxed{\text{z138}} \quad \mathbb{G}_{1,2}^{(c)}(T_{1g}, a) &= -\frac{\sqrt{6}\mathbb{T}_{1,1}^{(a)}(T_{1u})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{6} + \frac{\sqrt{6}\mathbb{T}_{1,3}^{(a)}(T_{1u})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} \\
\boxed{\text{z139}} \quad \mathbb{G}_{1,3}^{(c)}(T_{1g}, a) &= \frac{\sqrt{6}\mathbb{T}_{1,1}^{(a)}(T_{1u})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} - \frac{\sqrt{6}\mathbb{T}_{1,2}^{(a)}(T_{1u})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} \\
\boxed{\text{z140}} \quad \mathbb{G}_{1,1}^{(c)}(T_{1g}, b) &= \frac{\sqrt{6}\mathbb{T}_{1,2}^{(a)}(T_{1u})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{6} + \frac{\sqrt{6}\mathbb{T}_{1,3}^{(a)}(T_{1u})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{6} \\
\boxed{\text{z141}} \quad \mathbb{G}_{1,2}^{(c)}(T_{1g}, b) &= \frac{\sqrt{6}\mathbb{T}_{1,1}^{(a)}(T_{1u})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{6} + \frac{\sqrt{6}\mathbb{T}_{1,3}^{(a)}(T_{1u})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{6} \\
\boxed{\text{z142}} \quad \mathbb{G}_{1,3}^{(c)}(T_{1g}, b) &= \frac{\sqrt{6}\mathbb{T}_{1,1}^{(a)}(T_{1u})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{6} + \frac{\sqrt{6}\mathbb{T}_{1,2}^{(a)}(T_{1u})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{6} \\
\boxed{\text{z206}} \quad \mathbb{G}_{1,1}^{(1,-1;c)}(T_{1g}, a) &= -\frac{\sqrt{30}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{T}_{1,1}^{(b)}(T_{1u})}{30} + \frac{\sqrt{10}\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{T}_{1,1}^{(b)}(T_{1u})}{10} + \frac{\sqrt{10}\mathbb{M}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{10} + \frac{\sqrt{10}\mathbb{M}_{2,3}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{10} \\
\boxed{\text{z207}} \quad \mathbb{G}_{1,2}^{(1,-1;c)}(T_{1g}, a) &= -\frac{\sqrt{30}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{T}_{1,2}^{(b)}(T_{1u})}{30} + \frac{\sqrt{10}\mathbb{M}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{10} - \frac{\sqrt{10}\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{T}_{1,2}^{(b)}(T_{1u})}{10} + \frac{\sqrt{10}\mathbb{M}_{2,3}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{10} \\
\boxed{\text{z208}} \quad \mathbb{G}_{1,3}^{(1,-1;c)}(T_{1g}, a) &= \frac{\sqrt{30}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{T}_{1,3}^{(b)}(T_{1u})}{15} + \frac{\sqrt{10}\mathbb{M}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{10} + \frac{\sqrt{10}\mathbb{M}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{10} \\
\boxed{\text{z209}} \quad \mathbb{G}_{1,1}^{(1,-1;c)}(T_{1g}, b) &= -\frac{\sqrt{6}\mathbb{M}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{6} + \frac{\sqrt{6}\mathbb{M}_{2,3}^{(1,-1;a)}(T_{2u})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{6} \\
\boxed{\text{z210}} \quad \mathbb{G}_{1,2}^{(1,-1;c)}(T_{1g}, b) &= \frac{\sqrt{6}\mathbb{M}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{6} - \frac{\sqrt{6}\mathbb{M}_{2,3}^{(1,-1;a)}(T_{2u})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{6} \\
\boxed{\text{z211}} \quad \mathbb{G}_{1,3}^{(1,-1;c)}(T_{1g}, b) &= -\frac{\sqrt{6}\mathbb{M}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{6} + \frac{\sqrt{6}\mathbb{M}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{6} \\
\boxed{\text{z212}} \quad \mathbb{G}_{3,1}^{(1,-1;c)}(T_{1g}) &= -\frac{\sqrt{5}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{T}_{1,1}^{(b)}(T_{1u})}{10} + \frac{\sqrt{15}\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{T}_{1,1}^{(b)}(T_{1u})}{10} - \frac{\sqrt{15}\mathbb{M}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{15} - \frac{\sqrt{15}\mathbb{M}_{2,3}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{15}
\end{aligned}$$

$$\begin{aligned}
\boxed{\text{z213}} \quad \mathbb{G}_{3,2}^{(1,-1;c)}(T_{1g}) &= -\frac{\sqrt{5}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{T}_{1,2}^{(b)}(T_{1u})}{10} - \frac{\sqrt{15}\mathbb{M}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{15} - \frac{\sqrt{15}\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{T}_{1,2}^{(b)}(T_{1u})}{10} - \frac{\sqrt{15}\mathbb{M}_{2,3}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{15} \\
\boxed{\text{z214}} \quad \mathbb{G}_{3,3}^{(1,-1;c)}(T_{1g}) &= \frac{\sqrt{5}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{T}_{1,3}^{(b)}(T_{1u})}{5} - \frac{\sqrt{15}\mathbb{M}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{15} - \frac{\sqrt{15}\mathbb{M}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{15} \\
\boxed{\text{z215}} \quad \mathbb{G}_{1,1}^{(1,0;c)}(T_{1g}, a) &= \frac{\sqrt{6}\mathbb{T}_{1,2}^{(1,0;a)}(T_{1u})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{6} - \frac{\sqrt{6}\mathbb{T}_{1,3}^{(1,0;a)}(T_{1u})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} \\
\boxed{\text{z216}} \quad \mathbb{G}_{1,2}^{(1,0;c)}(T_{1g}, a) &= -\frac{\sqrt{6}\mathbb{T}_{1,1}^{(1,0;a)}(T_{1u})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{6} + \frac{\sqrt{6}\mathbb{T}_{1,3}^{(1,0;a)}(T_{1u})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} \\
\boxed{\text{z217}} \quad \mathbb{G}_{1,3}^{(1,0;c)}(T_{1g}, a) &= \frac{\sqrt{6}\mathbb{T}_{1,1}^{(1,0;a)}(T_{1u})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} - \frac{\sqrt{6}\mathbb{T}_{1,2}^{(1,0;a)}(T_{1u})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} \\
\boxed{\text{z218}} \quad \mathbb{G}_{1,1}^{(1,0;c)}(T_{1g}, b) &= \frac{\sqrt{6}\mathbb{T}_{1,2}^{(1,0;a)}(T_{1u})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{6} + \frac{\sqrt{6}\mathbb{T}_{1,3}^{(1,0;a)}(T_{1u})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{6} \\
\boxed{\text{z219}} \quad \mathbb{G}_{1,2}^{(1,0;c)}(T_{1g}, b) &= \frac{\sqrt{6}\mathbb{T}_{1,1}^{(1,0;a)}(T_{1u})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{6} + \frac{\sqrt{6}\mathbb{T}_{1,3}^{(1,0;a)}(T_{1u})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{6} \\
\boxed{\text{z220}} \quad \mathbb{G}_{1,3}^{(1,0;c)}(T_{1g}, b) &= \frac{\sqrt{6}\mathbb{T}_{1,1}^{(1,0;a)}(T_{1u})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{6} + \frac{\sqrt{6}\mathbb{T}_{1,2}^{(1,0;a)}(T_{1u})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{6} \\
\boxed{\text{z221}} \quad \mathbb{G}_{1,1}^{(1,1;c)}(T_{1g}) &= \frac{\sqrt{3}\mathbb{M}_0^{(1,1;a)}(A_{1u})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{3} \\
\boxed{\text{z222}} \quad \mathbb{G}_{1,2}^{(1,1;c)}(T_{1g}) &= \frac{\sqrt{3}\mathbb{M}_0^{(1,1;a)}(A_{1u})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{3} \\
\boxed{\text{z223}} \quad \mathbb{G}_{1,3}^{(1,1;c)}(T_{1g}) &= \frac{\sqrt{3}\mathbb{M}_0^{(1,1;a)}(A_{1u})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3} \\
\boxed{\text{z224}} \quad \mathbb{Q}_{1,1}^{(c)}(T_{1u}, a) &= \frac{\sqrt{3}\mathbb{Q}_{1,1}^{(a)}(T_{1u})\mathbb{Q}_0^{(b)}(A_{1g})}{3} \\
\boxed{\text{z225}} \quad \mathbb{Q}_{1,2}^{(c)}(T_{1u}, a) &= \frac{\sqrt{3}\mathbb{Q}_{1,2}^{(a)}(T_{1u})\mathbb{Q}_0^{(b)}(A_{1g})}{3} \\
\boxed{\text{z226}} \quad \mathbb{Q}_{1,3}^{(c)}(T_{1u}, a) &= \frac{\sqrt{3}\mathbb{Q}_{1,3}^{(a)}(T_{1u})\mathbb{Q}_0^{(b)}(A_{1g})}{3}
\end{aligned}$$

$$\boxed{\text{z227}} \quad \mathbb{Q}_{1,1}^{(c)}(T_{1u}, b) = -\frac{\sqrt{30}\mathbb{Q}_{1,1}^{(a)}(T_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{30} + \frac{\sqrt{10}\mathbb{Q}_{1,1}^{(a)}(T_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{10} + \frac{\sqrt{10}\mathbb{Q}_{1,2}^{(a)}(T_{1u})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{10} + \frac{\sqrt{10}\mathbb{Q}_{1,3}^{(a)}(T_{1u})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{10}$$

$$\boxed{\text{z228}} \quad \mathbb{Q}_{1,2}^{(c)}(T_{1u}, b) = \frac{\sqrt{10}\mathbb{Q}_{1,1}^{(a)}(T_{1u})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{10} - \frac{\sqrt{30}\mathbb{Q}_{1,2}^{(a)}(T_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{30} - \frac{\sqrt{10}\mathbb{Q}_{1,2}^{(a)}(T_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{10} + \frac{\sqrt{10}\mathbb{Q}_{1,3}^{(a)}(T_{1u})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{10}$$

$$\boxed{\text{z229}} \quad \mathbb{Q}_{1,3}^{(c)}(T_{1u}, b) = \frac{\sqrt{10}\mathbb{Q}_{1,1}^{(a)}(T_{1u})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{10} + \frac{\sqrt{10}\mathbb{Q}_{1,2}^{(a)}(T_{1u})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{10} + \frac{\sqrt{30}\mathbb{Q}_{1,3}^{(a)}(T_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{15}$$

$$\boxed{\text{z230}} \quad \mathbb{Q}_{3,1}^{(c)}(T_{1u}) = -\frac{\sqrt{5}\mathbb{Q}_{1,1}^{(a)}(T_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{10} + \frac{\sqrt{15}\mathbb{Q}_{1,1}^{(a)}(T_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{10} - \frac{\sqrt{15}\mathbb{Q}_{1,2}^{(a)}(T_{1u})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{15} - \frac{\sqrt{15}\mathbb{Q}_{1,3}^{(a)}(T_{1u})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{15}$$

$$\boxed{\text{z231}} \quad \mathbb{Q}_{3,2}^{(c)}(T_{1u}) = -\frac{\sqrt{15}\mathbb{Q}_{1,1}^{(a)}(T_{1u})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{15} - \frac{\sqrt{5}\mathbb{Q}_{1,2}^{(a)}(T_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{10} - \frac{\sqrt{15}\mathbb{Q}_{1,2}^{(a)}(T_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{10} - \frac{\sqrt{15}\mathbb{Q}_{1,3}^{(a)}(T_{1u})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{15}$$

$$\boxed{\text{z232}} \quad \mathbb{Q}_{3,3}^{(c)}(T_{1u}) = -\frac{\sqrt{15}\mathbb{Q}_{1,1}^{(a)}(T_{1u})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{15} - \frac{\sqrt{15}\mathbb{Q}_{1,2}^{(a)}(T_{1u})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{15} + \frac{\sqrt{5}\mathbb{Q}_{1,3}^{(a)}(T_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{5}$$

$$\boxed{\text{z278}} \quad \mathbb{Q}_{1,1}^{(1,-1;c)}(T_{1u}) = -\frac{\sqrt{10}\mathbb{G}_{2,1}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{10} + \frac{\sqrt{10}\mathbb{G}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{10} + \frac{\sqrt{30}\mathbb{G}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{30} \\ - \frac{\sqrt{30}\mathbb{G}_{2,2}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{30} - \frac{\sqrt{30}\mathbb{G}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{30} + \frac{\sqrt{30}\mathbb{G}_{2,3}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{30}$$

$$\boxed{\text{z279}} \quad \mathbb{Q}_{1,2}^{(1,-1;c)}(T_{1u}) = \frac{\sqrt{10}\mathbb{G}_{2,1}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{10} + \frac{\sqrt{30}\mathbb{G}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{30} - \frac{\sqrt{30}\mathbb{G}_{2,2}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{30} \\ - \frac{\sqrt{10}\mathbb{G}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{10} + \frac{\sqrt{30}\mathbb{G}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{30} - \frac{\sqrt{30}\mathbb{G}_{2,3}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{30}$$

$$\boxed{\text{z280}} \quad \mathbb{Q}_{1,3}^{(1,-1;c)}(T_{1u}) = -\frac{\sqrt{30}\mathbb{G}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{30} + \frac{\sqrt{30}\mathbb{G}_{2,2}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{15} + \frac{\sqrt{30}\mathbb{G}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{30} - \frac{\sqrt{30}\mathbb{G}_{2,3}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{15}$$

$$\boxed{\text{z291}} \quad \mathbb{Q}_{3,1}^{(1,-1;c)}(T_{1u}) = \frac{\sqrt{10}\mathbb{G}_{2,1}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{20} - \frac{\sqrt{10}\mathbb{G}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{20} - \frac{\sqrt{30}\mathbb{G}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{60} \\ + \frac{\sqrt{30}\mathbb{G}_{2,2}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{60} - \frac{\sqrt{30}\mathbb{G}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{15} + \frac{\sqrt{30}\mathbb{G}_{2,3}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{15}$$

$$\boxed{\text{z292}} \quad \mathbb{Q}_{3,2}^{(1,-1;c)}(T_{1u}) = -\frac{\sqrt{10}\mathbb{G}_{2,1}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{20} + \frac{\sqrt{30}\mathbb{G}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{15} + \frac{\sqrt{30}\mathbb{G}_{2,2}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{60} \\ + \frac{\sqrt{10}\mathbb{G}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{20} - \frac{\sqrt{30}\mathbb{G}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{60} - \frac{\sqrt{30}\mathbb{G}_{2,3}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{15}$$

$$\begin{aligned}
\boxed{\text{z293}} \quad \mathbb{Q}_{3,3}^{(1,-1;c)}(T_{1u}) &= -\frac{\sqrt{30}\mathbb{G}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{15} - \frac{\sqrt{30}\mathbb{G}_{2,2}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{30} + \frac{\sqrt{30}\mathbb{G}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{15} + \frac{\sqrt{30}\mathbb{G}_{2,3}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{30} \\
\boxed{\text{z326}} \quad \mathbb{Q}_{1,1}^{(1,0;c)}(T_{1u}, a) &= \frac{\sqrt{3}\mathbb{Q}_{1,1}^{(1,0;a)}(T_{1u})\mathbb{Q}_0^{(b)}(A_{1g})}{3} \\
\boxed{\text{z327}} \quad \mathbb{Q}_{1,2}^{(1,0;c)}(T_{1u}, a) &= \frac{\sqrt{3}\mathbb{Q}_{1,2}^{(1,0;a)}(T_{1u})\mathbb{Q}_0^{(b)}(A_{1g})}{3} \\
\boxed{\text{z328}} \quad \mathbb{Q}_{1,3}^{(1,0;c)}(T_{1u}, a) &= \frac{\sqrt{3}\mathbb{Q}_{1,3}^{(1,0;a)}(T_{1u})\mathbb{Q}_0^{(b)}(A_{1g})}{3} \\
\boxed{\text{z329}} \quad \mathbb{Q}_{1,1}^{(1,0;c)}(T_{1u}, b) &= -\frac{\sqrt{30}\mathbb{Q}_{1,1}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{30} + \frac{\sqrt{10}\mathbb{Q}_{1,1}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{10} + \frac{\sqrt{10}\mathbb{Q}_{1,2}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{10} + \frac{\sqrt{10}\mathbb{Q}_{1,3}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{10} \\
\boxed{\text{z330}} \quad \mathbb{Q}_{1,2}^{(1,0;c)}(T_{1u}, b) &= \frac{\sqrt{10}\mathbb{Q}_{1,1}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{10} - \frac{\sqrt{30}\mathbb{Q}_{1,2}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{30} - \frac{\sqrt{10}\mathbb{Q}_{1,2}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{10} + \frac{\sqrt{10}\mathbb{Q}_{1,3}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{10} \\
\boxed{\text{z331}} \quad \mathbb{Q}_{1,3}^{(1,0;c)}(T_{1u}, b) &= \frac{\sqrt{10}\mathbb{Q}_{1,1}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{10} + \frac{\sqrt{10}\mathbb{Q}_{1,2}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{10} + \frac{\sqrt{30}\mathbb{Q}_{1,3}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{15} \\
\boxed{\text{z332}} \quad \mathbb{Q}_{3,1}^{(1,0;c)}(T_{1u}) &= -\frac{\sqrt{5}\mathbb{Q}_{1,1}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{10} + \frac{\sqrt{15}\mathbb{Q}_{1,1}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{10} - \frac{\sqrt{15}\mathbb{Q}_{1,2}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{15} - \frac{\sqrt{15}\mathbb{Q}_{1,3}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{15} \\
\boxed{\text{z333}} \quad \mathbb{Q}_{3,2}^{(1,0;c)}(T_{1u}) &= -\frac{\sqrt{15}\mathbb{Q}_{1,1}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{15} - \frac{\sqrt{5}\mathbb{Q}_{1,2}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{10} - \frac{\sqrt{15}\mathbb{Q}_{1,2}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{10} - \frac{\sqrt{15}\mathbb{Q}_{1,3}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{15} \\
\boxed{\text{z334}} \quad \mathbb{Q}_{3,3}^{(1,0;c)}(T_{1u}) &= -\frac{\sqrt{15}\mathbb{Q}_{1,1}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{15} - \frac{\sqrt{15}\mathbb{Q}_{1,2}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{15} + \frac{\sqrt{5}\mathbb{Q}_{1,3}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{5} \\
\boxed{\text{z335}} \quad \mathbb{G}_{4,1}^{(1,-1;c)}(T_{1u}) &= -\frac{\sqrt{2}\mathbb{G}_{2,1}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{4} - \frac{\sqrt{2}\mathbb{G}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{4} - \frac{\sqrt{6}\mathbb{G}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{12} - \frac{\sqrt{6}\mathbb{G}_{2,2}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{12} \\
\boxed{\text{z336}} \quad \mathbb{G}_{4,2}^{(1,-1;c)}(T_{1u}) &= \frac{\sqrt{2}\mathbb{G}_{2,1}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{4} - \frac{\sqrt{6}\mathbb{G}_{2,2}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{12} + \frac{\sqrt{2}\mathbb{G}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{4} - \frac{\sqrt{6}\mathbb{G}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{12} \\
\boxed{\text{z337}} \quad \mathbb{G}_{4,3}^{(1,-1;c)}(T_{1u}) &= \frac{\sqrt{6}\mathbb{G}_{2,2}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{6} + \frac{\sqrt{6}\mathbb{G}_{2,3}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{6} \\
\boxed{\text{z413}} \quad \mathbb{Q}_{2,1}^{(c)}(T_{2g}, a) &= \frac{\sqrt{6}\mathbb{T}_{1,2}^{(a)}(T_{1u})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{6} + \frac{\sqrt{6}\mathbb{T}_{1,3}^{(a)}(T_{1u})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6}
\end{aligned}$$

