

# Model for “D4h1”

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## General Condition

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

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## Group and Unit Cell

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- Group: SG No. 123 D<sub>4h</sub><sup>1</sup> P4/mmm [ tetragonal ]
- Associated point group: PG No. 123 D<sub>4h</sub> 4/mmm [ tetragonal ]
- Unit cell:

*a* = 1.00000, *b* = 1.00000, *c* = 1.50000,  $\alpha$  = 90.0,  $\beta$  = 90.0,  $\gamma$  = 90.0
- Lattice vectors (conventional cell):

*a*<sub>1</sub> = [ 1.00000, 0.00000, 0.00000]  
*a*<sub>2</sub> = [ 0.00000, 1.00000, 0.00000]  
*a*<sub>3</sub> = [ 0.00000, 0.00000, 1.50000]

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**Symmetry Operation**


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Table 1: Symmetry operation

#	SO	#	SO	#	SO	#	SO	#	SO
1	{1 0}	2	{2 <sub>001</sub>  0}	3	{4 <sub>001</sub> <sup>+</sup>  0}	4	{4 <sub>001</sub> <sup>-</sup>  0}	5	{2 <sub>010</sub>  0}
6	{2 <sub>100</sub>  0}	7	{2 <sub>110</sub>  0}	8	{2 <sub>1-10</sub>  0}	9	{-1 0}	10	{m <sub>001</sub>  0}
11	{-4 <sub>001</sub> <sup>+</sup>  0}	12	{-4 <sub>001</sub> <sup>-</sup>  0}	13	{m <sub>010</sub>  0}	14	{m <sub>100</sub>  0}	15	{m <sub>110</sub>  0}
16	{m <sub>1-10</sub>  0}								

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**Harmonics**


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Table 2: Harmonics

#	symbol	irrep.	rank	X	multiplicity	component	symmetry
1	$\mathbb{Q}_0(A_{1g})$	$A_{1g}$	0	$Q, T$	-	-	1
2	$\mathbb{Q}_2(A_{1g})$	$A_{1g}$	2	$Q, T$	-	-	$-\frac{x^2}{2} - \frac{y^2}{2} + z^2$
3	$\mathbb{G}_0(A_{1u})$	$A_{1u}$	0	$G, M$	-	-	1
4	$\mathbb{G}_2(A_{1u})$	$A_{1u}$	2	$G, M$	-	-	$-\frac{x^2}{2} - \frac{y^2}{2} + z^2$
5	$\mathbb{G}_4(A_{1u}, 1)$	$A_{1u}$	4	$G, M$	1	-	$\frac{\sqrt{21}(x^4 - 3x^2y^2 - 3x^2z^2 + y^4 - 3y^2z^2 + z^4)}{6}$
6	$\mathbb{G}_4(A_{1u}, 2)$	$A_{1u}$	4	$G, M$	2	-	$-\frac{\sqrt{15}(x^4 - 12x^2y^2 + 6x^2z^2 + y^4 + 6y^2z^2 - 2z^4)}{12}$

continued ...

Table 2

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

continued ...

Table 2

#	symbol	irrep.	rank	X	multiplicity	component	symmetry
28	$\mathbb{Q}_{2,2}(E_g)$					2	$\sqrt{3}xz$
29	$\mathbb{G}_{3,1}(E_g, 1)$	$E_g$	3	$G, M$	1	1	$\frac{x(2x^2 - 3y^2 - 3z^2)}{2}$
30	$\mathbb{G}_{3,2}(E_g, 1)$					2	$\frac{y(3x^2 - 2y^2 + 3z^2)}{2}$
31	$\mathbb{G}_{3,1}(E_g, 2)$	$E_g$	3	$G, M$	2	1	$\frac{\sqrt{15}x(y-z)(y+z)}{2}$
32	$\mathbb{G}_{3,2}(E_g, 2)$					2	$-\frac{\sqrt{15}y(x-z)(x+z)}{2}$
33	$\mathbb{Q}_{4,1}(E_g, 1)$	$E_g$	4	$Q, T$	1	1	$\frac{\sqrt{35}yz(y-z)(y+z)}{2}$
34	$\mathbb{Q}_{4,2}(E_g, 1)$					2	$\frac{\sqrt{35}xz(x-z)(x+z)}{2}$
35	$\mathbb{Q}_{4,1}(E_g, 2)$	$E_g$	4	$Q, T$	2	1	$\frac{\sqrt{5}yz(6x^2 - y^2 - z^2)}{2}$
36	$\mathbb{Q}_{4,2}(E_g, 2)$					2	$-\frac{\sqrt{5}xz(x^2 - 6y^2 + z^2)}{2}$
37	$\mathbb{Q}_{1,1}(E_u)$	$E_u$	1	$Q, T$	-	1	$x$
38	$\mathbb{Q}_{1,2}(E_u)$					2	$y$
39	$\mathbb{G}_{2,1}(E_u)$	$E_u$	2	$G, M$	-	1	$\sqrt{3}yz$
40	$\mathbb{G}_{2,2}(E_u)$					2	$-\sqrt{3}xz$
41	$\mathbb{Q}_{3,1}(E_u, 1)$	$E_u$	3	$Q, T$	1	1	$\frac{x(2x^2 - 3y^2 - 3z^2)}{2}$
42	$\mathbb{Q}_{3,2}(E_u, 1)$					2	$-\frac{y(3x^2 - 2y^2 + 3z^2)}{2}$
43	$\mathbb{Q}_{3,1}(E_u, 2)$	$E_u$	3	$Q, T$	2	1	$\frac{\sqrt{15}x(y-z)(y+z)}{2}$
44	$\mathbb{Q}_{3,2}(E_u, 2)$					2	$\frac{\sqrt{15}y(x-z)(x+z)}{2}$
45	$\mathbb{G}_{4,1}(E_u, 1)$	$E_u$	4	$G, M$	1	1	$\frac{\sqrt{35}yz(y-z)(y+z)}{2}$
46	$\mathbb{G}_{4,2}(E_u, 1)$					2	$-\frac{\sqrt{35}xz(x-z)(x+z)}{2}$
47	$\mathbb{G}_{4,1}(E_u, 2)$	$E_u$	4	$G, M$	2	1	$\frac{\sqrt{5}yz(6x^2 - y^2 - z^2)}{2}$
48	$\mathbb{G}_{4,2}(E_u, 2)$					2	$\frac{\sqrt{5}xz(x^2 - 6y^2 + z^2)}{2}$

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**Basis in full matrix**

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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