$$\boxed{\text{z414}} \quad \mathbb{Q}_{2,2}^{(c)}(T_{2g}, a) = \frac{\sqrt{6}\mathbb{T}_{1,1}^{(a)}(T_{1u})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{6} + \frac{\sqrt{6}\mathbb{T}_{1,3}^{(a)}(T_{1u})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6}$$

$$\boxed{\text{z415}} \quad \mathbb{Q}_{2,3}^{(c)}(T_{2g}, a) = \frac{\sqrt{6}\mathbb{T}_{1,1}^{(a)}(T_{1u})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} + \frac{\sqrt{6}\mathbb{T}_{1,2}^{(a)}(T_{1u})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6}$$

$$\boxed{\text{z416}} \quad \mathbb{Q}_{2,1}^{(c)}(T_{2g}, b) = -\frac{\sqrt{6}\mathbb{T}_{1,2}^{(a)}(T_{1u})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{6} + \frac{\sqrt{6}\mathbb{T}_{1,3}^{(a)}(T_{1u})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{6}$$

$$\boxed{\text{z417}} \quad \mathbb{Q}_{2,2}^{(c)}(T_{2g}, b) = \frac{\sqrt{6}\mathbb{T}_{1,1}^{(a)}(T_{1u})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{6} - \frac{\sqrt{6}\mathbb{T}_{1,3}^{(a)}(T_{1u})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{6}$$

$$\boxed{\text{z418}} \quad \mathbb{Q}_{2,3}^{(c)}(T_{2g}, b) = -\frac{\sqrt{6}\mathbb{T}_{1,1}^{(a)}(T_{1u})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{6} + \frac{\sqrt{6}\mathbb{T}_{1,2}^{(a)}(T_{1u})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{6}$$

$$\boxed{\text{z419}} \quad \mathbb{Q}_{2,1}^{(1,-1;c)}(T_{2g}, a) = \frac{\sqrt{6}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} + \frac{\sqrt{2}\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} - \frac{\sqrt{2}\mathbb{M}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{6} + \frac{\sqrt{2}\mathbb{M}_{2,3}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6}$$

$$\boxed{\text{z420}} \quad \mathbb{Q}_{2,2}^{(1,-1;c)}(T_{2g}, a) = -\frac{\sqrt{6}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} + \frac{\sqrt{2}\mathbb{M}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{6} + \frac{\sqrt{2}\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} - \frac{\sqrt{2}\mathbb{M}_{2,3}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6}$$

$$\boxed{\text{z421}} \quad \mathbb{Q}_{2,3}^{(1,-1;c)}(T_{2g}, a) = -\frac{\sqrt{2}\mathbb{M}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} - \frac{\sqrt{2}\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3} + \frac{\sqrt{2}\mathbb{M}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6}$$

$$\boxed{\text{z422}} \quad \mathbb{Q}_{2,1}^{(1,-1;c)}(T_{2g}, b) = \frac{\sqrt{30}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{M}_{2,1}^{(b)}(T_{2u})}{30} - \frac{\sqrt{10}\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{M}_{2,1}^{(b)}(T_{2u})}{10} + \frac{\sqrt{10}\mathbb{M}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{10} + \frac{\sqrt{10}\mathbb{M}_{2,3}^{(1,-1;a)}(T_{2u})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{10}$$

$$\boxed{\text{z423}} \quad \mathbb{Q}_{2,2}^{(1,-1;c)}(T_{2g}, b) = \frac{\sqrt{30}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{M}_{2,2}^{(b)}(T_{2u})}{30} + \frac{\sqrt{10}\mathbb{M}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{10} + \frac{\sqrt{10}\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{M}_{2,2}^{(b)}(T_{2u})}{10} + \frac{\sqrt{10}\mathbb{M}_{2,3}^{(1,-1;a)}(T_{2u})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{10}$$

$$\boxed{\text{z424}} \quad \mathbb{Q}_{2,3}^{(1,-1;c)}(T_{2g}, b) = -\frac{\sqrt{30}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{M}_{2,3}^{(b)}(T_{2u})}{15} + \frac{\sqrt{10}\mathbb{M}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{10} + \frac{\sqrt{10}\mathbb{M}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{10}$$

$$\boxed{\text{z425}} \quad \mathbb{Q}_{4,1}^{(1,-1;c)}(T_{2g}) = -\frac{\sqrt{5}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{M}_{2,1}^{(b)}(T_{2u})}{10} + \frac{\sqrt{15}\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{M}_{2,1}^{(b)}(T_{2u})}{10} + \frac{\sqrt{15}\mathbb{M}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{15} + \frac{\sqrt{15}\mathbb{M}_{2,3}^{(1,-1;a)}(T_{2u})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{15}$$

$$\boxed{\text{z426}} \quad \mathbb{Q}_{4,2}^{(1,-1;c)}(T_{2g}) = -\frac{\sqrt{5}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{M}_{2,2}^{(b)}(T_{2u})}{10} + \frac{\sqrt{15}\mathbb{M}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{15} - \frac{\sqrt{15}\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{M}_{2,2}^{(b)}(T_{2u})}{10} + \frac{\sqrt{15}\mathbb{M}_{2,3}^{(1,-1;a)}(T_{2u})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{15}$$

$$\boxed{\text{z427}} \quad \mathbb{Q}_{4,3}^{(1,-1;c)}(T_{2g}) = \frac{\sqrt{5}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{M}_{2,3}^{(b)}(T_{2u})}{5} + \frac{\sqrt{15}\mathbb{M}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{15} + \frac{\sqrt{15}\mathbb{M}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{15}$$



$$\boxed{\text{z428}} \quad \mathbb{Q}_{2,1}^{(1,0;c)}(T_{2g}, a) = \frac{\sqrt{6}\mathbb{T}_{1,2}^{(1,0;a)}(T_{1u})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{6} + \frac{\sqrt{6}\mathbb{T}_{1,3}^{(1,0;a)}(T_{1u})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6}$$

$$\boxed{\text{z429}} \quad \mathbb{Q}_{2,2}^{(1,0;c)}(T_{2g}, a) = \frac{\sqrt{6}\mathbb{T}_{1,1}^{(1,0;a)}(T_{1u})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{6} + \frac{\sqrt{6}\mathbb{T}_{1,3}^{(1,0;a)}(T_{1u})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6}$$

$$\boxed{\text{z430}} \quad \mathbb{Q}_{2,3}^{(1,0;c)}(T_{2g}, a) = \frac{\sqrt{6}\mathbb{T}_{1,1}^{(1,0;a)}(T_{1u})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} + \frac{\sqrt{6}\mathbb{T}_{1,2}^{(1,0;a)}(T_{1u})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6}$$

$$\boxed{\text{z431}} \quad \mathbb{Q}_{2,1}^{(1,0;c)}(T_{2g}, b) = -\frac{\sqrt{6}\mathbb{T}_{1,2}^{(1,0;a)}(T_{1u})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{6} + \frac{\sqrt{6}\mathbb{T}_{1,3}^{(1,0;a)}(T_{1u})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{6}$$

$$\boxed{\text{z432}} \quad \mathbb{Q}_{2,2}^{(1,0;c)}(T_{2g}, b) = \frac{\sqrt{6}\mathbb{T}_{1,1}^{(1,0;a)}(T_{1u})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{6} - \frac{\sqrt{6}\mathbb{T}_{1,3}^{(1,0;a)}(T_{1u})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{6}$$

$$\boxed{\text{z433}} \quad \mathbb{Q}_{2,3}^{(1,0;c)}(T_{2g}, b) = -\frac{\sqrt{6}\mathbb{T}_{1,1}^{(1,0;a)}(T_{1u})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{6} + \frac{\sqrt{6}\mathbb{T}_{1,2}^{(1,0;a)}(T_{1u})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{6}$$

$$\boxed{\text{z434}} \quad \mathbb{Q}_{2,1}^{(1,1;c)}(T_{2g}) = \frac{\sqrt{3}\mathbb{M}_0^{(1,1;a)}(A_{1u})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{3}$$

$$\boxed{\text{z435}} \quad \mathbb{Q}_{2,2}^{(1,1;c)}(T_{2g}) = \frac{\sqrt{3}\mathbb{M}_0^{(1,1;a)}(A_{1u})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{3}$$

$$\boxed{\text{z436}} \quad \mathbb{Q}_{2,3}^{(1,1;c)}(T_{2g}) = \frac{\sqrt{3}\mathbb{M}_0^{(1,1;a)}(A_{1u})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{3}$$

$$\boxed{\text{z437}} \quad \mathbb{G}_{3,1}^{(1,-1;c)}(T_{2g}) = -\frac{\sqrt{3}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} - \frac{\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} - \frac{\mathbb{M}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3} + \frac{\mathbb{M}_{2,3}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{3}$$

$$\boxed{\text{z438}} \quad \mathbb{G}_{3,2}^{(1,-1;c)}(T_{2g}) = \frac{\sqrt{3}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} + \frac{\mathbb{M}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3} - \frac{\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} - \frac{\mathbb{M}_{2,3}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{3}$$

$$\boxed{\text{z439}} \quad \mathbb{G}_{3,3}^{(1,-1;c)}(T_{2g}) = -\frac{\mathbb{M}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{3} + \frac{\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3} + \frac{\mathbb{M}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{3}$$

$$\boxed{\text{z533}} \quad \mathbb{Q}_{3,1}^{(c)}(T_{2u}) = -\frac{\sqrt{3}\mathbb{Q}_{1,1}^{(a)}(T_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{6} - \frac{\mathbb{Q}_{1,1}^{(a)}(T_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{6} + \frac{\mathbb{Q}_{1,2}^{(a)}(T_{1u})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{3} - \frac{\mathbb{Q}_{1,3}^{(a)}(T_{1u})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{3}$$

$$\boxed{\text{z534}} \quad \mathbb{Q}_{3,2}^{(c)}(T_{2u}) = -\frac{\mathbb{Q}_{1,1}^{(a)}(T_{1u})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{3} + \frac{\sqrt{3}\mathbb{Q}_{1,2}^{(a)}(T_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{6} - \frac{\mathbb{Q}_{1,2}^{(a)}(T_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{6} + \frac{\mathbb{Q}_{1,3}^{(a)}(T_{1u})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{3}$$

$$\begin{aligned}
\text{z535} \quad \mathbb{Q}_{3,3}^{(c)}(T_{2u}) &= \frac{\mathbb{Q}_{1,1}^{(a)}(T_{1u})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{3} - \frac{\mathbb{Q}_{1,2}^{(a)}(T_{1u})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{3} + \frac{\mathbb{Q}_{1,3}^{(a)}(T_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{3} \\
\text{z536} \quad \mathbb{Q}_{3,1}^{(1,-1;c)}(T_{2u}) &= \frac{\sqrt{6}\mathbb{G}_{2,1}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{12} - \frac{\sqrt{6}\mathbb{G}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{12} + \frac{\sqrt{2}\mathbb{G}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{4} - \frac{\sqrt{2}\mathbb{G}_{2,2}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{4} \\
\text{z537} \quad \mathbb{Q}_{3,2}^{(1,-1;c)}(T_{2u}) &= \frac{\sqrt{6}\mathbb{G}_{2,1}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{12} + \frac{\sqrt{2}\mathbb{G}_{2,2}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{4} - \frac{\sqrt{6}\mathbb{G}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{12} - \frac{\sqrt{2}\mathbb{G}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{4} \\
\text{z538} \quad \mathbb{Q}_{3,3}^{(1,-1;c)}(T_{2u}) &= -\frac{\sqrt{6}\mathbb{G}_{2,1}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{6} + \frac{\sqrt{6}\mathbb{G}_{2,3}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{6} \\
\text{z539} \quad \mathbb{Q}_{3,1}^{(1,0;c)}(T_{2u}) &= -\frac{\sqrt{3}\mathbb{Q}_{1,1}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{6} - \frac{\mathbb{Q}_{1,1}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{6} + \frac{\mathbb{Q}_{1,2}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{3} - \frac{\mathbb{Q}_{1,3}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{3} \\
\text{z540} \quad \mathbb{Q}_{3,2}^{(1,0;c)}(T_{2u}) &= -\frac{\mathbb{Q}_{1,1}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{3} + \frac{\sqrt{3}\mathbb{Q}_{1,2}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{6} - \frac{\mathbb{Q}_{1,2}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{6} + \frac{\mathbb{Q}_{1,3}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{3} \\
\text{z541} \quad \mathbb{Q}_{3,3}^{(1,0;c)}(T_{2u}) &= \frac{\mathbb{Q}_{1,1}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{3} - \frac{\mathbb{Q}_{1,2}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{3} + \frac{\mathbb{Q}_{1,3}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{3} \\
\text{z542} \quad \mathbb{G}_{2,1}^{(c)}(T_{2u}) &= -\frac{\sqrt{6}\mathbb{Q}_{1,1}^{(a)}(T_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{6} - \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(T_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{6} - \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(T_{1u})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{6} + \frac{\sqrt{2}\mathbb{Q}_{1,3}^{(a)}(T_{1u})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{6} \\
\text{z543} \quad \mathbb{G}_{2,2}^{(c)}(T_{2u}) &= \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(T_{1u})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{6} + \frac{\sqrt{6}\mathbb{Q}_{1,2}^{(a)}(T_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{6} - \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(T_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{6} - \frac{\sqrt{2}\mathbb{Q}_{1,3}^{(a)}(T_{1u})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{6} \\
\text{z544} \quad \mathbb{G}_{2,3}^{(c)}(T_{2u}) &= -\frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(T_{1u})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{6} + \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(T_{1u})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{6} + \frac{\sqrt{2}\mathbb{Q}_{1,3}^{(a)}(T_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{3} \\
\text{z545} \quad \mathbb{G}_{2,1}^{(1,-1;c)}(T_{2u}, a) &= \frac{\sqrt{3}\mathbb{G}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{Q}_0^{(b)}(A_{1g})}{3} \\
\text{z546} \quad \mathbb{G}_{2,2}^{(1,-1;c)}(T_{2u}, a) &= \frac{\sqrt{3}\mathbb{G}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{Q}_0^{(b)}(A_{1g})}{3} \\
\text{z547} \quad \mathbb{G}_{2,3}^{(1,-1;c)}(T_{2u}, a) &= \frac{\sqrt{3}\mathbb{G}_{2,3}^{(1,-1;a)}(T_{2u})\mathbb{Q}_0^{(b)}(A_{1g})}{3}
\end{aligned}$$

$$\begin{aligned}
\text{z548} \quad \mathbb{G}_{2,1}^{(1,-1;c)}(T_{2u}, b) &= \frac{\sqrt{42}\mathbb{G}_{2,1}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{42} + \frac{\sqrt{42}\mathbb{G}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{42} - \frac{\sqrt{14}\mathbb{G}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{14} \\
&\quad - \frac{\sqrt{14}\mathbb{G}_{2,2}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{14} + \frac{\sqrt{14}\mathbb{G}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{14} + \frac{\sqrt{14}\mathbb{G}_{2,3}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{14} \\
\text{z549} \quad \mathbb{G}_{2,2}^{(1,-1;c)}(T_{2u}, b) &= \frac{\sqrt{42}\mathbb{G}_{2,1}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{42} + \frac{\sqrt{14}\mathbb{G}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{14} + \frac{\sqrt{14}\mathbb{G}_{2,2}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{14} \\
&\quad + \frac{\sqrt{42}\mathbb{G}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{42} + \frac{\sqrt{14}\mathbb{G}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{14} + \frac{\sqrt{14}\mathbb{G}_{2,3}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{14} \\
\text{z550} \quad \mathbb{G}_{2,3}^{(1,-1;c)}(T_{2u}, b) &= -\frac{\sqrt{42}\mathbb{G}_{2,1}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{21} + \frac{\sqrt{14}\mathbb{G}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{14} + \frac{\sqrt{14}\mathbb{G}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{14} - \frac{\sqrt{42}\mathbb{G}_{2,3}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{21} \\
\text{z551} \quad \mathbb{G}_{4,1}^{(1,-1;c)}(T_{2u}) &= -\frac{\sqrt{14}\mathbb{G}_{2,1}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{28} - \frac{\sqrt{14}\mathbb{G}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{28} + \frac{\sqrt{42}\mathbb{G}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{28} \\
&\quad + \frac{\sqrt{42}\mathbb{G}_{2,2}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{28} + \frac{\sqrt{42}\mathbb{G}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{21} + \frac{\sqrt{42}\mathbb{G}_{2,3}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{21} \\
\text{z552} \quad \mathbb{G}_{4,2}^{(1,-1;c)}(T_{2u}) &= -\frac{\sqrt{14}\mathbb{G}_{2,1}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{28} + \frac{\sqrt{42}\mathbb{G}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{21} - \frac{\sqrt{42}\mathbb{G}_{2,2}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{28} \\
&\quad - \frac{\sqrt{14}\mathbb{G}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{28} - \frac{\sqrt{42}\mathbb{G}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{28} + \frac{\sqrt{42}\mathbb{G}_{2,3}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{21} \\
\text{z553} \quad \mathbb{G}_{4,3}^{(1,-1;c)}(T_{2u}) &= \frac{\sqrt{14}\mathbb{G}_{2,1}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{14} + \frac{\sqrt{42}\mathbb{G}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{21} + \frac{\sqrt{42}\mathbb{G}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{21} + \frac{\sqrt{14}\mathbb{G}_{2,3}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{14} \\
\text{z554} \quad \mathbb{G}_{2,1}^{(1,0;c)}(T_{2u}) &= -\frac{\sqrt{6}\mathbb{Q}_{1,1}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{6} - \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{6} - \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{6} + \frac{\sqrt{2}\mathbb{Q}_{1,3}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{6} \\
\text{z555} \quad \mathbb{G}_{2,2}^{(1,0;c)}(T_{2u}) &= \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{6} + \frac{\sqrt{6}\mathbb{Q}_{1,2}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{6} - \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{6} - \frac{\sqrt{2}\mathbb{Q}_{1,3}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{6} \\
\text{z556} \quad \mathbb{G}_{2,3}^{(1,0;c)}(T_{2u}) &= -\frac{\sqrt{2}\mathbb{Q}_{1,1}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{6} + \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{6} + \frac{\sqrt{2}\mathbb{Q}_{1,3}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{3} \\
\text{z557} \quad \mathbb{G}_{2,1}^{(1,1;c)}(T_{2u}) &= \frac{\sqrt{3}\mathbb{G}_0^{(1,1;a)}(A_{1u})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{3} \\
\text{z558} \quad \mathbb{G}_{2,2}^{(1,1;c)}(T_{2u}) &= \frac{\sqrt{3}\mathbb{G}_0^{(1,1;a)}(A_{1u})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{3}
\end{aligned}$$

$$\boxed{\text{z559}} \quad \mathbb{G}_{2,3}^{(1,1;c)}(T_{2u}) = \frac{\sqrt{3}\mathbb{G}_0^{(1,1;a)}(A_{1u})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{3}$$

• 'A'-'A' bond-cluster : **A;A\_002\_1**

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

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

\* wyckoff: **6b03c**

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

$$\boxed{\text{z16}} \quad \mathbb{Q}_0^{(c)}(A_{1g}, b) = \frac{\sqrt{5}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(E_g)}{5} + \frac{\sqrt{5}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{5} + \frac{\sqrt{5}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(E_g)}{5} + \frac{\sqrt{5}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{5} + \frac{\sqrt{5}\mathbb{Q}_{2,3}^{(a)}(T_{2g})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{5}$$

$$\boxed{\text{z17}} \quad \mathbb{Q}_4^{(c)}(A_{1g}) = \frac{\sqrt{30}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(E_g)}{10} - \frac{\sqrt{30}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{15} + \frac{\sqrt{30}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(E_g)}{10} - \frac{\sqrt{30}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{15} - \frac{\sqrt{30}\mathbb{Q}_{2,3}^{(a)}(T_{2g})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{15}$$

$$\boxed{\text{z18}} \quad \mathbb{Q}_0^{(1,-1;c)}(A_{1g}) = \frac{\sqrt{5}\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(E_g)}{5} + \frac{\sqrt{5}\mathbb{Q}_{2,1}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{5} + \frac{\sqrt{5}\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(E_g)}{5} + \frac{\sqrt{5}\mathbb{Q}_{2,2}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{5} + \frac{\sqrt{5}\mathbb{Q}_{2,3}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{5}$$

$$\boxed{\text{z19}} \quad \mathbb{Q}_4^{(1,-1;c)}(A_{1g}) = \frac{\sqrt{30}\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(E_g)}{10} - \frac{\sqrt{30}\mathbb{Q}_{2,1}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{15} + \frac{\sqrt{30}\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(E_g)}{10} - \frac{\sqrt{30}\mathbb{Q}_{2,2}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{15} - \frac{\sqrt{30}\mathbb{Q}_{2,3}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{15}$$

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

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

$$\boxed{\text{z28}} \quad \mathbb{G}_0^{(1,-1;c)}(A_{1u}) = \frac{\sqrt{3}\mathbb{M}_{1,1}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{3} + \frac{\sqrt{3}\mathbb{M}_{1,2}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{3} + \frac{\sqrt{3}\mathbb{M}_{1,3}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3}$$

$$\boxed{\text{z29}} \quad \mathbb{G}_4^{(1,-1;c)}(A_{1u}, a) = \frac{\sqrt{3}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{3} + \frac{\sqrt{3}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{3} + \frac{\sqrt{3}\mathbb{M}_{3,3}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3}$$

$$\boxed{\text{z68}} \quad \mathbb{G}_4^{(1,-1;c)}(A_{1u}, b) = -\frac{\sqrt{3}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{2g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{3} - \frac{\sqrt{3}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{2g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{3} - \frac{\sqrt{3}\mathbb{M}_{3,3}^{(1,-1;a)}(T_{2g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{3}$$

$$\boxed{\text{z69}} \quad \mathbb{G}_0^{(1,0;c)}(A_{1u}) = \frac{\sqrt{3}\mathbb{T}_{2,1}^{(1,0;a)}(T_{2g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{3} + \frac{\sqrt{3}\mathbb{T}_{2,2}^{(1,0;a)}(T_{2g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{3} + \frac{\sqrt{3}\mathbb{T}_{2,3}^{(1,0;a)}(T_{2g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{3}$$

$$\boxed{\text{z70}} \quad \mathbb{G}_0^{(1,1;c)}(A_{1u}) = \frac{\sqrt{3}\mathbb{M}_{1,1}^{(1,1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{3} + \frac{\sqrt{3}\mathbb{M}_{1,2}^{(1,1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{3} + \frac{\sqrt{3}\mathbb{M}_{1,3}^{(1,1;a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3}$$

$$\boxed{\text{z71}} \quad \mathbb{G}_3^{(c)}(A_{2g}) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2} - \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z72}} \quad \mathbb{G}_3^{(1,-1;c)}(A_{2g}) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2} - \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z73}} \quad \mathbb{G}_3^{(1,0;c)}(A_{2g}) = \frac{\sqrt{3}\mathbb{G}_{1,1}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{3} + \frac{\sqrt{3}\mathbb{G}_{1,2}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{3} + \frac{\sqrt{3}\mathbb{G}_{1,3}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{3}$$

$$\boxed{\text{z74}} \quad \mathbb{Q}_3^{(c)}(A_{2u}) = \frac{\sqrt{3}\mathbb{M}_{1,1}^{(a)}(T_{1g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{3} + \frac{\sqrt{3}\mathbb{M}_{1,2}^{(a)}(T_{1g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{3} + \frac{\sqrt{3}\mathbb{M}_{1,3}^{(a)}(T_{1g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{3}$$

$$\boxed{\text{z75}} \quad \mathbb{Q}_3^{(1,-1;c)}(A_{2u},a) = -\frac{\sqrt{3}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{3} - \frac{\sqrt{3}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{3} - \frac{\sqrt{3}\mathbb{M}_{3,3}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3}$$

$$\boxed{\text{z76}} \quad \mathbb{Q}_3^{(1,-1;c)}(A_{2u},b) = -\frac{\sqrt{3}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{3} - \frac{\sqrt{3}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{3} - \frac{\sqrt{3}\mathbb{M}_{3,3}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{3}$$

$$\boxed{\text{z77}} \quad \mathbb{Q}_3^{(1,-1;c)}(A_{2u},c) = \frac{\sqrt{3}\mathbb{M}_{1,1}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{3} + \frac{\sqrt{3}\mathbb{M}_{1,2}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{3} + \frac{\sqrt{3}\mathbb{M}_{1,3}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{3}$$

$$\boxed{\text{z78}} \quad \mathbb{Q}_3^{(1,0;c)}(A_{2u}) = \frac{\sqrt{3}\mathbb{T}_{2,1}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{3} + \frac{\sqrt{3}\mathbb{T}_{2,2}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{3} + \frac{\sqrt{3}\mathbb{T}_{2,3}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3}$$

$$\boxed{\text{z79}} \quad \mathbb{Q}_3^{(1,1;c)}(A_{2u}) = \frac{\sqrt{3}\mathbb{M}_{1,1}^{(1,1;a)}(T_{1g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{3} + \frac{\sqrt{3}\mathbb{M}_{1,2}^{(1,1;a)}(T_{1g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{3} + \frac{\sqrt{3}\mathbb{M}_{1,3}^{(1,1;a)}(T_{1g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{3}$$

$$\boxed{\text{z80}} \quad \mathbb{Q}_{2,1}^{(c)}(E_g,a) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z81}} \quad \mathbb{Q}_{2,2}^{(c)}(E_g,a) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z82}} \quad \mathbb{Q}_{2,1}^{(c)}(E_g,b) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z83}} \quad \mathbb{Q}_{2,2}^{(c)}(E_g,b) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\begin{aligned}
\boxed{\text{z84}} \quad \mathbb{Q}_{2,1}^{(c)}(E_g, c) &= \frac{\sqrt{7}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(E_g)}{7} + \frac{\sqrt{7}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{14} - \frac{\sqrt{7}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(E_g)}{7} + \frac{\sqrt{7}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{14} - \frac{\sqrt{7}\mathbb{Q}_{2,3}^{(a)}(T_{2g})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{7} \\
\boxed{\text{z85}} \quad \mathbb{Q}_{2,2}^{(c)}(E_g, c) &= -\frac{\sqrt{7}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(E_g)}{7} - \frac{\sqrt{21}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{14} - \frac{\sqrt{7}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(E_g)}{7} + \frac{\sqrt{21}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{14} \\
\boxed{\text{z143}} \quad \mathbb{Q}_{4,1}^{(c)}(E_g) &= \frac{\sqrt{21}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(E_g)}{14} - \frac{\sqrt{21}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{21} - \frac{\sqrt{21}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(E_g)}{14} - \frac{\sqrt{21}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{21} + \frac{2\sqrt{21}\mathbb{Q}_{2,3}^{(a)}(T_{2g})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{21} \\
\boxed{\text{z144}} \quad \mathbb{Q}_{4,2}^{(c)}(E_g) &= -\frac{\sqrt{21}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(E_g)}{14} + \frac{\sqrt{7}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{7} - \frac{\sqrt{21}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(E_g)}{14} - \frac{\sqrt{7}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{7} \\
\boxed{\text{z145}} \quad \mathbb{Q}_{2,1}^{(1,-1;c)}(E_g, a) &= \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_0^{(b)}(A_{1g})}{2} \\
\boxed{\text{z146}} \quad \mathbb{Q}_{2,2}^{(1,-1;c)}(E_g, a) &= \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_0^{(b)}(A_{1g})}{2} \\
\boxed{\text{z147}} \quad \mathbb{Q}_{2,1}^{(1,-1;c)}(E_g, b) &= \frac{\sqrt{7}\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(E_g)}{7} + \frac{\sqrt{7}\mathbb{Q}_{2,1}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{14} - \frac{\sqrt{7}\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(E_g)}{7} + \frac{\sqrt{7}\mathbb{Q}_{2,2}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{14} - \frac{\sqrt{7}\mathbb{Q}_{2,3}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{7} \\
\boxed{\text{z148}} \quad \mathbb{Q}_{2,2}^{(1,-1;c)}(E_g, b) &= -\frac{\sqrt{7}\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(E_g)}{7} - \frac{\sqrt{21}\mathbb{Q}_{2,1}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{14} - \frac{\sqrt{7}\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(E_g)}{7} + \frac{\sqrt{21}\mathbb{Q}_{2,2}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{14} \\
\boxed{\text{z149}} \quad \mathbb{Q}_{4,1}^{(1,-1;c)}(E_g) &= \frac{\sqrt{21}\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(E_g)}{14} - \frac{\sqrt{21}\mathbb{Q}_{2,1}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{21} - \frac{\sqrt{21}\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(E_g)}{14} - \frac{\sqrt{21}\mathbb{Q}_{2,2}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{21} + \frac{2\sqrt{21}\mathbb{Q}_{2,3}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{21} \\
\boxed{\text{z150}} \quad \mathbb{Q}_{4,2}^{(1,-1;c)}(E_g) &= -\frac{\sqrt{21}\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(E_g)}{14} + \frac{\sqrt{7}\mathbb{Q}_{2,1}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{7} - \frac{\sqrt{21}\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(E_g)}{14} - \frac{\sqrt{7}\mathbb{Q}_{2,2}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{7} \\
\boxed{\text{z151}} \quad \mathbb{Q}_{2,1}^{(1,0;c)}(E_g) &= \frac{\mathbb{G}_{1,1}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{2} - \frac{\mathbb{G}_{1,2}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{2} \\
\boxed{\text{z152}} \quad \mathbb{Q}_{2,2}^{(1,0;c)}(E_g) &= \frac{\sqrt{3}\mathbb{G}_{1,1}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{6} + \frac{\sqrt{3}\mathbb{G}_{1,2}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{6} - \frac{\sqrt{3}\mathbb{G}_{1,3}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{3} \\
\boxed{\text{z153}} \quad \mathbb{Q}_{2,1}^{(1,1;c)}(E_g) &= \frac{\sqrt{2}\mathbb{Q}_0^{(1,1;a)}(A_{1g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} \\
\boxed{\text{z154}} \quad \mathbb{Q}_{2,2}^{(1,1;c)}(E_g) &= \frac{\sqrt{2}\mathbb{Q}_0^{(1,1;a)}(A_{1g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}
\end{aligned}$$

$$\begin{aligned}
\boxed{\text{z155}} \quad \mathbb{Q}_{5,1}^{(1,-1;c)}(E_u) &= \frac{\sqrt{70}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{28} - \frac{\sqrt{42}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{2g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{28} - \frac{\sqrt{70}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{28} - \frac{\sqrt{42}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{2g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{28} + \frac{\sqrt{42}\mathbb{M}_{3,3}^{(1,-1;a)}(T_{2g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{14} \\
\boxed{\text{z156}} \quad \mathbb{Q}_{5,2}^{(1,-1;c)}(E_u) &= \frac{\sqrt{210}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{84} + \frac{3\sqrt{14}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{2g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{28} + \frac{\sqrt{210}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{84} - \frac{3\sqrt{14}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{2g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{28} - \frac{\sqrt{210}\mathbb{M}_{3,3}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{42} \\
\boxed{\text{z157}} \quad \mathbb{G}_{2,1}^{(c)}(E_u, a) &= -\frac{\sqrt{3}\mathbb{M}_{1,1}^{(a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} - \frac{\sqrt{3}\mathbb{M}_{1,2}^{(a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} + \frac{\sqrt{3}\mathbb{M}_{1,3}^{(a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3} \\
\boxed{\text{z158}} \quad \mathbb{G}_{2,2}^{(c)}(E_u, a) &= \frac{\mathbb{M}_{1,1}^{(a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{2} - \frac{\mathbb{M}_{1,2}^{(a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{2} \\
\boxed{\text{z159}} \quad \mathbb{G}_{2,1}^{(c)}(E_u, b) &= \frac{\mathbb{M}_{1,1}^{(a)}(T_{1g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{2} - \frac{\mathbb{M}_{1,2}^{(a)}(T_{1g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{2} \\
\boxed{\text{z160}} \quad \mathbb{G}_{2,2}^{(c)}(E_u, b) &= \frac{\sqrt{3}\mathbb{M}_{1,1}^{(a)}(T_{1g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{6} + \frac{\sqrt{3}\mathbb{M}_{1,2}^{(a)}(T_{1g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{6} - \frac{\sqrt{3}\mathbb{M}_{1,3}^{(a)}(T_{1g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{3} \\
\boxed{\text{z161}} \quad \mathbb{G}_{2,1}^{(1,-1;c)}(E_u, a) &= -\frac{\sqrt{42}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{28} - \frac{\sqrt{70}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{28} - \frac{\sqrt{42}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{28} + \frac{\sqrt{70}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{28} + \frac{\sqrt{42}\mathbb{M}_{3,3}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{14} \\
\boxed{\text{z162}} \quad \mathbb{G}_{2,2}^{(1,-1;c)}(E_u, a) &= \frac{3\sqrt{14}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{28} - \frac{\sqrt{210}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{84} - \frac{3\sqrt{14}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{28} - \frac{\sqrt{210}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{84} + \frac{\sqrt{210}\mathbb{M}_{3,3}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{42} \\
\boxed{\text{z163}} \quad \mathbb{G}_{2,1}^{(1,-1;c)}(E_u, b) &= -\frac{3\sqrt{14}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{28} - \frac{\sqrt{210}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{2g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{84} + \frac{3\sqrt{14}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{28} \\
&\quad - \frac{\sqrt{210}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{2g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{84} + \frac{\sqrt{210}\mathbb{M}_{3,3}^{(1,-1;a)}(T_{2g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{42} \\
\boxed{\text{z164}} \quad \mathbb{G}_{2,2}^{(1,-1;c)}(E_u, b) &= -\frac{\sqrt{42}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{28} + \frac{\sqrt{70}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{2g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{28} - \frac{\sqrt{42}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{28} - \frac{\sqrt{70}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{2g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{28} + \frac{\sqrt{42}\mathbb{M}_{3,3}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{14} \\
\boxed{\text{z165}} \quad \mathbb{G}_{2,1}^{(1,-1;c)}(E_u, c) &= -\frac{\sqrt{3}\mathbb{M}_{1,1}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} - \frac{\sqrt{3}\mathbb{M}_{1,2}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} + \frac{\sqrt{3}\mathbb{M}_{1,3}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3} \\
\boxed{\text{z166}} \quad \mathbb{G}_{2,2}^{(1,-1;c)}(E_u, c) &= \frac{\mathbb{M}_{1,1}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{2} - \frac{\mathbb{M}_{1,2}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{2} \\
\boxed{\text{z167}} \quad \mathbb{G}_{2,1}^{(1,-1;c)}(E_u, d) &= \frac{\mathbb{M}_{1,1}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{2} - \frac{\mathbb{M}_{1,2}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{2}
\end{aligned}$$