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

- '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

$$\boxed{\text{z269}} \quad \mathbb{G}_2^{(1,-1;c)}(A_{1u}) = \mathbb{G}_2^{(1,-1;a)}(A_{1u})\mathbb{Q}_0^{(s)}(A_{1g})$$

$$\boxed{\text{z270}} \quad \mathbb{G}_0^{(1,1;c)}(A_{1u}) = \mathbb{G}_0^{(1,1;a)}(A_{1u})\mathbb{Q}_0^{(s)}(A_{1g})$$

$$\boxed{\text{z318}} \quad \mathbb{Q}_1^{(c)}(A_{2u}) = \mathbb{Q}_1^{(a)}(A_{2u})\mathbb{Q}_0^{(s)}(A_{1g})$$

$$\boxed{\text{z319}} \quad \mathbb{Q}_1^{(1,0;c)}(A_{2u}) = \mathbb{Q}_1^{(1,0;a)}(A_{2u})\mathbb{Q}_0^{(s)}(A_{1g})$$

$$\boxed{\text{z359}} \quad \mathbb{G}_2^{(1,-1;c)}(B_{1u}) = \mathbb{G}_2^{(1,-1;a)}(B_{1u})\mathbb{Q}_0^{(s)}(A_{1g})$$

$$\boxed{\text{z403}} \quad \mathbb{G}_2^{(1,-1;c)}(B_{2u}) = \mathbb{G}_2^{(1,-1;a)}(B_{2u})\mathbb{Q}_0^{(s)}(A_{1g})$$

$$\boxed{\text{z443}} \quad \mathbb{Q}_{1,1}^{(c)}(E_u) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

$$\boxed{\text{z444}} \quad \mathbb{Q}_{1,2}^{(c)}(E_u) = \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

$$\boxed{\text{z445}} \quad \mathbb{Q}_{1,1}^{(1,0;c)}(E_u) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(1,0;a)}(E_u)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

$$\boxed{\text{z446}} \quad \mathbb{Q}_{1,2}^{(1,0;c)}(E_u) = \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(1,0;a)}(E_u)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

$$\boxed{\text{z447}} \quad \mathbb{G}_{2,1}^{(1,-1;c)}(E_u) = \frac{\sqrt{2}\mathbb{G}_{2,1}^{(1,-1;a)}(E_u)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

$$\boxed{\text{z448}} \quad \mathbb{G}_{2,2}^{(1,-1;c)}(E_u) = \frac{\sqrt{2}\mathbb{G}_{2,2}^{(1,-1;a)}(E_u)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

- ' $\mathbb{A}$ ' site-cluster :  $\mathbb{A}$
- \* 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

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

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

$$\boxed{\text{z4}} \quad \mathbb{Q}_2^{(1,-1;c)}(A_{1g}) = \mathbb{Q}_2^{(1,-1;a)}(A_{1g})\mathbb{Q}_0^{(s)}(A_{1g})$$

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

$$\boxed{\text{z49}} \quad \mathbb{G}_1^{(1,0;c)}(A_{2g}) = \mathbb{G}_1^{(1,0;a)}(A_{2g})\mathbb{Q}_0^{(s)}(A_{1g})$$

$$\boxed{\text{z77}} \quad \mathbb{Q}_2^{(c)}(B_{1g}) = \mathbb{Q}_2^{(a)}(B_{1g})\mathbb{Q}_0^{(s)}(A_{1g})$$

$$\boxed{\text{z78}} \quad \mathbb{Q}_2^{(1,-1;c)}(B_{1g}) = \mathbb{Q}_2^{(1,-1;a)}(B_{1g})\mathbb{Q}_0^{(s)}(A_{1g})$$

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

$$\boxed{\text{z115}} \quad \mathbb{Q}_2^{(1,-1;c)}(B_{2g}) = \mathbb{Q}_2^{(1,-1;a)}(B_{2g})\mathbb{Q}_0^{(s)}(A_{1g})$$

$$\boxed{\text{z147}} \quad \mathbb{Q}_{2,1}^{(c)}(E_g) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

$$\boxed{\text{z148}} \quad \mathbb{Q}_{2,2}^{(c)}(E_g) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

$$\boxed{\text{z149}} \quad \mathbb{Q}_{2,1}^{(1,-1;c)}(E_g) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

$$\boxed{\text{z150}} \quad \mathbb{Q}_{2,2}^{(1,-1;c)}(E_g) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

$$\boxed{\text{z151}} \quad \mathbb{G}_{1,1}^{(1,0;c)}(E_g) = \frac{\sqrt{2}\mathbb{G}_{1,1}^{(1,0;a)}(E_g)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

$$\boxed{\text{z152}} \quad \mathbb{G}_{1,2}^{(1,0;c)}(E_g) = \frac{\sqrt{2}\mathbb{G}_{1,2}^{(1,0;a)}(E_g)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

• 'A'-A' bond-cluster : A;A\_001\_1

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

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

\* wyckoff: 2b@2f

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

$$\boxed{\text{z79}} \quad \mathbb{G}_0^{(1,-1;c)}(A_{1u}) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z271}} \quad \mathbb{Q}_1^{(1,-1;c)}(A_{2u}) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z320}} \quad \mathbb{Q}_2^{(c)}(B_{1g}) = \mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_2^{(b)}(B_{1g})$$

$$\boxed{\text{z360}} \quad \mathbb{G}_2^{(1,-1;c)}(B_{1u}) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z404}} \quad \mathbb{G}_2^{(1,-1;c)}(B_{2u}) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z449}} \quad \mathbb{Q}_{1,1}^{(1,-1;c)}(E_u) = -\frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z450}} \quad \mathbb{Q}_{1,2}^{(1,-1;c)}(E_u) = \frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

• '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: 2b@2f

$$\boxed{\text{z7}} \quad \mathbb{Q}_0^{(c)}(A_{1g}) = \frac{\sqrt{2}\mathbb{T}_{1,1}^{(a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{T}_{1,2}^{(a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z8}} \quad \mathbb{Q}_2^{(1,-1;c)}(A_{1g}) = -\frac{\sqrt{2}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z9}} \quad \mathbb{Q}_0^{(1,0;c)}(A_{1g}) = \frac{\sqrt{2}\mathbb{T}_{1,1}^{(1,0;a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{T}_{1,2}^{(1,0;a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