$$\begin{aligned}
\text{z168} \quad \mathbb{G}_{2,2}^{(1,-1;c)}(E_u, d) &= \frac{\sqrt{3}\mathbb{M}_{1,1}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{6} + \frac{\sqrt{3}\mathbb{M}_{1,2}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{6} - \frac{\sqrt{3}\mathbb{M}_{1,3}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{3} \\
\text{z169} \quad \mathbb{G}_{4,1}^{(1,-1;c)}(E_u) &= -\frac{\sqrt{210}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{84} + \frac{3\sqrt{14}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{28} - \frac{\sqrt{210}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{84} - \frac{3\sqrt{14}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{28} + \frac{\sqrt{210}\mathbb{M}_{3,3}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{42} \\
\text{z233} \quad \mathbb{G}_{4,2}^{(1,-1;c)}(E_u) &= \frac{\sqrt{70}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{28} + \frac{\sqrt{42}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{28} - \frac{\sqrt{70}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{28} + \frac{\sqrt{42}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{28} - \frac{\sqrt{42}\mathbb{M}_{3,3}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{14} \\
\text{z234} \quad \mathbb{G}_{2,1}^{(1,0;c)}(E_u, a) &= -\frac{\mathbb{T}_{2,1}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{2} + \frac{\mathbb{T}_{2,2}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{2} \\
\text{z235} \quad \mathbb{G}_{2,2}^{(1,0;c)}(E_u, a) &= -\frac{\sqrt{3}\mathbb{T}_{2,1}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} - \frac{\sqrt{3}\mathbb{T}_{2,2}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} + \frac{\sqrt{3}\mathbb{T}_{2,3}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3} \\
\text{z236} \quad \mathbb{G}_{2,1}^{(1,0;c)}(E_u, b) &= \frac{\sqrt{3}\mathbb{T}_{2,1}^{(1,0;a)}(T_{2g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{6} + \frac{\sqrt{3}\mathbb{T}_{2,2}^{(1,0;a)}(T_{2g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{6} - \frac{\sqrt{3}\mathbb{T}_{2,3}^{(1,0;a)}(T_{2g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{3} \\
\text{z237} \quad \mathbb{G}_{2,2}^{(1,0;c)}(E_u, b) &= -\frac{\mathbb{T}_{2,1}^{(1,0;a)}(T_{2g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{2} + \frac{\mathbb{T}_{2,2}^{(1,0;a)}(T_{2g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{2} \\
\text{z238} \quad \mathbb{G}_{2,1}^{(1,1;c)}(E_u, a) &= -\frac{\sqrt{3}\mathbb{M}_{1,1}^{(1,1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} - \frac{\sqrt{3}\mathbb{M}_{1,2}^{(1,1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} + \frac{\sqrt{3}\mathbb{M}_{1,3}^{(1,1;a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3} \\
\text{z239} \quad \mathbb{G}_{2,2}^{(1,1;c)}(E_u, a) &= \frac{\mathbb{M}_{1,1}^{(1,1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{2} - \frac{\mathbb{M}_{1,2}^{(1,1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{2} \\
\text{z240} \quad \mathbb{G}_{2,1}^{(1,1;c)}(E_u, b) &= \frac{\mathbb{M}_{1,1}^{(1,1;a)}(T_{1g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{2} - \frac{\mathbb{M}_{1,2}^{(1,1;a)}(T_{1g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{2} \\
\text{z241} \quad \mathbb{G}_{2,2}^{(1,1;c)}(E_u, b) &= \frac{\sqrt{3}\mathbb{M}_{1,1}^{(1,1;a)}(T_{1g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{6} + \frac{\sqrt{3}\mathbb{M}_{1,2}^{(1,1;a)}(T_{1g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{6} - \frac{\sqrt{3}\mathbb{M}_{1,3}^{(1,1;a)}(T_{1g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{3} \\
\text{z242} \quad \mathbb{Q}_{4,1}^{(c)}(T_{1g}) &= -\frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{4} - \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{4} - \frac{\sqrt{6}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{12} - \frac{\sqrt{6}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{12} \\
\text{z243} \quad \mathbb{Q}_{4,2}^{(c)}(T_{1g}) &= \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{4} - \frac{\sqrt{6}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{12} + \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{4} - \frac{\sqrt{6}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{12} \\
\text{z244} \quad \mathbb{Q}_{4,3}^{(c)}(T_{1g}) &= \frac{\sqrt{6}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{6} + \frac{\sqrt{6}\mathbb{Q}_{2,3}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{6}
\end{aligned}$$



$$\begin{aligned}
\boxed{\text{z245}} \quad \mathbb{Q}_{4,1}^{(1,-1;c)}(T_{1g}) &= -\frac{\sqrt{2}\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{4} - \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{4} - \frac{\sqrt{6}\mathbb{Q}_{2,1}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{12} - \frac{\sqrt{6}\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{12} \\
\boxed{\text{z246}} \quad \mathbb{Q}_{4,2}^{(1,-1;c)}(T_{1g}) &= \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{4} - \frac{\sqrt{6}\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{12} + \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{4} - \frac{\sqrt{6}\mathbb{Q}_{2,2}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{12} \\
\boxed{\text{z247}} \quad \mathbb{Q}_{4,3}^{(1,-1;c)}(T_{1g}) &= \frac{\sqrt{6}\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{6} + \frac{\sqrt{6}\mathbb{Q}_{2,3}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{6} \\
\boxed{\text{z248}} \quad \mathbb{G}_{1,1}^{(c)}(T_{1g}) &= -\frac{\sqrt{10}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{10} + \frac{\sqrt{10}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{10} + \frac{\sqrt{30}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{30} - \frac{\sqrt{30}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{30} - \frac{\sqrt{30}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{30} + \frac{\sqrt{30}\mathbb{Q}_{2,3}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{30} \\
\boxed{\text{z249}} \quad \mathbb{G}_{1,2}^{(c)}(T_{1g}) &= \frac{\sqrt{10}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{10} + \frac{\sqrt{30}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{30} - \frac{\sqrt{30}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{30} - \frac{\sqrt{10}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{10} + \frac{\sqrt{30}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{30} - \frac{\sqrt{30}\mathbb{Q}_{2,3}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{30} \\
\boxed{\text{z250}} \quad \mathbb{G}_{1,3}^{(c)}(T_{1g}) &= -\frac{\sqrt{30}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{30} + \frac{\sqrt{30}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{15} + \frac{\sqrt{30}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{30} - \frac{\sqrt{30}\mathbb{Q}_{2,3}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{15} \\
\boxed{\text{z251}} \quad \mathbb{G}_{3,1}^{(c)}(T_{1g}) &= \frac{\sqrt{10}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{20} - \frac{\sqrt{10}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{20} - \frac{\sqrt{30}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{60} + \frac{\sqrt{30}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{60} - \frac{\sqrt{30}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{15} + \frac{\sqrt{30}\mathbb{Q}_{2,3}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{15} \\
\boxed{\text{z252}} \quad \mathbb{G}_{3,2}^{(c)}(T_{1g}) &= -\frac{\sqrt{10}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{20} + \frac{\sqrt{30}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{15} + \frac{\sqrt{30}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{60} + \frac{\sqrt{10}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{20} - \frac{\sqrt{30}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{60} - \frac{\sqrt{30}\mathbb{Q}_{2,3}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{15} \\
\boxed{\text{z253}} \quad \mathbb{G}_{3,3}^{(c)}(T_{1g}) &= -\frac{\sqrt{30}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{15} - \frac{\sqrt{30}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{30} + \frac{\sqrt{30}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{15} + \frac{\sqrt{30}\mathbb{Q}_{2,3}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{30} \\
\boxed{\text{z254}} \quad \mathbb{G}_{1,1}^{(1,-1;c)}(T_{1g}) &= -\frac{\sqrt{10}\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{10} + \frac{\sqrt{10}\mathbb{Q}_{2,1}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{10} + \frac{\sqrt{30}\mathbb{Q}_{2,1}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{30} \\
&\quad - \frac{\sqrt{30}\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{30} - \frac{\sqrt{30}\mathbb{Q}_{2,2}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{30} + \frac{\sqrt{30}\mathbb{Q}_{2,3}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{30} \\
\boxed{\text{z255}} \quad \mathbb{G}_{1,2}^{(1,-1;c)}(T_{1g}) &= \frac{\sqrt{10}\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{10} + \frac{\sqrt{30}\mathbb{Q}_{2,1}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{30} - \frac{\sqrt{30}\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{30} \\
&\quad - \frac{\sqrt{10}\mathbb{Q}_{2,2}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{10} + \frac{\sqrt{30}\mathbb{Q}_{2,2}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{30} - \frac{\sqrt{30}\mathbb{Q}_{2,3}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{30} \\
\boxed{\text{z256}} \quad \mathbb{G}_{1,3}^{(1,-1;c)}(T_{1g}) &= -\frac{\sqrt{30}\mathbb{Q}_{2,1}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{30} + \frac{\sqrt{30}\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{15} + \frac{\sqrt{30}\mathbb{Q}_{2,2}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{30} - \frac{\sqrt{30}\mathbb{Q}_{2,3}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{15}
\end{aligned}$$

$$\begin{aligned}
\boxed{\text{z257}} \quad \mathbb{G}_{3,1}^{(1,-1;c)}(T_{1g}) &= \frac{\sqrt{10}\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{20} - \frac{\sqrt{10}\mathbb{Q}_{2,1}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{20} - \frac{\sqrt{30}\mathbb{Q}_{2,1}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{60} \\
&+ \frac{\sqrt{30}\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{60} - \frac{\sqrt{30}\mathbb{Q}_{2,2}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{15} + \frac{\sqrt{30}\mathbb{Q}_{2,3}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{15} \\
\boxed{\text{z258}} \quad \mathbb{G}_{3,2}^{(1,-1;c)}(T_{1g}) &= -\frac{\sqrt{10}\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{20} + \frac{\sqrt{30}\mathbb{Q}_{2,1}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{15} + \frac{\sqrt{30}\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{60} \\
&+ \frac{\sqrt{10}\mathbb{Q}_{2,2}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{20} - \frac{\sqrt{30}\mathbb{Q}_{2,2}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{60} - \frac{\sqrt{30}\mathbb{Q}_{2,3}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{15} \\
\boxed{\text{z259}} \quad \mathbb{G}_{3,3}^{(1,-1;c)}(T_{1g}) &= -\frac{\sqrt{30}\mathbb{Q}_{2,1}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{15} - \frac{\sqrt{30}\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{30} + \frac{\sqrt{30}\mathbb{Q}_{2,2}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{15} + \frac{\sqrt{30}\mathbb{Q}_{2,3}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{30} \\
\boxed{\text{z260}} \quad \mathbb{G}_{1,1}^{(1,0;c)}(T_{1g}, a) &= \frac{\sqrt{3}\mathbb{G}_{1,1}^{(1,0;a)}(T_{1g})\mathbb{Q}_0^{(b)}(A_{1g})}{3} \\
\boxed{\text{z261}} \quad \mathbb{G}_{1,2}^{(1,0;c)}(T_{1g}, a) &= \frac{\sqrt{3}\mathbb{G}_{1,2}^{(1,0;a)}(T_{1g})\mathbb{Q}_0^{(b)}(A_{1g})}{3} \\
\boxed{\text{z262}} \quad \mathbb{G}_{1,3}^{(1,0;c)}(T_{1g}, a) &= \frac{\sqrt{3}\mathbb{G}_{1,3}^{(1,0;a)}(T_{1g})\mathbb{Q}_0^{(b)}(A_{1g})}{3} \\
\boxed{\text{z263}} \quad \mathbb{G}_{1,1}^{(1,0;c)}(T_{1g}, b) &= -\frac{\sqrt{30}\mathbb{G}_{1,1}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{30} + \frac{\sqrt{10}\mathbb{G}_{1,1}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{10} + \frac{\sqrt{10}\mathbb{G}_{1,2}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{10} + \frac{\sqrt{10}\mathbb{G}_{1,3}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{10} \\
\boxed{\text{z264}} \quad \mathbb{G}_{1,2}^{(1,0;c)}(T_{1g}, b) &= \frac{\sqrt{10}\mathbb{G}_{1,1}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{10} - \frac{\sqrt{30}\mathbb{G}_{1,2}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{30} - \frac{\sqrt{10}\mathbb{G}_{1,2}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{10} + \frac{\sqrt{10}\mathbb{G}_{1,3}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{10} \\
\boxed{\text{z265}} \quad \mathbb{G}_{1,3}^{(1,0;c)}(T_{1g}, b) &= \frac{\sqrt{10}\mathbb{G}_{1,1}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{10} + \frac{\sqrt{10}\mathbb{G}_{1,2}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{10} + \frac{\sqrt{30}\mathbb{G}_{1,3}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{15} \\
\boxed{\text{z266}} \quad \mathbb{G}_{3,1}^{(1,0;c)}(T_{1g}) &= -\frac{\sqrt{5}\mathbb{G}_{1,1}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{10} + \frac{\sqrt{15}\mathbb{G}_{1,1}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{10} - \frac{\sqrt{15}\mathbb{G}_{1,2}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{15} - \frac{\sqrt{15}\mathbb{G}_{1,3}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{15} \\
\boxed{\text{z267}} \quad \mathbb{G}_{3,2}^{(1,0;c)}(T_{1g}) &= -\frac{\sqrt{15}\mathbb{G}_{1,1}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{15} - \frac{\sqrt{5}\mathbb{G}_{1,2}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{10} - \frac{\sqrt{15}\mathbb{G}_{1,2}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{10} - \frac{\sqrt{15}\mathbb{G}_{1,3}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{15} \\
\boxed{\text{z268}} \quad \mathbb{G}_{3,3}^{(1,0;c)}(T_{1g}) &= -\frac{\sqrt{15}\mathbb{G}_{1,1}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{15} - \frac{\sqrt{15}\mathbb{G}_{1,2}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{15} + \frac{\sqrt{5}\mathbb{G}_{1,3}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{5}
\end{aligned}$$

$$\begin{aligned}
\boxed{\text{z281}} \quad \mathbb{Q}_{1,1}^{(c)}(T_{1u}, a) &= \frac{\sqrt{6}\mathbb{M}_{1,2}^{(a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{6} - \frac{\sqrt{6}\mathbb{M}_{1,3}^{(a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} \\
\boxed{\text{z282}} \quad \mathbb{Q}_{1,2}^{(c)}(T_{1u}, a) &= -\frac{\sqrt{6}\mathbb{M}_{1,1}^{(a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{6} + \frac{\sqrt{6}\mathbb{M}_{1,3}^{(a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} \\
\boxed{\text{z283}} \quad \mathbb{Q}_{1,3}^{(c)}(T_{1u}, a) &= \frac{\sqrt{6}\mathbb{M}_{1,1}^{(a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} - \frac{\sqrt{6}\mathbb{M}_{1,2}^{(a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} \\
\boxed{\text{z284}} \quad \mathbb{Q}_{1,1}^{(c)}(T_{1u}, b) &= \frac{\sqrt{6}\mathbb{M}_{1,2}^{(a)}(T_{1g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{6} + \frac{\sqrt{6}\mathbb{M}_{1,3}^{(a)}(T_{1g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{6} \\
\boxed{\text{z285}} \quad \mathbb{Q}_{1,2}^{(c)}(T_{1u}, b) &= \frac{\sqrt{6}\mathbb{M}_{1,1}^{(a)}(T_{1g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{6} + \frac{\sqrt{6}\mathbb{M}_{1,3}^{(a)}(T_{1g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{6} \\
\boxed{\text{z286}} \quad \mathbb{Q}_{1,3}^{(c)}(T_{1u}, b) &= \frac{\sqrt{6}\mathbb{M}_{1,1}^{(a)}(T_{1g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{6} + \frac{\sqrt{6}\mathbb{M}_{1,2}^{(a)}(T_{1g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{6} \\
\boxed{\text{z294}} \quad \mathbb{Q}_{1,1}^{(1,-1;c)}(T_{1u}, a) &= -\frac{\sqrt{21}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{21} - \frac{\sqrt{35}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{2g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{21} - \frac{\sqrt{21}\mathbb{M}_{3,3}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{21} + \frac{\sqrt{35}\mathbb{M}_{3,3}^{(1,-1;a)}(T_{2g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{21} + \frac{\sqrt{35}\mathbb{M}_3^{(1,-1;a)}(A_{2g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{21} \\
\boxed{\text{z295}} \quad \mathbb{Q}_{1,2}^{(1,-1;c)}(T_{1u}, a) &= -\frac{\sqrt{21}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{21} + \frac{\sqrt{35}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{2g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{21} - \frac{\sqrt{21}\mathbb{M}_{3,3}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{21} - \frac{\sqrt{35}\mathbb{M}_{3,3}^{(1,-1;a)}(T_{2g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{21} + \frac{\sqrt{35}\mathbb{M}_3^{(1,-1;a)}(A_{2g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{21} \\
\boxed{\text{z296}} \quad \mathbb{Q}_{1,3}^{(1,-1;c)}(T_{1u}, a) &= -\frac{\sqrt{21}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{21} - \frac{\sqrt{35}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{2g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{21} - \frac{\sqrt{21}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{21} + \frac{\sqrt{35}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{2g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{21} + \frac{\sqrt{35}\mathbb{M}_3^{(1,-1;a)}(A_{2g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{21} \\
\boxed{\text{z297}} \quad \mathbb{Q}_{1,1}^{(1,-1;c)}(T_{1u}, b) &= \frac{\sqrt{6}\mathbb{M}_{1,2}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{6} - \frac{\sqrt{6}\mathbb{M}_{1,3}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} \\
\boxed{\text{z298}} \quad \mathbb{Q}_{1,2}^{(1,-1;c)}(T_{1u}, b) &= -\frac{\sqrt{6}\mathbb{M}_{1,1}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{6} + \frac{\sqrt{6}\mathbb{M}_{1,3}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} \\
\boxed{\text{z299}} \quad \mathbb{Q}_{1,3}^{(1,-1;c)}(T_{1u}, b) &= \frac{\sqrt{6}\mathbb{M}_{1,1}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} - \frac{\sqrt{6}\mathbb{M}_{1,2}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} \\
\boxed{\text{z338}} \quad \mathbb{Q}_{1,1}^{(1,-1;c)}(T_{1u}, c) &= \frac{\sqrt{6}\mathbb{M}_{1,2}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{6} + \frac{\sqrt{6}\mathbb{M}_{1,3}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{6} \\
\boxed{\text{z339}} \quad \mathbb{Q}_{1,2}^{(1,-1;c)}(T_{1u}, c) &= \frac{\sqrt{6}\mathbb{M}_{1,1}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{6} + \frac{\sqrt{6}\mathbb{M}_{1,3}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{6}
\end{aligned}$$

$$\begin{aligned}
\text{z340} \quad \mathbb{Q}_{1,3}^{(1,-1;c)}(T_{1u}, c) &= \frac{\sqrt{6}\mathbb{M}_{1,1}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{6} + \frac{\sqrt{6}\mathbb{M}_{1,2}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{6} \\
\text{z341} \quad \mathbb{Q}_{3,1}^{(1,-1;c)}(T_{1u}, a) &= -\frac{\mathbb{M}_{3,2}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{4} - \frac{\sqrt{15}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{12} + \frac{\mathbb{M}_{3,3}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{4} - \frac{\sqrt{15}\mathbb{M}_{3,3}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{12} \\
\text{z342} \quad \mathbb{Q}_{3,2}^{(1,-1;c)}(T_{1u}, a) &= \frac{\mathbb{M}_{3,1}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{4} - \frac{\sqrt{15}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{12} - \frac{\mathbb{M}_{3,3}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{4} - \frac{\sqrt{15}\mathbb{M}_{3,3}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{12} \\
\text{z343} \quad \mathbb{Q}_{3,3}^{(1,-1;c)}(T_{1u}, a) &= -\frac{\mathbb{M}_{3,1}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{4} - \frac{\sqrt{15}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{12} + \frac{\mathbb{M}_{3,2}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{4} - \frac{\sqrt{15}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{12} \\
\text{z344} \quad \mathbb{Q}_{3,1}^{(1,-1;c)}(T_{1u}, b) &= -\frac{\sqrt{105}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{84} - \frac{5\sqrt{7}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{2g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{84} - \frac{\sqrt{105}\mathbb{M}_{3,3}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{84} \\
&\quad + \frac{5\sqrt{7}\mathbb{M}_{3,3}^{(1,-1;a)}(T_{2g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{84} - \frac{4\sqrt{7}\mathbb{M}_3^{(1,-1;a)}(A_{2g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{21} \\
\text{z345} \quad \mathbb{Q}_{3,2}^{(1,-1;c)}(T_{1u}, b) &= -\frac{\sqrt{105}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{84} + \frac{5\sqrt{7}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{2g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{84} - \frac{\sqrt{105}\mathbb{M}_{3,3}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{84} \\
&\quad - \frac{5\sqrt{7}\mathbb{M}_{3,3}^{(1,-1;a)}(T_{2g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{84} - \frac{4\sqrt{7}\mathbb{M}_3^{(1,-1;a)}(A_{2g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{21} \\
\text{z346} \quad \mathbb{Q}_{3,3}^{(1,-1;c)}(T_{1u}, b) &= -\frac{\sqrt{105}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{84} - \frac{5\sqrt{7}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{2g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{84} - \frac{\sqrt{105}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{84} \\
&\quad + \frac{5\sqrt{7}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{2g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{84} - \frac{4\sqrt{7}\mathbb{M}_3^{(1,-1;a)}(A_{2g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{21} \\
\text{z347} \quad \mathbb{Q}_{5,1}^{(1,-1;c)}(T_{1u}, 2) &= \frac{\sqrt{15}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{12} - \frac{\mathbb{M}_{3,2}^{(1,-1;a)}(T_{2g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{4} + \frac{\sqrt{15}\mathbb{M}_{3,3}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{12} + \frac{\mathbb{M}_{3,3}^{(1,-1;a)}(T_{2g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{4} \\
\text{z348} \quad \mathbb{Q}_{5,2}^{(1,-1;c)}(T_{1u}, 2) &= \frac{\sqrt{15}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{12} + \frac{\mathbb{M}_{3,1}^{(1,-1;a)}(T_{2g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{4} + \frac{\sqrt{15}\mathbb{M}_{3,3}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{12} - \frac{\mathbb{M}_{3,3}^{(1,-1;a)}(T_{2g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{4} \\
\text{z349} \quad \mathbb{Q}_{5,3}^{(1,-1;c)}(T_{1u}, 2) &= \frac{\sqrt{15}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{12} - \frac{\mathbb{M}_{3,1}^{(1,-1;a)}(T_{2g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{4} + \frac{\sqrt{15}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{12} + \frac{\mathbb{M}_{3,2}^{(1,-1;a)}(T_{2g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{4} \\
\text{z350} \quad \mathbb{Q}_{1,1}^{(1,0;c)}(T_{1u}, a) &= -\frac{\sqrt{30}\mathbb{T}_{2,1}^{(1,0;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(T_{1u})}{30} + \frac{\sqrt{10}\mathbb{T}_{2,2}^{(1,0;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(T_{1u})}{10} + \frac{\sqrt{10}\mathbb{T}_{2,2}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{10} + \frac{\sqrt{10}\mathbb{T}_{2,3}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{10}
\end{aligned}$$

$$\begin{aligned}
\text{z351} \quad \mathbb{Q}_{1,2}^{(1,0;c)}(T_{1u}, a) &= -\frac{\sqrt{30}\mathbb{T}_{2,1}^{(1,0;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(T_{1u})}{30} + \frac{\sqrt{10}\mathbb{T}_{2,1}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{10} - \frac{\sqrt{10}\mathbb{T}_{2,2}^{(1,0;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(T_{1u})}{10} + \frac{\sqrt{10}\mathbb{T}_{2,3}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{10} \\
\text{z352} \quad \mathbb{Q}_{1,3}^{(1,0;c)}(T_{1u}, a) &= \frac{\sqrt{30}\mathbb{T}_{2,1}^{(1,0;a)}(E_g)\mathbb{T}_{1,3}^{(b)}(T_{1u})}{15} + \frac{\sqrt{10}\mathbb{T}_{2,1}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{10} + \frac{\sqrt{10}\mathbb{T}_{2,2}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{10} \\
\text{z353} \quad \mathbb{Q}_{1,1}^{(1,0;c)}(T_{1u}, b) &= -\frac{\sqrt{6}\mathbb{T}_{2,1}^{(1,0;a)}(E_g)\mathbb{M}_{2,1}^{(b)}(T_{2u})}{6} - \frac{\sqrt{2}\mathbb{T}_{2,2}^{(1,0;a)}(E_g)\mathbb{M}_{2,1}^{(b)}(T_{2u})}{6} - \frac{\sqrt{2}\mathbb{T}_{2,2}^{(1,0;a)}(T_{2g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{6} + \frac{\sqrt{2}\mathbb{T}_{2,3}^{(1,0;a)}(T_{2g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{6} \\
\text{z354} \quad \mathbb{Q}_{1,2}^{(1,0;c)}(T_{1u}, b) &= \frac{\sqrt{6}\mathbb{T}_{2,1}^{(1,0;a)}(E_g)\mathbb{M}_{2,2}^{(b)}(T_{2u})}{6} + \frac{\sqrt{2}\mathbb{T}_{2,1}^{(1,0;a)}(T_{2g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{6} - \frac{\sqrt{2}\mathbb{T}_{2,2}^{(1,0;a)}(E_g)\mathbb{M}_{2,2}^{(b)}(T_{2u})}{6} - \frac{\sqrt{2}\mathbb{T}_{2,3}^{(1,0;a)}(T_{2g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{6} \\
\text{z355} \quad \mathbb{Q}_{1,3}^{(1,0;c)}(T_{1u}, b) &= -\frac{\sqrt{2}\mathbb{T}_{2,1}^{(1,0;a)}(T_{2g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{6} + \frac{\sqrt{2}\mathbb{T}_{2,2}^{(1,0;a)}(E_g)\mathbb{M}_{2,3}^{(b)}(T_{2u})}{3} + \frac{\sqrt{2}\mathbb{T}_{2,2}^{(1,0;a)}(T_{2g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{6} \\
\text{z356} \quad \mathbb{Q}_{3,1}^{(1,0;c)}(T_{1u}, a) &= -\frac{\sqrt{5}\mathbb{T}_{2,1}^{(1,0;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(T_{1u})}{10} + \frac{\sqrt{15}\mathbb{T}_{2,2}^{(1,0;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(T_{1u})}{10} - \frac{\sqrt{15}\mathbb{T}_{2,2}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{15} - \frac{\sqrt{15}\mathbb{T}_{2,3}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{15} \\
\text{z357} \quad \mathbb{Q}_{3,2}^{(1,0;c)}(T_{1u}, a) &= -\frac{\sqrt{5}\mathbb{T}_{2,1}^{(1,0;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(T_{1u})}{10} - \frac{\sqrt{15}\mathbb{T}_{2,1}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{15} - \frac{\sqrt{15}\mathbb{T}_{2,2}^{(1,0;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(T_{1u})}{10} - \frac{\sqrt{15}\mathbb{T}_{2,3}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{15} \\
\text{z358} \quad \mathbb{Q}_{3,3}^{(1,0;c)}(T_{1u}, a) &= \frac{\sqrt{5}\mathbb{T}_{2,1}^{(1,0;a)}(E_g)\mathbb{T}_{1,3}^{(b)}(T_{1u})}{5} - \frac{\sqrt{15}\mathbb{T}_{2,1}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{15} - \frac{\sqrt{15}\mathbb{T}_{2,2}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{15} \\
\text{z359} \quad \mathbb{Q}_{3,1}^{(1,0;c)}(T_{1u}, b) &= \frac{\sqrt{3}\mathbb{T}_{2,1}^{(1,0;a)}(E_g)\mathbb{M}_{2,1}^{(b)}(T_{2u})}{6} + \frac{\mathbb{T}_{2,2}^{(1,0;a)}(E_g)\mathbb{M}_{2,1}^{(b)}(T_{2u})}{6} - \frac{\mathbb{T}_{2,2}^{(1,0;a)}(T_{2g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{3} + \frac{\mathbb{T}_{2,3}^{(1,0;a)}(T_{2g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{3} \\
\text{z360} \quad \mathbb{Q}_{3,2}^{(1,0;c)}(T_{1u}, b) &= -\frac{\sqrt{3}\mathbb{T}_{2,1}^{(1,0;a)}(E_g)\mathbb{M}_{2,2}^{(b)}(T_{2u})}{6} + \frac{\mathbb{T}_{2,1}^{(1,0;a)}(T_{2g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{3} + \frac{\mathbb{T}_{2,2}^{(1,0;a)}(E_g)\mathbb{M}_{2,2}^{(b)}(T_{2u})}{6} - \frac{\mathbb{T}_{2,3}^{(1,0;a)}(T_{2g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{3} \\
\text{z361} \quad \mathbb{Q}_{3,3}^{(1,0;c)}(T_{1u}, b) &= -\frac{\mathbb{T}_{2,1}^{(1,0;a)}(T_{2g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{3} - \frac{\mathbb{T}_{2,2}^{(1,0;a)}(E_g)\mathbb{M}_{2,3}^{(b)}(T_{2u})}{3} + \frac{\mathbb{T}_{2,2}^{(1,0;a)}(T_{2g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{3} \\
\text{z440} \quad \mathbb{Q}_{1,1}^{(1,1;c)}(T_{1u}, a) &= \frac{\sqrt{6}\mathbb{M}_{1,2}^{(1,1;a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{6} - \frac{\sqrt{6}\mathbb{M}_{1,3}^{(1,1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} \\
\text{z441} \quad \mathbb{Q}_{1,2}^{(1,1;c)}(T_{1u}, a) &= -\frac{\sqrt{6}\mathbb{M}_{1,1}^{(1,1;a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{6} + \frac{\sqrt{6}\mathbb{M}_{1,3}^{(1,1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} \\
\text{z442} \quad \mathbb{Q}_{1,3}^{(1,1;c)}(T_{1u}, a) &= \frac{\sqrt{6}\mathbb{M}_{1,1}^{(1,1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} - \frac{\sqrt{6}\mathbb{M}_{1,2}^{(1,1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6}
\end{aligned}$$

$$\boxed{\text{z443}} \quad \mathbb{Q}_{1,1}^{(1,1;c)}(T_{1u}, b) = \frac{\sqrt{6}\mathbb{M}_{1,2}^{(1,1;a)}(T_{1g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{6} + \frac{\sqrt{6}\mathbb{M}_{1,3}^{(1,1;a)}(T_{1g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{6}$$

$$\boxed{\text{z444}} \quad \mathbb{Q}_{1,2}^{(1,1;c)}(T_{1u}, b) = \frac{\sqrt{6}\mathbb{M}_{1,1}^{(1,1;a)}(T_{1g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{6} + \frac{\sqrt{6}\mathbb{M}_{1,3}^{(1,1;a)}(T_{1g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{6}$$

$$\boxed{\text{z445}} \quad \mathbb{Q}_{1,3}^{(1,1;c)}(T_{1u}, b) = \frac{\sqrt{6}\mathbb{M}_{1,1}^{(1,1;a)}(T_{1g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{6} + \frac{\sqrt{6}\mathbb{M}_{1,2}^{(1,1;a)}(T_{1g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{6}$$

$$\boxed{\text{z446}} \quad \mathbb{G}_{4,1}^{(1,-1;c)}(T_{1u}) = \frac{\sqrt{15}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{12} - \frac{\mathbb{M}_{3,2}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{4} - \frac{\sqrt{15}\mathbb{M}_{3,3}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{12} - \frac{\mathbb{M}_{3,3}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{4}$$

$$\boxed{\text{z447}} \quad \mathbb{G}_{4,2}^{(1,-1;c)}(T_{1u}) = -\frac{\sqrt{15}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{12} - \frac{\mathbb{M}_{3,1}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{4} + \frac{\sqrt{15}\mathbb{M}_{3,3}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{12} - \frac{\mathbb{M}_{3,3}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{4}$$

$$\boxed{\text{z448}} \quad \mathbb{G}_{4,3}^{(1,-1;c)}(T_{1u}) = \frac{\sqrt{15}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{12} - \frac{\mathbb{M}_{3,1}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{4} - \frac{\sqrt{15}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{12} - \frac{\mathbb{M}_{3,2}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{4}$$

$$\boxed{\text{z449}} \quad \mathbb{Q}_{2,1}^{(c)}(T_{2g}, a) = \frac{\sqrt{3}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{3}$$

$$\boxed{\text{z450}} \quad \mathbb{Q}_{2,2}^{(c)}(T_{2g}, a) = \frac{\sqrt{3}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{3}$$

$$\boxed{\text{z451}} \quad \mathbb{Q}_{2,3}^{(c)}(T_{2g}, a) = \frac{\sqrt{3}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{3}$$

$$\boxed{\text{z452}} \quad \mathbb{Q}_{2,1}^{(c)}(T_{2g}, b) = \frac{\sqrt{3}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_0^{(b)}(A_{1g})}{3}$$

$$\boxed{\text{z453}} \quad \mathbb{Q}_{2,2}^{(c)}(T_{2g}, b) = \frac{\sqrt{3}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_0^{(b)}(A_{1g})}{3}$$

$$\boxed{\text{z454}} \quad \mathbb{Q}_{2,3}^{(c)}(T_{2g}, b) = \frac{\sqrt{3}\mathbb{Q}_{2,3}^{(a)}(T_{2g})\mathbb{Q}_0^{(b)}(A_{1g})}{3}$$

$$\boxed{\text{z455}} \quad \mathbb{Q}_{2,1}^{(c)}(T_{2g}, c) = \frac{\sqrt{42}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{42} + \frac{\sqrt{42}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{42} - \frac{\sqrt{14}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{14} - \frac{\sqrt{14}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{14} + \frac{\sqrt{14}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{14} + \frac{\sqrt{14}\mathbb{Q}_{2,3}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{14}$$

$$\boxed{\text{z456}} \quad \mathbb{Q}_{2,2}^{(c)}(T_{2g}, c) = \frac{\sqrt{42}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{42} + \frac{\sqrt{14}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{14} + \frac{\sqrt{14}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{14} + \frac{\sqrt{42}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{42} + \frac{\sqrt{14}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{14} + \frac{\sqrt{14}\mathbb{Q}_{2,3}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{14}$$

$$\begin{aligned}
\text{z457} \quad \mathbb{Q}_{2,3}^{(c)}(T_{2g}, c) &= -\frac{\sqrt{42}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{21} + \frac{\sqrt{14}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{14} + \frac{\sqrt{14}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{14} - \frac{\sqrt{42}\mathbb{Q}_{2,3}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{21} \\
\text{z458} \quad \mathbb{Q}_{4,1}^{(c)}(T_{2g}) &= -\frac{\sqrt{14}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{28} - \frac{\sqrt{14}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{28} + \frac{\sqrt{42}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{28} + \frac{\sqrt{42}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{28} + \frac{\sqrt{42}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{21} + \frac{\sqrt{42}\mathbb{Q}_{2,3}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{21} \\
\text{z459} \quad \mathbb{Q}_{4,2}^{(c)}(T_{2g}) &= -\frac{\sqrt{14}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{28} + \frac{\sqrt{42}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{21} - \frac{\sqrt{42}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{28} - \frac{\sqrt{14}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{28} - \frac{\sqrt{42}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{28} + \frac{\sqrt{42}\mathbb{Q}_{2,3}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{21} \\
\text{z460} \quad \mathbb{Q}_{4,3}^{(c)}(T_{2g}) &= \frac{\sqrt{14}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{14} + \frac{\sqrt{42}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{21} + \frac{\sqrt{42}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{21} + \frac{\sqrt{14}\mathbb{Q}_{2,3}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{14} \\
\text{z461} \quad \mathbb{Q}_{2,1}^{(1,-1;c)}(T_{2g}, a) &= \frac{\sqrt{3}\mathbb{Q}_{2,1}^{(1,-1;a)}(T_{2g})\mathbb{Q}_0^{(b)}(A_{1g})}{3} \\
\text{z462} \quad \mathbb{Q}_{2,2}^{(1,-1;c)}(T_{2g}, a) &= \frac{\sqrt{3}\mathbb{Q}_{2,2}^{(1,-1;a)}(T_{2g})\mathbb{Q}_0^{(b)}(A_{1g})}{3} \\
\text{z463} \quad \mathbb{Q}_{2,3}^{(1,-1;c)}(T_{2g}, a) &= \frac{\sqrt{3}\mathbb{Q}_{2,3}^{(1,-1;a)}(T_{2g})\mathbb{Q}_0^{(b)}(A_{1g})}{3} \\
\text{z464} \quad \mathbb{Q}_{2,1}^{(1,-1;c)}(T_{2g}, b) &= \frac{\sqrt{42}\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{42} + \frac{\sqrt{42}\mathbb{Q}_{2,1}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{42} - \frac{\sqrt{14}\mathbb{Q}_{2,1}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{14} \\
&\quad - \frac{\sqrt{14}\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{14} + \frac{\sqrt{14}\mathbb{Q}_{2,2}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{14} + \frac{\sqrt{14}\mathbb{Q}_{2,3}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{14} \\
\text{z465} \quad \mathbb{Q}_{2,2}^{(1,-1;c)}(T_{2g}, b) &= \frac{\sqrt{42}\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{42} + \frac{\sqrt{14}\mathbb{Q}_{2,1}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{14} + \frac{\sqrt{14}\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{14} \\
&\quad + \frac{\sqrt{42}\mathbb{Q}_{2,2}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{42} + \frac{\sqrt{14}\mathbb{Q}_{2,2}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{14} + \frac{\sqrt{14}\mathbb{Q}_{2,3}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{14} \\
\text{z466} \quad \mathbb{Q}_{2,3}^{(1,-1;c)}(T_{2g}, b) &= -\frac{\sqrt{42}\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{21} + \frac{\sqrt{14}\mathbb{Q}_{2,1}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{14} + \frac{\sqrt{14}\mathbb{Q}_{2,2}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{14} - \frac{\sqrt{42}\mathbb{Q}_{2,3}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{21} \\
\text{z467} \quad \mathbb{Q}_{4,1}^{(1,-1;c)}(T_{2g}) &= -\frac{\sqrt{14}\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{28} - \frac{\sqrt{14}\mathbb{Q}_{2,1}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{28} + \frac{\sqrt{42}\mathbb{Q}_{2,1}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{28} \\
&\quad + \frac{\sqrt{42}\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{28} + \frac{\sqrt{42}\mathbb{Q}_{2,2}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{21} + \frac{\sqrt{42}\mathbb{Q}_{2,3}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{21}
\end{aligned}$$