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

$$\boxed{\text{z51}} \quad \mathbb{G}_2^{(1,-1;c)}(A_{1u}) = \mathbb{G}_2^{(1,-1;a)}(A_{1u})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z52}} \quad \mathbb{G}_0^{(1,1;c)}(A_{1u}) = \mathbb{G}_0^{(1,1;a)}(A_{1u})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z80}} \quad \mathbb{G}_1^{(c)}(A_{2g}) = \frac{\sqrt{2}\mathbb{T}_{1,1}^{(a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{T}_{1,2}^{(a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z81}} \quad \mathbb{G}_1^{(1,-1;c)}(A_{2g}) = \frac{\sqrt{2}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z82}} \quad \mathbb{G}_1^{(1,0;c)}(A_{2g}) = \frac{\sqrt{2}\mathbb{T}_{1,1}^{(1,0;a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{T}_{1,2}^{(1,0;a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z116}} \quad \mathbb{Q}_1^{(c)}(A_{2u}) = \mathbb{Q}_1^{(a)}(A_{2u})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z117}} \quad \mathbb{Q}_1^{(1,-1;c)}(A_{2u}) = -\mathbb{G}_2^{(1,-1;a)}(B_{2u})\mathbb{Q}_2^{(b)}(B_{1g})$$

$$\boxed{\text{z118}} \quad \mathbb{Q}_1^{(1,0;c)}(A_{2u}) = \mathbb{Q}_1^{(1,0;a)}(A_{2u})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z153}} \quad \mathbb{Q}_2^{(c)}(B_{1g}) = \frac{\sqrt{2}\mathbb{T}_{1,1}^{(a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{T}_{1,2}^{(a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z154}} \quad \mathbb{Q}_2^{(1,-1;c)}(B_{1g}) = -\frac{\sqrt{2}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z155}} \quad \mathbb{Q}_2^{(1,0;c)}(B_{1g}) = \frac{\sqrt{2}\mathbb{T}_{1,1}^{(1,0;a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{T}_{1,2}^{(1,0;a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z156}} \quad \mathbb{Q}_3^{(1,-1;c)}(B_{1u}) = \mathbb{G}_2^{(1,-1;a)}(A_{1u})\mathbb{Q}_2^{(b)}(B_{1g})$$

$$\boxed{\text{z157}} \quad \mathbb{G}_2^{(1,-1;c)}(B_{1u}) = \mathbb{G}_2^{(1,-1;a)}(B_{1u})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z158}} \quad \mathbb{G}_2^{(1,1;c)}(B_{1u}) = \mathbb{G}_0^{(1,1;a)}(A_{1u})\mathbb{Q}_2^{(b)}(B_{1g})$$

$$\boxed{\text{z159}} \quad \mathbb{Q}_2^{(c)}(B_{2g}) = \frac{\sqrt{2}\mathbb{T}_{1,1}^{(a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{T}_{1,2}^{(a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z160}} \quad \mathbb{Q}_2^{(1,-1;c)}(B_{2g}) = -\frac{\sqrt{2}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z161}} \quad \mathbb{Q}_2^{(1,0;c)}(B_{2g}) = \frac{\sqrt{2}\mathbb{T}_{1,1}^{(1,0;a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{T}_{1,2}^{(1,0;a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z162}} \quad \mathbb{Q}_3^{(c)}(B_{2u}) = \mathbb{Q}_1^{(a)}(A_{2u})\mathbb{Q}_2^{(b)}(B_{1g})$$

$$\boxed{\text{z163}} \quad \mathbb{Q}_3^{(1,0;c)}(B_{2u}) = \mathbb{Q}_1^{(1,0;a)}(A_{2u})\mathbb{Q}_2^{(b)}(B_{1g})$$

$$\boxed{\text{z164}} \quad \mathbb{G}_2^{(1,-1;c)}(B_{2u}) = \mathbb{G}_2^{(1,-1;a)}(B_{2u})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z272}} \quad \mathbb{Q}_{2,1}^{(c)}(E_g) = \frac{\sqrt{2}\mathbb{T}_1^{(a)}(A_{2u})\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z273}} \quad \mathbb{Q}_{2,2}^{(c)}(E_g) = \frac{\sqrt{2}\mathbb{T}_1^{(a)}(A_{2u})\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z274}} \quad \mathbb{Q}_{2,1}^{(1,-1;c)}(E_g) = \frac{\sqrt{30}\mathbb{M}_2^{(1,-1;a)}(A_{1u})\mathbb{T}_{1,1}^{(b)}(E_u)}{10} + \frac{\sqrt{10}\mathbb{M}_2^{(1,-1;a)}(B_{1u})\mathbb{T}_{1,1}^{(b)}(E_u)}{10} + \frac{\sqrt{10}\mathbb{M}_2^{(1,-1;a)}(B_{2u})\mathbb{T}_{1,2}^{(b)}(E_u)}{10}$$

$$\boxed{\text{z321}} \quad \mathbb{Q}_{2,2}^{(1,-1;c)}(E_g) = -\frac{\sqrt{30}\mathbb{M}_2^{(1,-1;a)}(A_{1u})\mathbb{T}_{1,2}^{(b)}(E_u)}{10} + \frac{\sqrt{10}\mathbb{M}_2^{(1,-1;a)}(B_{1u})\mathbb{T}_{1,2}^{(b)}(E_u)}{10} - \frac{\sqrt{10}\mathbb{M}_2^{(1,-1;a)}(B_{2u})\mathbb{T}_{1,1}^{(b)}(E_u)}{10}$$

$$\boxed{\text{z322}} \quad \mathbb{Q}_{2,1}^{(1,0;c)}(E_g) = \frac{\sqrt{2}\mathbb{T}_1^{(1,0;a)}(A_{2u})\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z323}} \quad \mathbb{Q}_{2,2}^{(1,0;c)}(E_g) = \frac{\sqrt{2}\mathbb{T}_1^{(1,0;a)}(A_{2u})\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z361}} \quad \mathbb{G}_{1,1}^{(1,-1;c)}(E_g) = -\frac{\sqrt{5}\mathbb{M}_2^{(1,-1;a)}(A_{1u})\mathbb{T}_{1,1}^{(b)}(E_u)}{5} + \frac{\sqrt{15}\mathbb{M}_2^{(1,-1;a)}(B_{1u})\mathbb{T}_{1,1}^{(b)}(E_u)}{10} + \frac{\sqrt{15}\mathbb{M}_2^{(1,-1;a)}(B_{2u})\mathbb{T}_{1,2}^{(b)}(E_u)}{10}$$

$$\boxed{\text{z362}} \quad \mathbb{G}_{1,2}^{(1,-1;c)}(E_g) = \frac{\sqrt{5}\mathbb{M}_2^{(1,-1;a)}(A_{1u})\mathbb{T}_{1,2}^{(b)}(E_u)}{5} + \frac{\sqrt{15}\mathbb{M}_2^{(1,-1;a)}(B_{1u})\mathbb{T}_{1,2}^{(b)}(E_u)}{10} - \frac{\sqrt{15}\mathbb{M}_2^{(1,-1;a)}(B_{2u})\mathbb{T}_{1,1}^{(b)}(E_u)}{10}$$