$$\begin{aligned}
\text{z468} \quad \mathbb{Q}_{4,2}^{(1,-1;c)}(T_{2g}) &= -\frac{\sqrt{14}\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{28} + \frac{\sqrt{42}\mathbb{Q}_{2,1}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{21} - \frac{\sqrt{42}\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{28} \\
&\quad - \frac{\sqrt{14}\mathbb{Q}_{2,2}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{28} - \frac{\sqrt{42}\mathbb{Q}_{2,2}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{28} + \frac{\sqrt{42}\mathbb{Q}_{2,3}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{21} \\
\text{z469} \quad \mathbb{Q}_{4,3}^{(1,-1;c)}(T_{2g}) &= \frac{\sqrt{14}\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{14} + \frac{\sqrt{42}\mathbb{Q}_{2,1}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{21} + \frac{\sqrt{42}\mathbb{Q}_{2,2}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{21} + \frac{\sqrt{14}\mathbb{Q}_{2,3}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{14} \\
\text{z470} \quad \mathbb{Q}_{2,1}^{(1,0;c)}(T_{2g}) &= -\frac{\sqrt{6}\mathbb{G}_{1,1}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{6} - \frac{\sqrt{2}\mathbb{G}_{1,1}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{6} - \frac{\sqrt{2}\mathbb{G}_{1,2}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{6} + \frac{\sqrt{2}\mathbb{G}_{1,3}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{6} \\
\text{z471} \quad \mathbb{Q}_{2,2}^{(1,0;c)}(T_{2g}) &= \frac{\sqrt{2}\mathbb{G}_{1,1}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{6} + \frac{\sqrt{6}\mathbb{G}_{1,2}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{6} - \frac{\sqrt{2}\mathbb{G}_{1,2}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{6} - \frac{\sqrt{2}\mathbb{G}_{1,3}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{6} \\
\text{z472} \quad \mathbb{Q}_{2,3}^{(1,0;c)}(T_{2g}) &= -\frac{\sqrt{2}\mathbb{G}_{1,1}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{6} + \frac{\sqrt{2}\mathbb{G}_{1,2}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{6} + \frac{\sqrt{2}\mathbb{G}_{1,3}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{3} \\
\text{z473} \quad \mathbb{Q}_{2,1}^{(1,1;c)}(T_{2g}) &= \frac{\sqrt{3}\mathbb{Q}_0^{(1,1;a)}(A_{1g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{3} \\
\text{z474} \quad \mathbb{Q}_{2,2}^{(1,1;c)}(T_{2g}) &= \frac{\sqrt{3}\mathbb{Q}_0^{(1,1;a)}(A_{1g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{3} \\
\text{z475} \quad \mathbb{Q}_{2,3}^{(1,1;c)}(T_{2g}) &= \frac{\sqrt{3}\mathbb{Q}_0^{(1,1;a)}(A_{1g})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{3} \\
\text{z476} \quad \mathbb{G}_{3,1}^{(c)}(T_{2g}) &= \frac{\sqrt{6}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{12} - \frac{\sqrt{6}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{12} + \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{4} - \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{4} \\
\text{z477} \quad \mathbb{G}_{3,2}^{(c)}(T_{2g}) &= \frac{\sqrt{6}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{12} + \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{4} - \frac{\sqrt{6}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{12} - \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{4} \\
\text{z478} \quad \mathbb{G}_{3,3}^{(c)}(T_{2g}) &= -\frac{\sqrt{6}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{6} + \frac{\sqrt{6}\mathbb{Q}_{2,3}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{6} \\
\text{z479} \quad \mathbb{G}_{3,1}^{(1,-1;c)}(T_{2g}) &= \frac{\sqrt{6}\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{12} - \frac{\sqrt{6}\mathbb{Q}_{2,1}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{12} + \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{4} - \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{4} \\
\text{z480} \quad \mathbb{G}_{3,2}^{(1,-1;c)}(T_{2g}) &= \frac{\sqrt{6}\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{12} + \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{4} - \frac{\sqrt{6}\mathbb{Q}_{2,2}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{12} - \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{4}
\end{aligned}$$



$$\begin{aligned}
\text{z481} \quad \mathbb{G}_{3,3}^{(1,-1;c)}(T_{2g}) &= -\frac{\sqrt{6}\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{6} + \frac{\sqrt{6}\mathbb{Q}_{2,3}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{6} \\
\text{z482} \quad \mathbb{G}_{3,1}^{(1,0;c)}(T_{2g}) &= -\frac{\sqrt{3}\mathbb{G}_{1,1}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{6} - \frac{\mathbb{G}_{1,1}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{6} + \frac{\mathbb{G}_{1,2}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{3} - \frac{\mathbb{G}_{1,3}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{3} \\
\text{z483} \quad \mathbb{G}_{3,2}^{(1,0;c)}(T_{2g}) &= -\frac{\mathbb{G}_{1,1}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{3} + \frac{\sqrt{3}\mathbb{G}_{1,2}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{6} - \frac{\mathbb{G}_{1,2}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{6} + \frac{\mathbb{G}_{1,3}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{3} \\
\text{z484} \quad \mathbb{G}_{3,3}^{(1,0;c)}(T_{2g}) &= \frac{\mathbb{G}_{1,1}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{3} - \frac{\mathbb{G}_{1,2}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{3} + \frac{\mathbb{G}_{1,3}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{3} \\
\text{z560} \quad \mathbb{Q}_{3,1}^{(c)}(T_{2u}) &= \frac{\sqrt{6}\mathbb{M}_{1,2}^{(a)}(T_{1g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{6} - \frac{\sqrt{6}\mathbb{M}_{1,3}^{(a)}(T_{1g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{6} \\
\text{z561} \quad \mathbb{Q}_{3,2}^{(c)}(T_{2u}) &= -\frac{\sqrt{6}\mathbb{M}_{1,1}^{(a)}(T_{1g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{6} + \frac{\sqrt{6}\mathbb{M}_{1,3}^{(a)}(T_{1g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{6} \\
\text{z562} \quad \mathbb{Q}_{3,3}^{(c)}(T_{2u}) &= \frac{\sqrt{6}\mathbb{M}_{1,1}^{(a)}(T_{1g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{6} - \frac{\sqrt{6}\mathbb{M}_{1,2}^{(a)}(T_{1g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{6} \\
\text{z563} \quad \mathbb{Q}_{3,1}^{(1,-1;c)}(T_{2u},a) &= \frac{\sqrt{15}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{12} + \frac{\mathbb{M}_{3,2}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{12} + \frac{\sqrt{15}\mathbb{M}_{3,3}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{12} - \frac{\mathbb{M}_{3,3}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{12} + \frac{\mathbb{M}_3^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{3} \\
\text{z564} \quad \mathbb{Q}_{3,2}^{(1,-1;c)}(T_{2u},a) &= \frac{\sqrt{15}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{12} - \frac{\mathbb{M}_{3,1}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{12} + \frac{\sqrt{15}\mathbb{M}_{3,3}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{12} + \frac{\mathbb{M}_{3,3}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{12} + \frac{\mathbb{M}_3^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{3} \\
\text{z565} \quad \mathbb{Q}_{3,3}^{(1,-1;c)}(T_{2u},a) &= \frac{\sqrt{15}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{12} + \frac{\mathbb{M}_{3,1}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{12} + \frac{\sqrt{15}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{12} - \frac{\mathbb{M}_{3,2}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{12} + \frac{\mathbb{M}_3^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3} \\
\text{z566} \quad \mathbb{Q}_{3,1}^{(1,-1;c)}(T_{2u},b) &= \frac{\sqrt{6}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{24} - \frac{\sqrt{10}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{2g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{8} - \frac{\sqrt{6}\mathbb{M}_{3,3}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{24} - \frac{\sqrt{10}\mathbb{M}_{3,3}^{(1,-1;a)}(T_{2g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{8} \\
\text{z567} \quad \mathbb{Q}_{3,2}^{(1,-1;c)}(T_{2u},b) &= -\frac{\sqrt{6}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{24} - \frac{\sqrt{10}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{2g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{8} + \frac{\sqrt{6}\mathbb{M}_{3,3}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{24} - \frac{\sqrt{10}\mathbb{M}_{3,3}^{(1,-1;a)}(T_{2g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{8} \\
\text{z568} \quad \mathbb{Q}_{3,3}^{(1,-1;c)}(T_{2u},b) &= \frac{\sqrt{6}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{24} - \frac{\sqrt{10}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{2g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{8} - \frac{\sqrt{6}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{24} - \frac{\sqrt{10}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{2g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{8} \\
\text{z569} \quad \mathbb{Q}_{3,1}^{(1,-1;c)}(T_{2u},c) &= \frac{\sqrt{6}\mathbb{M}_{1,2}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{6} - \frac{\sqrt{6}\mathbb{M}_{1,3}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{6}
\end{aligned}$$

$$\begin{aligned}
\text{z570} \quad \mathbb{Q}_{3,2}^{(1,-1;c)}(T_{2u}, c) &= -\frac{\sqrt{6}\mathbb{M}_{1,1}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{6} + \frac{\sqrt{6}\mathbb{M}_{1,3}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{6} \\
\text{z571} \quad \mathbb{Q}_{3,3}^{(1,-1;c)}(T_{2u}, c) &= \frac{\sqrt{6}\mathbb{M}_{1,1}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{6} - \frac{\sqrt{6}\mathbb{M}_{1,2}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{6} \\
\text{z572} \quad \mathbb{Q}_{5,1}^{(1,-1;c)}(T_{2u}) &= -\frac{\sqrt{10}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{8} - \frac{\sqrt{6}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{2g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{24} + \frac{\sqrt{10}\mathbb{M}_{3,3}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{8} - \frac{\sqrt{6}\mathbb{M}_{3,3}^{(1,-1;a)}(T_{2g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{24} \\
\text{z573} \quad \mathbb{Q}_{5,2}^{(1,-1;c)}(T_{2u}) &= \frac{\sqrt{10}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{8} - \frac{\sqrt{6}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{2g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{24} - \frac{\sqrt{10}\mathbb{M}_{3,3}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{8} - \frac{\sqrt{6}\mathbb{M}_{3,3}^{(1,-1;a)}(T_{2g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{24} \\
\text{z574} \quad \mathbb{Q}_{5,3}^{(1,-1;c)}(T_{2u}) &= -\frac{\sqrt{10}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{8} - \frac{\sqrt{6}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{2g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{24} + \frac{\sqrt{10}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{8} - \frac{\sqrt{6}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{2g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{24} \\
\text{z575} \quad \mathbb{Q}_{3,1}^{(1,0;c)}(T_{2u}, a) &= -\frac{\sqrt{3}\mathbb{T}_{2,1}^{(1,0;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} - \frac{\mathbb{T}_{2,2}^{(1,0;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} - \frac{\mathbb{T}_{2,2}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3} + \frac{\mathbb{T}_{2,3}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{3} \\
\text{z576} \quad \mathbb{Q}_{3,2}^{(1,0;c)}(T_{2u}, a) &= \frac{\sqrt{3}\mathbb{T}_{2,1}^{(1,0;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} + \frac{\mathbb{T}_{2,1}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3} - \frac{\mathbb{T}_{2,2}^{(1,0;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} - \frac{\mathbb{T}_{2,3}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{3} \\
\text{z577} \quad \mathbb{Q}_{3,3}^{(1,0;c)}(T_{2u}, a) &= -\frac{\mathbb{T}_{2,1}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{3} + \frac{\mathbb{T}_{2,2}^{(1,0;a)}(E_g)\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3} + \frac{\mathbb{T}_{2,2}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{3} \\
\text{z578} \quad \mathbb{Q}_{3,1}^{(1,0;c)}(T_{2u}, b) &= \frac{\sqrt{3}\mathbb{T}_{2,1}^{(1,0;a)}(E_g)\mathbb{M}_{2,1}^{(b)}(T_{2u})}{6} - \frac{\mathbb{T}_{2,2}^{(1,0;a)}(E_g)\mathbb{M}_{2,1}^{(b)}(T_{2u})}{2} \\
\text{z579} \quad \mathbb{Q}_{3,2}^{(1,0;c)}(T_{2u}, b) &= \frac{\sqrt{3}\mathbb{T}_{2,1}^{(1,0;a)}(E_g)\mathbb{M}_{2,2}^{(b)}(T_{2u})}{6} + \frac{\mathbb{T}_{2,2}^{(1,0;a)}(E_g)\mathbb{M}_{2,2}^{(b)}(T_{2u})}{2} \\
\text{z580} \quad \mathbb{Q}_{3,3}^{(1,0;c)}(T_{2u}, b) &= -\frac{\sqrt{3}\mathbb{T}_{2,1}^{(1,0;a)}(E_g)\mathbb{M}_{2,3}^{(b)}(T_{2u})}{3} \\
\text{z581} \quad \mathbb{Q}_{3,1}^{(1,1;c)}(T_{2u}) &= \frac{\sqrt{6}\mathbb{M}_{1,2}^{(1,1;a)}(T_{1g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{6} - \frac{\sqrt{6}\mathbb{M}_{1,3}^{(1,1;a)}(T_{1g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{6} \\
\text{z582} \quad \mathbb{Q}_{3,2}^{(1,1;c)}(T_{2u}) &= -\frac{\sqrt{6}\mathbb{M}_{1,1}^{(1,1;a)}(T_{1g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{6} + \frac{\sqrt{6}\mathbb{M}_{1,3}^{(1,1;a)}(T_{1g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{6} \\
\text{z583} \quad \mathbb{Q}_{3,3}^{(1,1;c)}(T_{2u}) &= \frac{\sqrt{6}\mathbb{M}_{1,1}^{(1,1;a)}(T_{1g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{6} - \frac{\sqrt{6}\mathbb{M}_{1,2}^{(1,1;a)}(T_{1g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{6}
\end{aligned}$$



$$\boxed{\text{z598}} \quad \mathbb{G}_{2,3}^{(1,0;c)}(T_{2u}, a) = -\frac{\sqrt{2}\mathbb{T}_{2,1}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} - \frac{\sqrt{2}\mathbb{T}_{2,2}^{(1,0;a)}(E_g)\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3} + \frac{\sqrt{2}\mathbb{T}_{2,2}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6}$$

$$\boxed{\text{z599}} \quad \mathbb{G}_{2,1}^{(1,0;c)}(T_{2u}, b) = \frac{\sqrt{6}\mathbb{T}_{2,2}^{(1,0;a)}(T_{2g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{6} + \frac{\sqrt{6}\mathbb{T}_{2,3}^{(1,0;a)}(T_{2g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{6}$$

$$\boxed{\text{z600}} \quad \mathbb{G}_{2,2}^{(1,0;c)}(T_{2u}, b) = \frac{\sqrt{6}\mathbb{T}_{2,1}^{(1,0;a)}(T_{2g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{6} + \frac{\sqrt{6}\mathbb{T}_{2,3}^{(1,0;a)}(T_{2g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{6}$$

$$\boxed{\text{z601}} \quad \mathbb{G}_{2,3}^{(1,0;c)}(T_{2u}, b) = \frac{\sqrt{6}\mathbb{T}_{2,1}^{(1,0;a)}(T_{2g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{6} + \frac{\sqrt{6}\mathbb{T}_{2,2}^{(1,0;a)}(T_{2g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{6}$$

$$\boxed{\text{z602}} \quad \mathbb{G}_{2,1}^{(1,1;c)}(T_{2u}) = \frac{\sqrt{6}\mathbb{M}_{1,2}^{(1,1;a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{6} + \frac{\sqrt{6}\mathbb{M}_{1,3}^{(1,1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6}$$

$$\boxed{\text{z603}} \quad \mathbb{G}_{2,2}^{(1,1;c)}(T_{2u}) = \frac{\sqrt{6}\mathbb{M}_{1,1}^{(1,1;a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{6} + \frac{\sqrt{6}\mathbb{M}_{1,3}^{(1,1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6}$$

$$\boxed{\text{z604}} \quad \mathbb{G}_{2,3}^{(1,1;c)}(T_{2u}) = \frac{\sqrt{6}\mathbb{M}_{1,1}^{(1,1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} + \frac{\sqrt{6}\mathbb{M}_{1,2}^{(1,1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6}$$

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## Atomic SAMB

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- bra:  $\langle s, \uparrow |, \langle s, \downarrow |$
- ket:  $|s, \uparrow\rangle, |s, \downarrow\rangle$

$$\boxed{\text{x1}} \quad \mathbb{Q}_0^{(a)}(A_{1g}) = \begin{bmatrix} \frac{\sqrt{2}}{2} & 0 \\ 0 & \frac{\sqrt{2}}{2} \end{bmatrix}$$

$$\boxed{\text{x2}} \quad \mathbb{M}_{1,1}^{(1,-1;a)}(T_{1g}) = \begin{bmatrix} 0 & \frac{\sqrt{2}}{2} \\ \frac{\sqrt{2}}{2} & 0 \end{bmatrix}$$

$$\boxed{\text{x3}} \quad \mathbb{M}_{1,2}^{(1,-1;a)}(T_{1g}) = \begin{bmatrix} 0 & -\frac{\sqrt{2}i}{2} \\ \frac{\sqrt{2}i}{2} & 0 \end{bmatrix}$$

$$\boxed{\text{x4}} \quad \mathbb{M}_{1,3}^{(1,-1;a)}(T_{1g}) = \begin{bmatrix} \frac{\sqrt{2}}{2} & 0 \\ 0 & -\frac{\sqrt{2}}{2} \end{bmatrix}$$