$$\boxed{\text{z363}} \quad \mathbb{G}_{3,1}^{(1,-1;c)}(E_g, 1) = \frac{\mathbb{M}_2^{(1,-1;a)}(B_{1u})\mathbb{T}_{1,1}^{(b)}(E_u)}{2} - \frac{\mathbb{M}_2^{(1,-1;a)}(B_{2u})\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z405}} \quad \mathbb{G}_{3,2}^{(1,-1;c)}(E_g, 1) = \frac{\mathbb{M}_2^{(1,-1;a)}(B_{1u})\mathbb{T}_{1,2}^{(b)}(E_u)}{2} + \frac{\mathbb{M}_2^{(1,-1;a)}(B_{2u})\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z406}} \quad \mathbb{G}_{1,1}^{(1,1;c)}(E_g) = \frac{\sqrt{2}\mathbb{M}_0^{(1,1;a)}(A_{1u})\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z407}} \quad \mathbb{G}_{1,2}^{(1,1;c)}(E_g) = -\frac{\sqrt{2}\mathbb{M}_0^{(1,1;a)}(A_{1u})\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

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

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

$$\boxed{\text{z453}} \quad \mathbb{Q}_{1,1}^{(c)}(E_u, b) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_2^{(b)}(B_{1g})}{2}$$

$$\boxed{\text{z454}} \quad \mathbb{Q}_{1,2}^{(c)}(E_u, b) = -\frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_2^{(b)}(B_{1g})}{2}$$

$$\boxed{\text{z455}} \quad \mathbb{Q}_{1,1}^{(1,-1;c)}(E_u) = \frac{\sqrt{2}\mathbb{G}_{2,1}^{(1,-1;a)}(E_u)\mathbb{Q}_2^{(b)}(B_{1g})}{2}$$

$$\boxed{\text{z456}} \quad \mathbb{Q}_{1,2}^{(1,-1;c)}(E_u) = -\frac{\sqrt{2}\mathbb{G}_{2,2}^{(1,-1;a)}(E_u)\mathbb{Q}_2^{(b)}(B_{1g})}{2}$$

$$\boxed{\text{z457}} \quad \mathbb{Q}_{1,1}^{(1,0;c)}(E_u, a) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(1,0;a)}(E_u)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z458}} \quad \mathbb{Q}_{1,2}^{(1,0;c)}(E_u, a) = \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(1,0;a)}(E_u)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z459}} \quad \mathbb{Q}_{1,1}^{(1,0;c)}(E_u, b) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(1,0;a)}(E_u)\mathbb{Q}_2^{(b)}(B_{1g})}{2}$$

$$\boxed{\text{z460}} \quad \mathbb{Q}_{1,2}^{(1,0;c)}(E_u, b) = -\frac{\sqrt{2}\mathbb{Q}_{1,2}^{(1,0;a)}(E_u)\mathbb{Q}_2^{(b)}(B_{1g})}{2}$$

$$\boxed{\text{z461}} \quad \mathbb{G}_{2,1}^{(1,-1;c)}(E_u) = \frac{\sqrt{2}\mathbb{G}_{2,1}^{(1,-1;a)}(E_u)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z462}} \quad \mathbb{G}_{2,2}^{(1,-1;c)}(E_u) = \frac{\sqrt{2}\mathbb{G}_{2,2}^{(1,-1;a)}(E_u)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

• '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: 2b@2f

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

$$\boxed{\text{z11}} \quad \mathbb{Q}_0^{(c)}(A_{1g}, b) = \mathbb{Q}_2^{(a)}(B_{1g})\mathbb{Q}_2^{(b)}(B_{1g})$$

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

$$\boxed{\text{z13}} \quad \mathbb{Q}_0^{(1,-1;c)}(A_{1g}) = \mathbb{Q}_2^{(1,-1;a)}(B_{1g})\mathbb{Q}_2^{(b)}(B_{1g})$$

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

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

$$\boxed{\text{z53}} \quad \mathbb{G}_0^{(c)}(A_{1u}) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{M}_{1,2}^{(a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

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

$$\boxed{\text{z55}} \quad \mathbb{G}_2^{(1,-1;c)}(A_{1u}) = -\frac{\sqrt{3}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g, 1)\mathbb{T}_{1,1}^{(b)}(E_u)}{4} - \frac{\sqrt{5}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g, 2)\mathbb{T}_{1,1}^{(b)}(E_u)}{4} + \frac{\sqrt{3}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g, 1)\mathbb{T}_{1,2}^{(b)}(E_u)}{4} + \frac{\sqrt{5}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g, 2)\mathbb{T}_{1,2}^{(b)}(E_u)}{4}$$

$$\boxed{\text{z83}} \quad \mathbb{G}_4^{(1,-1;c)}(A_{1u}, 1) = \frac{\sqrt{5}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g, 1)\mathbb{T}_{1,1}^{(b)}(E_u)}{4} - \frac{\sqrt{3}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g, 2)\mathbb{T}_{1,1}^{(b)}(E_u)}{4} - \frac{\sqrt{5}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g, 1)\mathbb{T}_{1,2}^{(b)}(E_u)}{4} + \frac{\sqrt{3}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g, 2)\mathbb{T}_{1,2}^{(b)}(E_u)}{4}$$

$$\boxed{\text{z84}} \quad \mathbb{G}_2^{(1,0;c)}(A_{1u}) = -\frac{\sqrt{2}\mathbb{T}_{2,1}^{(1,0;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{T}_{2,2}^{(1,0;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z85}} \quad \mathbb{G}_0^{(1,1;c)}(A_{1u}) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z86}} \quad \mathbb{Q}_4^{(c)}(A_{2g}) = \mathbb{Q}_2^{(a)}(B_{2g})\mathbb{Q}_2^{(b)}(B_{1g})$$

$$\boxed{\text{z87}} \quad \mathbb{Q}_4^{(1,-1;c)}(A_{2g}) = \mathbb{Q}_2^{(1,-1;a)}(B_{2g})\mathbb{Q}_2^{(b)}(B_{1g})$$

$$\boxed{\text{z88}} \quad \mathbb{G}_1^{(1,0;c)}(A_{2g}) = \mathbb{G}_1^{(1,0;a)}(A_{2g})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z119}} \quad \mathbb{Q}_1^{(e)}(A_{2u}) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{M}_{1,2}^{(a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z120}} \quad \mathbb{Q}_1^{(1,-1;c)}(A_{2u}) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z121}} \quad \mathbb{Q}_3^{(1,-1;c)}(A_{2u}) = -\frac{\sqrt{3}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,1)\mathbb{T}_{1,2}^{(b)}(E_u)}{4} - \frac{\sqrt{5}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,2}^{(b)}(E_u)}{4} - \frac{\sqrt{3}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,1)\mathbb{T}_{1,1}^{(b)}(E_u)}{4} - \frac{\sqrt{5}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,1}^{(b)}(E_u)}{4}$$

$$\boxed{\text{z165}} \quad \mathbb{Q}_1^{(1,0;c)}(A_{2u}) = \frac{\sqrt{2}\mathbb{T}_{2,1}^{(1,0;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{T}_{2,2}^{(1,0;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z166}} \quad \mathbb{Q}_1^{(1,1;c)}(A_{2u}) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z167}} \quad \mathbb{G}_4^{(1,-1;c)}(A_{2u}) = \frac{\sqrt{5}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,1)\mathbb{T}_{1,2}^{(b)}(E_u)}{4} - \frac{\sqrt{3}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,2}^{(b)}(E_u)}{4} + \frac{\sqrt{5}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,1)\mathbb{T}_{1,1}^{(b)}(E_u)}{4} - \frac{\sqrt{3}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,1}^{(b)}(E_u)}{4}$$

$$\boxed{\text{z168}} \quad \mathbb{Q}_2^{(c)}(B_{1g}, a) = \mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_2^{(b)}(B_{1g})$$

$$\boxed{\text{z169}} \quad \mathbb{Q}_2^{(c)}(B_{1g}, b) = \mathbb{Q}_2^{(a)}(B_{1g})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z170}} \quad \mathbb{Q}_2^{(c)}(B_{1g}, c) = -\mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_2^{(b)}(B_{1g})$$

$$\boxed{\text{z171}} \quad \mathbb{Q}_2^{(1,-1;c)}(B_{1g}, a) = \mathbb{Q}_2^{(1,-1;a)}(B_{1g})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z172}} \quad \mathbb{Q}_2^{(1,-1;c)}(B_{1g}, b) = -\mathbb{Q}_2^{(1,-1;a)}(A_{1g})\mathbb{Q}_2^{(b)}(B_{1g})$$

$$\boxed{\text{z173}} \quad \mathbb{Q}_2^{(1,1;c)}(B_{1g}) = \mathbb{Q}_0^{(1,1;a)}(A_{1g})\mathbb{Q}_2^{(b)}(B_{1g})$$

$$\boxed{\text{z174}} \quad \mathbb{Q}_3^{(1,-1;c)}(B_{1u}) = -\frac{\sqrt{2}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z175}} \quad \mathbb{Q}_3^{(1,0;c)}(B_{1u}) = \frac{\sqrt{2}\mathbb{T}_{2,1}^{(1,0;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{T}_{2,2}^{(1,0;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z176}} \quad \mathbb{G}_2^{(c)}(B_{1u}) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{M}_{1,2}^{(a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z275}} \quad \mathbb{G}_2^{(1,-1;c)}(B_{1u}, a) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z276}} \quad \mathbb{G}_2^{(1,-1;c)}(B_{1u}, b) = \frac{\sqrt{2}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g, 1)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g, 1)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z277}} \quad \mathbb{G}_2^{(1,1;c)}(B_{1u}) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z278}} \quad \mathbb{Q}_2^{(c)}(B_{2g}) = \mathbb{Q}_2^{(a)}(B_{2g})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z279}} \quad \mathbb{Q}_2^{(1,-1;c)}(B_{2g}) = \mathbb{Q}_2^{(1,-1;a)}(B_{2g})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z280}} \quad \mathbb{Q}_2^{(1,0;c)}(B_{2g}) = \mathbb{G}_1^{(1,0;a)}(A_{2g})\mathbb{Q}_2^{(b)}(B_{1g})$$

$$\boxed{\text{z324}} \quad \mathbb{Q}_3^{(1,-1;c)}(B_{2u}) = \frac{\sqrt{30}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g, 1)\mathbb{T}_{1,2}^{(b)}(E_u)}{8} + \frac{\sqrt{2}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g, 2)\mathbb{T}_{1,2}^{(b)}(E_u)}{8} - \frac{\sqrt{30}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g, 1)\mathbb{T}_{1,1}^{(b)}(E_u)}{8} - \frac{\sqrt{2}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g, 2)\mathbb{T}_{1,1}^{(b)}(E_u)}{8}$$

$$\boxed{\text{z325}} \quad \mathbb{Q}_3^{(1,0;c)}(B_{2u}) = -\frac{\sqrt{2}\mathbb{T}_{2,1}^{(1,0;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{T}_{2,2}^{(1,0;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z326}} \quad \mathbb{G}_2^{(c)}(B_{2u}) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{M}_{1,2}^{(a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z327}} \quad \mathbb{G}_2^{(1,-1;c)}(B_{2u}, a) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z328}} \quad \mathbb{G}_2^{(1,-1;c)}(B_{2u}, b) = -\frac{\sqrt{2}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g, 1)\mathbb{T}_{1,2}^{(b)}(E_u)}{8} + \frac{\sqrt{30}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g, 2)\mathbb{T}_{1,2}^{(b)}(E_u)}{8} + \frac{\sqrt{2}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g, 1)\mathbb{T}_{1,1}^{(b)}(E_u)}{8} - \frac{\sqrt{30}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g, 2)\mathbb{T}_{1,1}^{(b)}(E_u)}{8}$$

$$\boxed{\text{z329}} \quad \mathbb{G}_2^{(1,1;c)}(B_{2u}) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z364}} \quad \mathbb{Q}_{2,1}^{(c)}(E_g, a) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z365}} \quad \mathbb{Q}_{2,2}^{(c)}(E_g, a) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z366}} \quad \mathbb{Q}_{2,1}^{(c)}(E_g, b) = -\frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_2^{(b)}(B_{1g})}{2}$$

$$\boxed{\text{z367}} \quad \mathbb{Q}_{2,2}^{(c)}(E_g, b) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_2^{(b)}(B_{1g})}{2}$$