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

$$\boxed{\text{x5}} \quad \mathbb{Q}_{1,1}^{(a)}(T_{1u}) = \begin{bmatrix} \frac{1}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x6}} \quad \mathbb{Q}_{1,2}^{(a)}(T_{1u}) = \begin{bmatrix} 0 & 0 & \frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2} & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x7}} \quad \mathbb{Q}_{1,3}^{(a)}(T_{1u}) = \begin{bmatrix} 0 & 0 & 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{2} \end{bmatrix}$$

$$\boxed{\text{x8}} \quad \mathbb{Q}_{1,1}^{(1,0;a)}(T_{1u}) = \begin{bmatrix} 0 & 0 & -\frac{\sqrt{2}i}{4} & 0 & 0 & \frac{\sqrt{2}}{4} \\ 0 & 0 & 0 & \frac{\sqrt{2}i}{4} & -\frac{\sqrt{2}}{4} & 0 \end{bmatrix}$$

$$\boxed{\text{x9}} \quad \mathbb{Q}_{1,2}^{(1,0;a)}(T_{1u}) = \begin{bmatrix} \frac{\sqrt{2}i}{4} & 0 & 0 & 0 & 0 & -\frac{\sqrt{2}i}{4} \\ 0 & -\frac{\sqrt{2}i}{4} & 0 & 0 & -\frac{\sqrt{2}i}{4} & 0 \end{bmatrix}$$

$$\boxed{\text{x10}} \quad \mathbb{Q}_{1,3}^{(1,0;a)}(T_{1u}) = \begin{bmatrix} 0 & -\frac{\sqrt{2}}{4} & 0 & \frac{\sqrt{2}i}{4} & 0 & 0 \\ \frac{\sqrt{2}}{4} & 0 & \frac{\sqrt{2}i}{4} & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x11}} \quad \mathbb{G}_{2,1}^{(1,-1;a)}(E_u) = \begin{bmatrix} 0 & -\frac{\sqrt{6}i}{12} & 0 & -\frac{\sqrt{6}}{12} & \frac{\sqrt{6}i}{6} & 0 \\ -\frac{\sqrt{6}i}{12} & 0 & \frac{\sqrt{6}}{12} & 0 & 0 & -\frac{\sqrt{6}i}{6} \end{bmatrix}$$

$$\boxed{\text{x12}} \quad \mathbb{G}_{2,2}^{(1,-1;a)}(E_u) = \begin{bmatrix} 0 & \frac{\sqrt{2}i}{4} & 0 & -\frac{\sqrt{2}}{4} & 0 & 0 \\ \frac{\sqrt{2}i}{4} & 0 & \frac{\sqrt{2}}{4} & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x13}} \quad \mathbb{G}_{2,1}^{(1,-1;a)}(T_{2u}) = \begin{bmatrix} 0 & 0 & \frac{\sqrt{2}i}{4} & 0 & 0 & \frac{\sqrt{2}}{4} \\ 0 & 0 & 0 & -\frac{\sqrt{2}i}{4} & -\frac{\sqrt{2}}{4} & 0 \end{bmatrix}$$

$$\boxed{\text{x14}} \quad \mathbb{G}_{2,2}^{(1,-1;a)}(T_{2u}) = \begin{bmatrix} \frac{\sqrt{2}i}{4} & 0 & 0 & 0 & 0 & \frac{\sqrt{2}i}{4} \\ 0 & -\frac{\sqrt{2}i}{4} & 0 & 0 & \frac{\sqrt{2}i}{4} & 0 \end{bmatrix}$$

$$\boxed{\text{x15}} \quad \mathbb{G}_{2,3}^{(1,-1;a)}(T_{2u}) = \begin{bmatrix} 0 & \frac{\sqrt{2}}{4} & 0 & \frac{\sqrt{2}i}{4} & 0 & 0 \\ -\frac{\sqrt{2}}{4} & 0 & \frac{\sqrt{2}i}{4} & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x16}} \quad \mathbb{G}_0^{(1,1;a)}(A_{1u}) = \begin{bmatrix} 0 & \frac{\sqrt{3}i}{6} & 0 & \frac{\sqrt{3}}{6} & \frac{\sqrt{3}i}{6} & 0 \\ \frac{\sqrt{3}i}{6} & 0 & -\frac{\sqrt{3}}{6} & 0 & 0 & -\frac{\sqrt{3}i}{6} \end{bmatrix}$$

$$\boxed{\text{x17}} \quad \mathbb{M}_{2,1}^{(1,-1;a)}(E_u) = \begin{bmatrix} 0 & -\frac{\sqrt{6}}{12} & 0 & \frac{\sqrt{6}i}{12} & \frac{\sqrt{6}}{6} & 0 \\ -\frac{\sqrt{6}}{12} & 0 & -\frac{\sqrt{6}i}{12} & 0 & 0 & -\frac{\sqrt{6}}{6} \end{bmatrix}$$

$$\boxed{\text{x18}} \quad \mathbb{M}_{2,2}^{(1,-1;a)}(E_u) = \begin{bmatrix} 0 & \frac{\sqrt{2}}{4} & 0 & \frac{\sqrt{2}i}{4} & 0 & 0 \\ \frac{\sqrt{2}}{4} & 0 & -\frac{\sqrt{2}i}{4} & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x19}} \quad \mathbb{M}_{2,1}^{(1,-1;a)}(T_{2u}) = \begin{bmatrix} 0 & 0 & \frac{\sqrt{2}}{4} & 0 & 0 & -\frac{\sqrt{2}i}{4} \\ 0 & 0 & 0 & -\frac{\sqrt{2}}{4} & \frac{\sqrt{2}i}{4} & 0 \end{bmatrix}$$

$$\boxed{\text{x20}} \quad \mathbb{M}_{2,2}^{(1,-1;a)}(T_{2u}) = \begin{bmatrix} \frac{\sqrt{2}}{4} & 0 & 0 & 0 & 0 & \frac{\sqrt{2}}{4} \\ 0 & -\frac{\sqrt{2}}{4} & 0 & 0 & \frac{\sqrt{2}}{4} & 0 \end{bmatrix}$$

$$\boxed{\text{x21}} \quad \mathbb{M}_{2,3}^{(1,-1;a)}(T_{2u}) = \begin{bmatrix} 0 & -\frac{\sqrt{2}i}{4} & 0 & \frac{\sqrt{2}}{4} & 0 & 0 \\ \frac{\sqrt{2}i}{4} & 0 & \frac{\sqrt{2}}{4} & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x22}} \quad \mathbb{M}_0^{(1,1;a)}(A_{1u}) = \begin{bmatrix} 0 & \frac{\sqrt{3}}{6} & 0 & -\frac{\sqrt{3}i}{6} & \frac{\sqrt{3}}{6} & 0 \\ \frac{\sqrt{3}}{6} & 0 & \frac{\sqrt{3}i}{6} & 0 & 0 & -\frac{\sqrt{3}}{6} \end{bmatrix}$$

$$\boxed{\text{x23}} \quad \mathbb{T}_{1,1}^{(a)}(T_{1u}) = \begin{bmatrix} \frac{i}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{i}{2} & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x24}} \quad \mathbb{T}_{1,2}^{(a)}(T_{1u}) = \begin{bmatrix} 0 & 0 & \frac{i}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{i}{2} & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x25}} \quad \mathbb{T}_{1,3}^{(a)}(T_{1u}) = \begin{bmatrix} 0 & 0 & 0 & 0 & \frac{i}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{i}{2} \end{bmatrix}$$

$$\boxed{\text{x26}} \quad \mathbb{T}_{1,1}^{(1,0;a)}(T_{1u}) = \begin{bmatrix} 0 & 0 & -\frac{\sqrt{2}}{4} & 0 & 0 & -\frac{\sqrt{2}i}{4} \\ 0 & 0 & 0 & \frac{\sqrt{2}}{4} & \frac{\sqrt{2}i}{4} & 0 \end{bmatrix}$$

$$\boxed{\text{x27}} \quad \mathbb{T}_{1,2}^{(1,0;a)}(T_{1u}) = \begin{bmatrix} \frac{\sqrt{2}}{4} & 0 & 0 & 0 & 0 & -\frac{\sqrt{2}}{4} \\ 0 & -\frac{\sqrt{2}}{4} & 0 & 0 & -\frac{\sqrt{2}}{4} & 0 \end{bmatrix}$$

$$\boxed{\text{x28}} \quad \mathbb{T}_{1,3}^{(1,0;a)}(T_{1u}) = \begin{bmatrix} 0 & \frac{\sqrt{2}i}{4} & 0 & \frac{\sqrt{2}}{4} & 0 & 0 \\ -\frac{\sqrt{2}i}{4} & 0 & \frac{\sqrt{2}}{4} & 0 & 0 & 0 \end{bmatrix}$$

• bra:  $\langle p_x, \uparrow |, \langle p_x, \downarrow |, \langle p_y, \uparrow |, \langle p_y, \downarrow |, \langle p_z, \uparrow |, \langle p_z, \downarrow |$

- ket:  $|p_x, \uparrow\rangle, |p_x, \downarrow\rangle, |p_y, \uparrow\rangle, |p_y, \downarrow\rangle, |p_z, \uparrow\rangle, |p_z, \downarrow\rangle$

$$\boxed{\text{x29}} \quad \mathbb{Q}_0^{(a)}(A_{1g}) = \begin{bmatrix} \frac{\sqrt{6}}{6} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{6}}{6} & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{6}}{6} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{6}}{6} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{6}}{6} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{6}}{6} \end{bmatrix}$$

$$\boxed{\text{x30}} \quad \mathbb{Q}_{2,1}^{(a)}(E_g) = \begin{bmatrix} -\frac{\sqrt{3}}{6} & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{3}}{6} & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{3}}{6} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{3}}{6} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{3}}{3} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{3}}{3} \end{bmatrix}$$

$$\boxed{\text{x31}} \quad \mathbb{Q}_{2,2}^{(a)}(E_g) = \begin{bmatrix} \frac{1}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{1}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x32}} \quad \mathbb{Q}_{2,1}^{(a)}(T_{2g}) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{2} \\ 0 & 0 & \frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2} & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x33}} \quad \mathbb{Q}_{2,2}^{(a)}(T_{2g}) = \begin{bmatrix} 0 & 0 & 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{2} \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{1}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x34}} \quad \mathbb{Q}_{2,3}^{(a)}(T_{2g}) = \begin{bmatrix} 0 & 0 & \frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2} & 0 & 0 \\ \frac{1}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x35}} \quad \mathbb{Q}_{2,1}^{(1,-1;a)}(E_g) = \begin{bmatrix} 0 & 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 & -\frac{\sqrt{6}}{12} \\ 0 & 0 & 0 & \frac{\sqrt{6}i}{6} & \frac{\sqrt{6}}{12} & 0 \\ \frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 & \frac{\sqrt{6}i}{12} \\ 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 & \frac{\sqrt{6}i}{12} & 0 \\ 0 & \frac{\sqrt{6}}{12} & 0 & -\frac{\sqrt{6}i}{12} & 0 & 0 \\ -\frac{\sqrt{6}}{12} & 0 & -\frac{\sqrt{6}i}{12} & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x36}} \quad \mathbb{Q}_{2,2}^{(1,-1;a)}(E_g) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{2}}{4} \\ 0 & 0 & 0 & 0 & \frac{\sqrt{2}}{4} & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{2}i}{4} \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{2}i}{4} & 0 \\ 0 & \frac{\sqrt{2}}{4} & 0 & \frac{\sqrt{2}i}{4} & 0 & 0 \\ -\frac{\sqrt{2}}{4} & 0 & \frac{\sqrt{2}i}{4} & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x37}} \quad \mathbb{Q}_{2,1}^{(1,-1;a)}(T_{2g}) = \begin{bmatrix} 0 & 0 & 0 & -\frac{\sqrt{2}}{4} & \frac{\sqrt{2}i}{4} & 0 \\ 0 & 0 & \frac{\sqrt{2}}{4} & 0 & 0 & -\frac{\sqrt{2}i}{4} \\ 0 & \frac{\sqrt{2}}{4} & 0 & 0 & 0 & 0 \\ -\frac{\sqrt{2}}{4} & 0 & 0 & 0 & 0 & 0 \\ -\frac{\sqrt{2}i}{4} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{2}i}{4} & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x38}} \quad \mathbb{Q}_{2,2}^{(1,-1;a)}(T_{2g}) = \begin{bmatrix} 0 & 0 & 0 & -\frac{\sqrt{2}i}{4} & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{2}i}{4} & 0 & 0 & 0 \\ 0 & \frac{\sqrt{2}i}{4} & 0 & 0 & -\frac{\sqrt{2}i}{4} & 0 \\ \frac{\sqrt{2}i}{4} & 0 & 0 & 0 & 0 & \frac{\sqrt{2}i}{4} \\ 0 & 0 & \frac{\sqrt{2}i}{4} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{2}i}{4} & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x39}} \quad \mathbb{Q}_{2,3}^{(1,-1;a)}(T_{2g}) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{2}i}{4} \\ 0 & 0 & 0 & 0 & \frac{\sqrt{2}i}{4} & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{2}}{4} \\ 0 & 0 & 0 & 0 & \frac{\sqrt{2}}{4} & 0 \\ 0 & -\frac{\sqrt{2}i}{4} & 0 & \frac{\sqrt{2}}{4} & 0 & 0 \\ -\frac{\sqrt{2}i}{4} & 0 & -\frac{\sqrt{2}}{4} & 0 & 0 & 0 \end{bmatrix}$$



$$\boxed{\text{x40}} \quad \mathbb{Q}_0^{(1,1;a)}(A_{1g}) = \begin{bmatrix} 0 & 0 & -\frac{\sqrt{3}i}{6} & 0 & 0 & \frac{\sqrt{3}}{6} \\ 0 & 0 & 0 & \frac{\sqrt{3}i}{6} & -\frac{\sqrt{3}}{6} & 0 \\ \frac{\sqrt{3}i}{6} & 0 & 0 & 0 & 0 & -\frac{\sqrt{3}i}{6} \\ 0 & -\frac{\sqrt{3}i}{6} & 0 & 0 & -\frac{\sqrt{3}}{6} & 0 \\ 0 & -\frac{\sqrt{3}}{6} & 0 & \frac{\sqrt{3}i}{6} & 0 & 0 \\ \frac{\sqrt{3}}{6} & 0 & \frac{\sqrt{3}i}{6} & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x41}} \quad \mathbb{G}_{1,1}^{(1,0;a)}(T_{1g}) = \begin{bmatrix} 0 & 0 & 0 & -\frac{\sqrt{2}}{4} & -\frac{\sqrt{2}i}{4} & 0 \\ 0 & 0 & \frac{\sqrt{2}}{4} & 0 & 0 & \frac{\sqrt{2}i}{4} \\ 0 & \frac{\sqrt{2}}{4} & 0 & 0 & 0 & 0 \\ -\frac{\sqrt{2}}{4} & 0 & 0 & 0 & 0 & 0 \\ \frac{\sqrt{2}i}{4} & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{2}i}{4} & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x42}} \quad \mathbb{G}_{1,2}^{(1,0;a)}(T_{1g}) = \begin{bmatrix} 0 & 0 & 0 & \frac{\sqrt{2}i}{4} & 0 & 0 \\ 0 & 0 & \frac{\sqrt{2}i}{4} & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{2}i}{4} & 0 & 0 & -\frac{\sqrt{2}}{4} & 0 \\ -\frac{\sqrt{2}i}{4} & 0 & 0 & 0 & 0 & \frac{\sqrt{2}i}{4} \\ 0 & 0 & \frac{\sqrt{2}i}{4} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{2}i}{4} & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x43}} \quad \mathbb{G}_{1,3}^{(1,0;a)}(T_{1g}) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{2}i}{4} \\ 0 & 0 & 0 & 0 & \frac{\sqrt{2}i}{4} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{2}}{4} \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{2}}{4} & 0 \\ 0 & -\frac{\sqrt{2}i}{4} & 0 & -\frac{\sqrt{2}}{4} & 0 & 0 \\ -\frac{\sqrt{2}i}{4} & 0 & \frac{\sqrt{2}}{4} & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x44}} \quad \mathbb{M}_{1,1}^{(a)}(T_{1g}) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{i}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{i}{2} \\ 0 & 0 & \frac{i}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{i}{2} & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x45}} \quad \mathbb{M}_{1,2}^{(a)}(T_{1g}) = \begin{bmatrix} 0 & 0 & 0 & 0 & \frac{i}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{i}{2} \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ -\frac{i}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{i}{2} & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x46}} \quad \mathbb{M}_{1,3}^{(a)}(T_{1g}) = \begin{bmatrix} 0 & 0 & -\frac{i}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{i}{2} & 0 & 0 \\ \frac{i}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{i}{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x47}} \quad \mathbb{M}_3^{(1,-1;a)}(A_{2g}) = \begin{bmatrix} 0 & 0 & \frac{\sqrt{3}}{6} & 0 & 0 & -\frac{\sqrt{3}i}{6} \\ 0 & 0 & 0 & -\frac{\sqrt{3}}{6} & \frac{\sqrt{3}i}{6} & 0 \\ \frac{\sqrt{3}}{6} & 0 & 0 & 0 & 0 & \frac{\sqrt{3}}{6} \\ 0 & -\frac{\sqrt{3}}{6} & 0 & 0 & \frac{\sqrt{3}}{6} & 0 \\ 0 & -\frac{\sqrt{3}i}{6} & 0 & \frac{\sqrt{3}}{6} & 0 & 0 \\ \frac{\sqrt{3}i}{6} & 0 & \frac{\sqrt{3}}{6} & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x48}} \quad \mathbb{M}_{1,1}^{(1,-1;a)}(T_{1g}) = \begin{bmatrix} 0 & \frac{\sqrt{6}}{6} & 0 & 0 & 0 & 0 \\ \frac{\sqrt{6}}{6} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{6}}{6} & 0 & 0 \\ 0 & 0 & \frac{\sqrt{6}}{6} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{6}}{6} \\ 0 & 0 & 0 & 0 & \frac{\sqrt{6}}{6} & 0 \end{bmatrix}$$

$$\boxed{\text{x49}} \quad \mathbb{M}_{1,2}^{(1,-1;a)}(T_{1g}) = \begin{bmatrix} 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 \\ \frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 \\ 0 & 0 & \frac{\sqrt{6}i}{6} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{6}i}{6} \\ 0 & 0 & 0 & 0 & \frac{\sqrt{6}i}{6} & 0 \end{bmatrix}$$

$$\boxed{\text{x50}} \quad \mathbb{M}_{1,3}^{(1,-1;a)}(T_{1g}) = \begin{bmatrix} \frac{\sqrt{6}}{6} & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{6}}{6} & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{6}}{6} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{6}}{6} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{6}}{6} & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{6}}{6} \end{bmatrix}$$

$$\boxed{\text{x51}} \quad \mathbb{M}_{3,1}^{(1,-1;a)}(T_{1g}) = \begin{bmatrix} 0 & \frac{\sqrt{5}}{5} & 0 & \frac{\sqrt{5}i}{10} & -\frac{\sqrt{5}}{10} & 0 \\ \frac{\sqrt{5}}{5} & 0 & -\frac{\sqrt{5}i}{10} & 0 & 0 & \frac{\sqrt{5}}{10} \\ 0 & \frac{\sqrt{5}i}{10} & 0 & -\frac{\sqrt{5}}{10} & 0 & 0 \\ -\frac{\sqrt{5}i}{10} & 0 & -\frac{\sqrt{5}}{10} & 0 & 0 & 0 \\ -\frac{\sqrt{5}}{10} & 0 & 0 & 0 & 0 & -\frac{\sqrt{5}}{10} \\ 0 & \frac{\sqrt{5}}{10} & 0 & 0 & -\frac{\sqrt{5}}{10} & 0 \end{bmatrix}$$