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

$$\boxed{\text{z369}} \quad \mathbb{Q}_{2,2}^{(1,-1;c)}(E_g, a) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z408}} \quad \mathbb{Q}_{2,1}^{(1,-1;c)}(E_g, b) = -\frac{\sqrt{2}\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_2^{(b)}(B_{1g})}{2}$$

$$\boxed{\text{z409}} \quad \mathbb{Q}_{2,2}^{(1,-1;c)}(E_g, b) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_2^{(b)}(B_{1g})}{2}$$

$$\boxed{\text{z410}} \quad \mathbb{Q}_{2,1}^{(1,0;c)}(E_g) = -\frac{\sqrt{2}\mathbb{G}_{1,1}^{(1,0;a)}(E_g)\mathbb{Q}_2^{(b)}(B_{1g})}{2}$$

$$\boxed{\text{z411}} \quad \mathbb{Q}_{2,2}^{(1,0;c)}(E_g) = \frac{\sqrt{2}\mathbb{G}_{1,2}^{(1,0;a)}(E_g)\mathbb{Q}_2^{(b)}(B_{1g})}{2}$$

$$\boxed{\text{z412}} \quad \mathbb{G}_{1,1}^{(1,0;c)}(E_g) = \frac{\sqrt{2}\mathbb{G}_{1,1}^{(1,0;a)}(E_g)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z413}} \quad \mathbb{G}_{1,2}^{(1,0;c)}(E_g) = \frac{\sqrt{2}\mathbb{G}_{1,2}^{(1,0;a)}(E_g)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z463}} \quad \mathbb{Q}_{1,1}^{(c)}(E_u) = -\frac{\sqrt{2}\mathbb{M}_1^{(a)}(A_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z464}} \quad \mathbb{Q}_{1,2}^{(c)}(E_u) = \frac{\sqrt{2}\mathbb{M}_1^{(a)}(A_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z465}} \quad \mathbb{Q}_{1,1}^{(1,-1;c)}(E_u) = -\frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z466}} \quad \mathbb{Q}_{1,2}^{(1,-1;c)}(E_u) = \frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z467}} \quad \mathbb{Q}_{3,1}^{(1,-1;c)}(E_u, 1) = \frac{\sqrt{3}\mathbb{M}_3^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{4} - \frac{\sqrt{5}\mathbb{M}_3^{(1,-1;a)}(B_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{4}$$

$$\boxed{\text{z468}} \quad \mathbb{Q}_{3,2}^{(1,-1;c)}(E_u, 1) = -\frac{\sqrt{3}\mathbb{M}_3^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{4} - \frac{\sqrt{5}\mathbb{M}_3^{(1,-1;a)}(B_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{4}$$

$$\boxed{\text{z469}} \quad \mathbb{Q}_{3,1}^{(1,-1;c)}(E_u, 2) = \frac{\sqrt{165}\mathbb{M}_3^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{44} + \frac{2\sqrt{11}\mathbb{M}_3^{(1,-1;a)}(B_{1g})\mathbb{T}_{1,1}^{(b)}(E_u)}{11} + \frac{3\sqrt{11}\mathbb{M}_3^{(1,-1;a)}(B_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{44}$$

$$\boxed{\text{z470}} \quad \mathbb{Q}_{3,2}^{(1,-1;c)}(E_u, 2) = -\frac{\sqrt{165}\mathbb{M}_3^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{44} - \frac{2\sqrt{11}\mathbb{M}_3^{(1,-1;a)}(B_{1g})\mathbb{T}_{1,2}^{(b)}(E_u)}{11} + \frac{3\sqrt{11}\mathbb{M}_3^{(1,-1;a)}(B_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{44}$$

$$\boxed{\text{z471}} \quad \mathbb{Q}_{1,1}^{(1,0;c)}(E_u) = -\frac{\sqrt{14}\mathbb{T}_2^{(1,0;a)}(A_{1g})\mathbb{T}_{1,1}^{(b)}(E_u)}{14} + \frac{\sqrt{42}\mathbb{T}_2^{(1,0;a)}(B_{1g})\mathbb{T}_{1,1}^{(b)}(E_u)}{14} + \frac{\sqrt{42}\mathbb{T}_2^{(1,0;a)}(B_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{14}$$

$$\boxed{\text{z472}} \quad \mathbb{Q}_{1,2}^{(1,0;c)}(E_u) = -\frac{\sqrt{14}\mathbb{T}_2^{(1,0;a)}(A_{1g})\mathbb{T}_{1,2}^{(b)}(E_u)}{14} - \frac{\sqrt{42}\mathbb{T}_2^{(1,0;a)}(B_{1g})\mathbb{T}_{1,2}^{(b)}(E_u)}{14} + \frac{\sqrt{42}\mathbb{T}_2^{(1,0;a)}(B_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{14}$$

$$\boxed{\text{z473}} \quad \mathbb{Q}_{3,1}^{(1,0;c)}(E_u, 1) = -\frac{\sqrt{42}\mathbb{T}_2^{(1,0;a)}(A_{1g})\mathbb{T}_{1,1}^{(b)}(E_u)}{28} + \frac{3\sqrt{14}\mathbb{T}_2^{(1,0;a)}(B_{1g})\mathbb{T}_{1,1}^{(b)}(E_u)}{28} - \frac{\sqrt{14}\mathbb{T}_2^{(1,0;a)}(B_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{7}$$

$$\boxed{\text{z474}} \quad \mathbb{Q}_{3,2}^{(1,0;c)}(E_u, 1) = -\frac{\sqrt{42}\mathbb{T}_2^{(1,0;a)}(A_{1g})\mathbb{T}_{1,2}^{(b)}(E_u)}{28} - \frac{3\sqrt{14}\mathbb{T}_2^{(1,0;a)}(B_{1g})\mathbb{T}_{1,2}^{(b)}(E_u)}{28} - \frac{\sqrt{14}\mathbb{T}_2^{(1,0;a)}(B_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{7}$$

$$\boxed{\text{z475}} \quad \mathbb{Q}_{3,1}^{(1,0;c)}(E_u, 2) = -\frac{\sqrt{6}\mathbb{T}_2^{(1,0;a)}(A_{1g})\mathbb{T}_{1,1}^{(b)}(E_u)}{4} - \frac{\sqrt{2}\mathbb{T}_2^{(1,0;a)}(B_{1g})\mathbb{T}_{1,1}^{(b)}(E_u)}{4}$$

$$\boxed{\text{z476}} \quad \mathbb{Q}_{3,2}^{(1,0;c)}(E_u, 2) = -\frac{\sqrt{6}\mathbb{T}_2^{(1,0;a)}(A_{1g})\mathbb{T}_{1,2}^{(b)}(E_u)}{4} + \frac{\sqrt{2}\mathbb{T}_2^{(1,0;a)}(B_{1g})\mathbb{T}_{1,2}^{(b)}(E_u)}{4}$$

$$\boxed{\text{z477}} \quad \mathbb{Q}_{1,1}^{(1,1;c)}(E_u) = -\frac{\sqrt{2}\mathbb{M}_1^{(1,1;a)}(A_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z478}} \quad \mathbb{Q}_{1,2}^{(1,1;c)}(E_u) = \frac{\sqrt{2}\mathbb{M}_1^{(1,1;a)}(A_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z479}} \quad \mathbb{G}_{2,1}^{(1,-1;c)}(E_u) = -\frac{\sqrt{110}\mathbb{M}_3^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{22} + \frac{\sqrt{66}\mathbb{M}_3^{(1,-1;a)}(B_{1g})\mathbb{T}_{1,1}^{(b)}(E_u)}{22} - \frac{\sqrt{66}\mathbb{M}_3^{(1,-1;a)}(B_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{22}$$

$$\boxed{\text{z480}} \quad \mathbb{G}_{2,2}^{(1,-1;c)}(E_u) = \frac{\sqrt{110}\mathbb{M}_3^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{22} - \frac{\sqrt{66}\mathbb{M}_3^{(1,-1;a)}(B_{1g})\mathbb{T}_{1,2}^{(b)}(E_u)}{22} - \frac{\sqrt{66}\mathbb{M}_3^{(1,-1;a)}(B_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{22}$$

• 'A'-A' bond-cluster : A;A\_002\_1

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

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

\* wyckoff: 2c@1c

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

$$\boxed{\text{z122}} \quad \mathbb{G}_0^{(1,-1;c)}(A_{1u}) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z281}} \quad \mathbb{Q}_1^{(1,-1;c)}(A_{2u}) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z330}} \quad \mathbb{G}_2^{(1,-1;c)}(B_{1u}) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z370}} \quad \mathbb{Q}_2^{(c)}(B_{2g}) = \mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_2^{(b)}(B_{2g})$$

$$\boxed{\text{z414}} \quad \mathbb{G}_2^{(1,-1;c)}(B_{2u}) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z481}} \quad \mathbb{Q}_{1,1}^{(1,-1;c)}(E_u) = -\frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z482}} \quad \mathbb{Q}_{1,2}^{(1,-1;c)}(E_u) = \frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

• '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: 2c@1c

$$\boxed{\text{z17}} \quad \mathbb{Q}_0^{(c)}(A_{1g}) = \frac{\sqrt{2}\mathbb{T}_{1,1}^{(a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{T}_{1,2}^{(a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z18}} \quad \mathbb{Q}_2^{(1,-1;c)}(A_{1g}) = -\frac{\sqrt{2}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z19}} \quad \mathbb{Q}_0^{(1,0;c)}(A_{1g}) = \frac{\sqrt{2}\mathbb{T}_{1,1}^{(1,0;a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{T}_{1,2}^{(1,0;a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z56}} \quad \mathbb{G}_0^{(1,-1;c)}(A_{1u}) = \mathbb{G}_2^{(1,-1;a)}(B_{2u})\mathbb{Q}_2^{(b)}(B_{2g})$$

$$\boxed{\text{z57}} \quad \mathbb{G}_2^{(1,-1;c)}(A_{1u}) = \mathbb{G}_2^{(1,-1;a)}(A_{1u})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z58}} \quad \mathbb{G}_0^{(1,1;c)}(A_{1u}) = \mathbb{G}_0^{(1,1;a)}(A_{1u})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z89}} \quad \mathbb{G}_1^{(c)}(A_{2g}) = \frac{\sqrt{2}\mathbb{T}_{1,1}^{(a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{T}_{1,2}^{(a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z90}} \quad \mathbb{G}_1^{(1,-1;c)}(A_{2g}) = \frac{\sqrt{2}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z91}} \quad \mathbb{G}_1^{(1,0;c)}(A_{2g}) = \frac{\sqrt{2}\mathbb{T}_{1,1}^{(1,0;a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{T}_{1,2}^{(1,0;a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z123}} \quad \mathbb{Q}_1^{(c)}(A_{2u}) = \mathbb{Q}_1^{(a)}(A_{2u})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z124}} \quad \mathbb{Q}_1^{(1,-1;c)}(A_{2u}) = \mathbb{G}_2^{(1,-1;a)}(B_{1u})\mathbb{Q}_2^{(b)}(B_{2g})$$

$$\boxed{\text{z125}} \quad \mathbb{Q}_1^{(1,0;c)}(A_{2u}) = \mathbb{Q}_1^{(1,0;a)}(A_{2u})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z177}} \quad \mathbb{Q}_2^{(c)}(B_{1g}) = \frac{\sqrt{2}\mathbb{T}_{1,1}^{(a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{T}_{1,2}^{(a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z178}} \quad \mathbb{Q}_2^{(1,-1;c)}(B_{1g}) = -\frac{\sqrt{2}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z179}} \quad \mathbb{Q}_2^{(1,0;c)}(B_{1g}) = \frac{\sqrt{2}\mathbb{T}_{1,1}^{(1,0;a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{T}_{1,2}^{(1,0;a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z180}} \quad \mathbb{Q}_3^{(c)}(B_{1u}) = \mathbb{Q}_1^{(a)}(A_{2u})\mathbb{Q}_2^{(b)}(B_{2g})$$

$$\boxed{\text{z181}} \quad \mathbb{Q}_3^{(1,0;c)}(B_{1u}) = \mathbb{Q}_1^{(1,0;a)}(A_{2u})\mathbb{Q}_2^{(b)}(B_{2g})$$

$$\boxed{\text{z182}} \quad \mathbb{G}_2^{(1,-1;c)}(B_{1u}) = \mathbb{G}_2^{(1,-1;a)}(B_{1u})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z183}} \quad \mathbb{Q}_2^{(c)}(B_{2g}) = \frac{\sqrt{2}\mathbb{T}_{1,1}^{(a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{T}_{1,2}^{(a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z184}} \quad \mathbb{Q}_2^{(1,-1;c)}(B_{2g}) = -\frac{\sqrt{2}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z185}} \quad \mathbb{Q}_2^{(1,0;c)}(B_{2g}) = \frac{\sqrt{2}\mathbb{T}_{1,1}^{(1,0;a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{T}_{1,2}^{(1,0;a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z186}} \quad \mathbb{Q}_3^{(1,-1;c)}(B_{2u}) = -\mathbb{G}_2^{(1,-1;a)}(A_{1u})\mathbb{Q}_2^{(b)}(B_{2g})$$

$$\boxed{\text{z187}} \quad \mathbb{G}_2^{(1,-1;c)}(B_{2u}) = \mathbb{G}_2^{(1,-1;a)}(B_{2u})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z188}} \quad \mathbb{G}_2^{(1,1;c)}(B_{2u}) = \mathbb{G}_0^{(1,1;a)}(A_{1u})\mathbb{Q}_2^{(b)}(B_{2g})$$