$$\boxed{\text{x52}} \quad \mathbb{M}_{3,2}^{(1,-1;a)}(T_{1g}) = \begin{bmatrix} 0 & \frac{\sqrt{5}i}{10} & 0 & -\frac{\sqrt{5}}{10} & 0 & 0 \\ -\frac{\sqrt{5}i}{10} & 0 & -\frac{\sqrt{5}}{10} & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{5}}{10} & 0 & -\frac{\sqrt{5}i}{5} & -\frac{\sqrt{5}}{10} & 0 \\ -\frac{\sqrt{5}}{10} & 0 & \frac{\sqrt{5}i}{5} & 0 & 0 & \frac{\sqrt{5}}{10} \\ 0 & 0 & -\frac{\sqrt{5}}{10} & 0 & 0 & \frac{\sqrt{5}i}{10} \\ 0 & 0 & 0 & \frac{\sqrt{5}}{10} & -\frac{\sqrt{5}i}{10} & 0 \end{bmatrix}$$

$$\boxed{\text{x53}} \quad \mathbb{M}_{3,3}^{(1,-1;a)}(T_{1g}) = \begin{bmatrix} -\frac{\sqrt{5}}{10} & 0 & 0 & 0 & 0 & -\frac{\sqrt{5}}{10} \\ 0 & \frac{\sqrt{5}}{10} & 0 & 0 & -\frac{\sqrt{5}}{10} & 0 \\ 0 & 0 & -\frac{\sqrt{5}}{10} & 0 & 0 & \frac{\sqrt{5}i}{10} \\ 0 & 0 & 0 & \frac{\sqrt{5}}{10} & -\frac{\sqrt{5}i}{10} & 0 \\ 0 & -\frac{\sqrt{5}}{10} & 0 & \frac{\sqrt{5}i}{10} & \frac{\sqrt{5}}{5} & 0 \\ -\frac{\sqrt{5}}{10} & 0 & -\frac{\sqrt{5}i}{10} & 0 & 0 & -\frac{\sqrt{5}}{5} \end{bmatrix}$$

$$\boxed{\text{x54}} \quad \mathbb{M}_{3,1}^{(1,-1;a)}(T_{2g}) = \begin{bmatrix} 0 & 0 & 0 & -\frac{\sqrt{3}i}{6} & -\frac{\sqrt{3}}{6} & 0 \\ 0 & 0 & \frac{\sqrt{3}i}{6} & 0 & 0 & \frac{\sqrt{3}}{6} \\ 0 & -\frac{\sqrt{3}i}{6} & 0 & \frac{\sqrt{3}}{6} & 0 & 0 \\ \frac{\sqrt{3}i}{6} & 0 & \frac{\sqrt{3}}{6} & 0 & 0 & 0 \\ -\frac{\sqrt{3}}{6} & 0 & 0 & 0 & 0 & -\frac{\sqrt{3}}{6} \\ 0 & \frac{\sqrt{3}}{6} & 0 & 0 & -\frac{\sqrt{3}}{6} & 0 \end{bmatrix}$$

$$\boxed{\text{x55}} \quad \mathbb{M}_{3,2}^{(1,-1;a)}(T_{2g}) = \begin{bmatrix} 0 & \frac{\sqrt{3}i}{6} & 0 & -\frac{\sqrt{3}}{6} & 0 & 0 \\ -\frac{\sqrt{3}i}{6} & 0 & -\frac{\sqrt{3}}{6} & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{3}}{6} & 0 & 0 & \frac{\sqrt{3}}{6} & 0 \\ -\frac{\sqrt{3}}{6} & 0 & 0 & 0 & 0 & -\frac{\sqrt{3}}{6} \\ 0 & 0 & \frac{\sqrt{3}}{6} & 0 & 0 & -\frac{\sqrt{3}i}{6} \\ 0 & 0 & 0 & -\frac{\sqrt{3}}{6} & \frac{\sqrt{3}i}{6} & 0 \end{bmatrix}$$

$$\boxed{\text{x56}} \quad \mathbb{M}_{3,3}^{(1,-1;a)}(T_{2g}) = \begin{bmatrix} \frac{\sqrt{3}}{6} & 0 & 0 & 0 & 0 & \frac{\sqrt{3}}{6} \\ 0 & -\frac{\sqrt{3}}{6} & 0 & 0 & \frac{\sqrt{3}}{6} & 0 \\ 0 & 0 & -\frac{\sqrt{3}}{6} & 0 & 0 & \frac{\sqrt{3}i}{6} \\ 0 & 0 & 0 & \frac{\sqrt{3}}{6} & -\frac{\sqrt{3}i}{6} & 0 \\ 0 & \frac{\sqrt{3}}{6} & 0 & \frac{\sqrt{3}i}{6} & 0 & 0 \\ \frac{\sqrt{3}}{6} & 0 & -\frac{\sqrt{3}i}{6} & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x57}} \quad \mathbb{M}_{1,1}^{(1,1;a)}(T_{1g}) = \begin{bmatrix} 0 & \frac{\sqrt{30}}{15} & 0 & -\frac{\sqrt{30}i}{20} & \frac{\sqrt{30}}{20} & 0 \\ \frac{\sqrt{30}}{15} & 0 & \frac{\sqrt{30}i}{20} & 0 & 0 & -\frac{\sqrt{30}}{20} \\ 0 & -\frac{\sqrt{30}i}{20} & 0 & -\frac{\sqrt{30}}{30} & 0 & 0 \\ \frac{\sqrt{30}i}{20} & 0 & -\frac{\sqrt{30}}{30} & 0 & 0 & 0 \\ \frac{\sqrt{30}}{20} & 0 & 0 & 0 & 0 & -\frac{\sqrt{30}}{30} \\ 0 & -\frac{\sqrt{30}}{20} & 0 & 0 & -\frac{\sqrt{30}}{30} & 0 \end{bmatrix}$$

$$\boxed{\text{x58}} \quad \mathbb{M}_{1,2}^{(1,1;a)}(T_{1g}) = \begin{bmatrix} 0 & \frac{\sqrt{30}i}{30} & 0 & \frac{\sqrt{30}}{20} & 0 & 0 \\ -\frac{\sqrt{30}i}{30} & 0 & \frac{\sqrt{30}}{20} & 0 & 0 & 0 \\ 0 & \frac{\sqrt{30}}{20} & 0 & -\frac{\sqrt{30}i}{15} & \frac{\sqrt{30}}{20} & 0 \\ \frac{\sqrt{30}}{20} & 0 & \frac{\sqrt{30}i}{15} & 0 & 0 & -\frac{\sqrt{30}}{20} \\ 0 & 0 & \frac{\sqrt{30}}{20} & 0 & 0 & \frac{\sqrt{30}i}{30} \\ 0 & 0 & 0 & -\frac{\sqrt{30}}{20} & -\frac{\sqrt{30}i}{30} & 0 \end{bmatrix}$$

$$\boxed{\text{x59}} \quad \mathbb{M}_{1,3}^{(1,1;a)}(T_{1g}) = \begin{bmatrix} -\frac{\sqrt{30}}{30} & 0 & 0 & 0 & 0 & \frac{\sqrt{30}}{20} \\ 0 & \frac{\sqrt{30}}{30} & 0 & 0 & \frac{\sqrt{30}}{20} & 0 \\ 0 & 0 & -\frac{\sqrt{30}}{30} & 0 & 0 & -\frac{\sqrt{30}i}{20} \\ 0 & 0 & 0 & \frac{\sqrt{30}}{30} & \frac{\sqrt{30}i}{20} & 0 \\ 0 & \frac{\sqrt{30}}{20} & 0 & -\frac{\sqrt{30}i}{20} & \frac{\sqrt{30}}{15} & 0 \\ \frac{\sqrt{30}}{20} & 0 & \frac{\sqrt{30}i}{20} & 0 & 0 & -\frac{\sqrt{30}}{15} \end{bmatrix}$$

$$\boxed{\text{x60}} \quad \mathbb{T}_{2,1}^{(1,0;a)}(E_g) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{2}i}{4} \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{2}i}{4} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{2}}{4} \\ 0 & 0 & 0 & 0 & \frac{\sqrt{2}}{4} & 0 \\ 0 & \frac{\sqrt{2}i}{4} & 0 & \frac{\sqrt{2}}{4} & 0 & 0 \\ -\frac{\sqrt{2}i}{4} & 0 & \frac{\sqrt{2}}{4} & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x61}} \quad \mathbb{T}_{2,2}^{(1,0;a)}(E_g) = \begin{bmatrix} 0 & 0 & -\frac{\sqrt{6}}{6} & 0 & 0 & -\frac{\sqrt{6}i}{12} \\ 0 & 0 & 0 & \frac{\sqrt{6}}{6} & \frac{\sqrt{6}i}{12} & 0 \\ -\frac{\sqrt{6}}{6} & 0 & 0 & 0 & 0 & \frac{\sqrt{6}}{12} \\ 0 & \frac{\sqrt{6}}{6} & 0 & 0 & \frac{\sqrt{6}}{12} & 0 \\ 0 & -\frac{\sqrt{6}i}{12} & 0 & \frac{\sqrt{6}}{12} & 0 & 0 \\ \frac{\sqrt{6}i}{12} & 0 & \frac{\sqrt{6}}{12} & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x62}} \quad \mathbb{T}_{2,1}^{(1,0;a)}(T_{2g}) = \begin{bmatrix} 0 & 0 & 0 & \frac{\sqrt{6}i}{12} & \frac{\sqrt{6}}{12} & 0 \\ 0 & 0 & -\frac{\sqrt{6}i}{12} & 0 & 0 & -\frac{\sqrt{6}}{12} \\ 0 & \frac{\sqrt{6}i}{12} & 0 & \frac{\sqrt{6}}{6} & 0 & 0 \\ -\frac{\sqrt{6}i}{12} & 0 & \frac{\sqrt{6}}{6} & 0 & 0 & 0 \\ \frac{\sqrt{6}}{12} & 0 & 0 & 0 & 0 & -\frac{\sqrt{6}}{6} \\ 0 & -\frac{\sqrt{6}}{12} & 0 & 0 & -\frac{\sqrt{6}}{6} & 0 \end{bmatrix}$$

$$\boxed{\text{x63}} \quad \mathbb{T}_{2,2}^{(1,0;a)}(T_{2g}) = \begin{bmatrix} 0 & \frac{\sqrt{6}i}{6} & 0 & \frac{\sqrt{6}}{12} & 0 & 0 \\ -\frac{\sqrt{6}i}{6} & 0 & \frac{\sqrt{6}}{12} & 0 & 0 & 0 \\ 0 & \frac{\sqrt{6}}{12} & 0 & 0 & -\frac{\sqrt{6}}{12} & 0 \\ \frac{\sqrt{6}}{12} & 0 & 0 & 0 & 0 & \frac{\sqrt{6}}{12} \\ 0 & 0 & -\frac{\sqrt{6}}{12} & 0 & 0 & -\frac{\sqrt{6}i}{6} \\ 0 & 0 & 0 & \frac{\sqrt{6}}{12} & \frac{\sqrt{6}i}{6} & 0 \end{bmatrix}$$

$$\boxed{\text{x64}} \quad \mathbb{T}_{2,3}^{(1,0;a)}(T_{2g}) = \begin{bmatrix} \frac{\sqrt{6}}{6} & 0 & 0 & 0 & 0 & -\frac{\sqrt{6}}{12} \\ 0 & -\frac{\sqrt{6}}{6} & 0 & 0 & -\frac{\sqrt{6}}{12} & 0 \\ 0 & 0 & -\frac{\sqrt{6}}{6} & 0 & 0 & -\frac{\sqrt{6}i}{12} \\ 0 & 0 & 0 & \frac{\sqrt{6}}{6} & \frac{\sqrt{6}i}{12} & 0 \\ 0 & -\frac{\sqrt{6}}{12} & 0 & -\frac{\sqrt{6}i}{12} & 0 & 0 \\ -\frac{\sqrt{6}}{12} & 0 & \frac{\sqrt{6}i}{12} & 0 & 0 & 0 \end{bmatrix}$$

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## Cluster SAMB

- Site cluster

\*\* Wyckoff: 1a

$$\boxed{\text{y1}} \quad \mathbb{Q}_0^{(s)}(A_{1g}) = [1]$$

- Bond cluster

\*\* Wyckoff: 3a@3d

$$\boxed{\text{y2}} \quad \mathbb{Q}_0^{(s)}(A_{1g}) = \left[ \frac{\sqrt{3}}{3}, \frac{\sqrt{3}}{3}, \frac{\sqrt{3}}{3} \right]$$

$$\boxed{\text{y3}} \quad \mathbb{Q}_{2,1}^{(s)}(E_g) = \left[ -\frac{\sqrt{6}}{6}, -\frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{3} \right]$$

$$\boxed{\text{y4}} \quad \mathbb{Q}_{2,2}^{(s)}(E_g) = \left[ \frac{\sqrt{2}}{2}, -\frac{\sqrt{2}}{2}, 0 \right]$$

$$\boxed{\text{y5}} \quad \mathbb{T}_{1,1}^{(s)}(T_{1u}) = [i, 0, 0]$$

$$\boxed{\text{y6}} \quad \mathbb{T}_{1,2}^{(s)}(T_{1u}) = [0, i, 0]$$

$$\boxed{\text{y7}} \quad \mathbb{T}_{1,3}^{(s)}(T_{1u}) = [0, 0, i]$$

\*\* Wyckoff: 6b@3c

$$\boxed{\text{y8}} \quad \mathbb{Q}_0^{(s)}(A_{1g}) = \left[ \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6} \right]$$

$$\boxed{\text{y9}} \quad \mathbb{Q}_{2,1}^{(s)}(E_g) = \left[ -\frac{\sqrt{3}}{6}, -\frac{\sqrt{3}}{6}, -\frac{\sqrt{3}}{6}, -\frac{\sqrt{3}}{6}, \frac{\sqrt{3}}{3}, \frac{\sqrt{3}}{3} \right]$$

$$\boxed{\text{y10}} \quad \mathbb{Q}_{2,2}^{(s)}(E_g) = \left[ \frac{1}{2}, \frac{1}{2}, -\frac{1}{2}, -\frac{1}{2}, 0, 0 \right]$$

$$\boxed{\text{y11}} \quad \mathbb{T}_{1,1}^{(s)}(T_{1u}) = \left[ 0, 0, \frac{i}{2}, \frac{i}{2}, \frac{i}{2}, -\frac{i}{2} \right]$$

$$\boxed{\text{y12}} \quad \mathbb{T}_{1,2}^{(s)}(T_{1u}) = \left[ \frac{i}{2}, -\frac{i}{2}, 0, 0, \frac{i}{2}, \frac{i}{2} \right]$$

$$\boxed{\text{y13}} \quad \mathbb{T}_{1,3}^{(s)}(T_{1u}) = \left[ \frac{i}{2}, \frac{i}{2}, \frac{i}{2}, -\frac{i}{2}, 0, 0 \right]$$

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

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

$$\boxed{\text{y16}} \quad \mathbb{Q}_{2,3}^{(s)}(T_{2g}) = \left[ 0, 0, 0, 0, \frac{\sqrt{2}}{2}, -\frac{\sqrt{2}}{2} \right]$$

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

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

$$\boxed{\text{y19}} \quad \mathbb{M}_{2,3}^{(s)}(T_{2u}) = \left[ \frac{i}{2}, \frac{i}{2}, -\frac{i}{2}, \frac{i}{2}, 0, 0 \right]$$

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**Site and Bond**


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Table 5: Orbital of each site

#	site	orbital
1	<b>A</b>	$ s, \uparrow\rangle,  s, \downarrow\rangle,  p_x, \uparrow\rangle,  p_x, \downarrow\rangle,  p_y, \uparrow\rangle,  p_y, \downarrow\rangle,  p_z, \uparrow\rangle,  p_z, \downarrow\rangle$

Table 6: Neighbor and bra-ket of each bond

#	head	tail	neighbor	head (bra)	tail (ket)
1	<b>A</b>	<b>A</b>	[1,2]	[s,p]	[s,p]

## Site in Unit Cell

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

Table 7: 'A' (#1) site cluster (1a),  $m\bar{3}m$

SL	position ( $\mathbf{s}$ )	mapping
1	[ 0.00000, 0.00000, 0.00000]	[1,2,3,4, $\dots$ ,48]

## 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 8: 1-th 'A'-'A' [1] (#1) bond cluster (3a@3d), ND,  $|\mathbf{v}|=1.0$  (cartesian)

SL	vector ( $\mathbf{v}$ )	center ( $\mathbf{c}$ )	mapping	head	tail	$\mathbf{R}$ (primitive)
1	[-1.00000, 0.00000, 0.00000]	[ 0.50000, 0.00000, 0.00000]	[1,-2,-3,4,17,-18,-19,20,-25,26,27,-28,-41,42,43,-44]	(1,1)	(1,1)	[1,0,0]
2	[ 0.00000,-1.00000, 0.00000]	[ 0.00000, 0.50000, 0.00000]	[5,-6,-7,8,13,-14,-15,16,-29,30,31,-32,-37,38,39,-40]	(1,1)	(1,1)	[0,1,0]
3	[ 0.00000, 0.00000,-1.00000]	[ 0.00000, 0.00000, 0.50000]	[9,-10,-11,12,-21,22,23,-24,-33,34,35,-36,45,-46,-47,48]	(1,1)	(1,1)	[0,0,1]



Table 9: 2-th 'A'-'A' [1] (#2) bond cluster (6b03c), ND,  $|\mathbf{v}|= 1.41421$  (cartesian)

SL	vector ( $\mathbf{v}$ )	center ( $\mathbf{c}$ )	mapping	head	tail	$\mathbf{R}$ (primitive)
1	[ 0.00000, -1.00000, -1.00000]	[ 0.00000, 0.50000, 0.50000]	[1, -4, 18, -19, -25, 28, -42, 43]	(1, 1)	(1, 1)	[0, 1, 1]
2	[ 0.00000, 1.00000, -1.00000]	[ 0.00000, 0.50000, 0.50000]	[2, -3, -17, 20, -26, 27, 41, -44]	(1, 1)	(1, 1)	[0, -1, 1]
3	[-1.00000, 0.00000, -1.00000]	[ 0.50000, 0.00000, 0.50000]	[5, -8, -14, 15, -29, 32, 38, -39]	(1, 1)	(1, 1)	[1, 0, 1]
4	[-1.00000, 0.00000, 1.00000]	[ 0.50000, 0.00000, 0.50000]	[6, -7, 13, -16, -30, 31, -37, 40]	(1, 1)	(1, 1)	[1, 0, -1]
5	[-1.00000, -1.00000, 0.00000]	[ 0.50000, 0.50000, 0.00000]	[9, -12, 21, -24, -33, 36, -45, 48]	(1, 1)	(1, 1)	[1, 1, 0]
6	[ 1.00000, -1.00000, 0.00000]	[ 0.50000, 0.50000, 0.00000]	[10, -11, -22, 23, -34, 35, 46, -47]	(1, 1)	(1, 1)	[-1, 1, 0]