$$\boxed{\text{z282}} \quad \mathbb{Q}_{2,1}^{(c)}(E_g) = \frac{\sqrt{2}\mathbb{T}_1^{(a)}(A_{2u})\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z283}} \quad \mathbb{Q}_{2,2}^{(c)}(E_g) = \frac{\sqrt{2}\mathbb{T}_1^{(a)}(A_{2u})\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z284}} \quad \mathbb{Q}_{2,1}^{(1,-1;c)}(E_g) = \frac{\sqrt{30}\mathbb{M}_2^{(1,-1;a)}(A_{1u})\mathbb{T}_{1,1}^{(b)}(E_u)}{10} + \frac{\sqrt{10}\mathbb{M}_2^{(1,-1;a)}(B_{1u})\mathbb{T}_{1,1}^{(b)}(E_u)}{10} + \frac{\sqrt{10}\mathbb{M}_2^{(1,-1;a)}(B_{2u})\mathbb{T}_{1,2}^{(b)}(E_u)}{10}$$

$$\boxed{\text{z331}} \quad \mathbb{Q}_{2,2}^{(1,-1;c)}(E_g) = -\frac{\sqrt{30}\mathbb{M}_2^{(1,-1;a)}(A_{1u})\mathbb{T}_{1,2}^{(b)}(E_u)}{10} + \frac{\sqrt{10}\mathbb{M}_2^{(1,-1;a)}(B_{1u})\mathbb{T}_{1,2}^{(b)}(E_u)}{10} - \frac{\sqrt{10}\mathbb{M}_2^{(1,-1;a)}(B_{2u})\mathbb{T}_{1,1}^{(b)}(E_u)}{10}$$

$$\boxed{\text{z332}} \quad \mathbb{Q}_{2,1}^{(1,0;c)}(E_g) = \frac{\sqrt{2}\mathbb{T}_1^{(1,0;a)}(A_{2u})\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z333}} \quad \mathbb{Q}_{2,2}^{(1,0;c)}(E_g) = \frac{\sqrt{2}\mathbb{T}_1^{(1,0;a)}(A_{2u})\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

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

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

$$\boxed{\text{z373}} \quad \mathbb{G}_{3,1}^{(1,-1;c)}(E_g, 1) = \frac{\mathbb{M}_2^{(1,-1;a)}(B_{1u})\mathbb{T}_{1,1}^{(b)}(E_u)}{2} - \frac{\mathbb{M}_2^{(1,-1;a)}(B_{2u})\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z415}} \quad \mathbb{G}_{3,2}^{(1,-1;c)}(E_g, 1) = \frac{\mathbb{M}_2^{(1,-1;a)}(B_{1u})\mathbb{T}_{1,2}^{(b)}(E_u)}{2} + \frac{\mathbb{M}_2^{(1,-1;a)}(B_{2u})\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z416}} \quad \mathbb{G}_{1,1}^{(1,1;c)}(E_g) = \frac{\sqrt{2}\mathbb{M}_0^{(1,1;a)}(A_{1u})\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z417}} \quad \mathbb{G}_{1,2}^{(1,1;c)}(E_g) = -\frac{\sqrt{2}\mathbb{M}_0^{(1,1;a)}(A_{1u})\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z483}} \quad \mathbb{Q}_{1,1}^{(c)}(E_u, a) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z484}} \quad \mathbb{Q}_{1,2}^{(c)}(E_u, a) = \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z485}} \quad \mathbb{Q}_{1,1}^{(c)}(E_u, b) = \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_2^{(b)}(B_{2g})}{2}$$

$$\boxed{\text{z486}} \quad \mathbb{Q}_{1,2}^{(c)}(E_u, b) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_2^{(b)}(B_{2g})}{2}$$

$$\boxed{\text{z487}} \quad \mathbb{Q}_{1,1}^{(1,-1;c)}(E_u) = \frac{\sqrt{2}\mathbb{G}_{2,2}^{(1,-1;a)}(E_u)\mathbb{Q}_2^{(b)}(B_{2g})}{2}$$

$$\boxed{\text{z488}} \quad \mathbb{Q}_{1,2}^{(1,-1;c)}(E_u) = \frac{\sqrt{2}\mathbb{G}_{2,1}^{(1,-1;a)}(E_u)\mathbb{Q}_2^{(b)}(B_{2g})}{2}$$

$$\boxed{\text{z489}} \quad \mathbb{Q}_{1,1}^{(1,0;c)}(E_u, a) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(1,0;a)}(E_u)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z490}} \quad \mathbb{Q}_{1,2}^{(1,0;c)}(E_u, a) = \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(1,0;a)}(E_u)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z491}} \quad \mathbb{Q}_{1,1}^{(1,0;c)}(E_u, b) = \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(1,0;a)}(E_u)\mathbb{Q}_2^{(b)}(B_{2g})}{2}$$

$$\boxed{\text{z492}} \quad \mathbb{Q}_{1,2}^{(1,0;c)}(E_u, b) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(1,0;a)}(E_u)\mathbb{Q}_2^{(b)}(B_{2g})}{2}$$

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

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

• '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: 2c@1c

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

$$\boxed{\text{z21}} \quad \mathbb{Q}_0^{(c)}(A_{1g}, b) = \mathbb{Q}_2^{(a)}(B_{2g})\mathbb{Q}_2^{(b)}(B_{2g})$$

$$\boxed{\text{z22}} \quad \mathbb{Q}_2^{(c)}(A_{1g}) = \mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z23}} \quad \mathbb{Q}_0^{(1,-1;c)}(A_{1g}) = \mathbb{Q}_2^{(1,-1;a)}(B_{2g})\mathbb{Q}_2^{(b)}(B_{2g})$$

$$\boxed{\text{z24}} \quad \mathbb{Q}_2^{(1,-1;c)}(A_{1g}) = \mathbb{Q}_2^{(1,-1;a)}(A_{1g})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z25}} \quad \mathbb{Q}_0^{(1,1;c)}(A_{1g}) = \mathbb{Q}_0^{(1,1;a)}(A_{1g})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z59}} \quad \mathbb{G}_0^{(c)}(A_{1u}) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{M}_{1,2}^{(a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z60}} \quad \mathbb{G}_0^{(1,-1;c)}(A_{1u}) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z61}} \quad \mathbb{G}_2^{(1,-1;c)}(A_{1u}) = -\frac{\sqrt{3}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g, 1)\mathbb{T}_{1,1}^{(b)}(E_u)}{4} - \frac{\sqrt{5}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g, 2)\mathbb{T}_{1,1}^{(b)}(E_u)}{4} + \frac{\sqrt{3}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g, 1)\mathbb{T}_{1,2}^{(b)}(E_u)}{4} + \frac{\sqrt{5}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g, 2)\mathbb{T}_{1,2}^{(b)}(E_u)}{4}$$

$$\boxed{\text{z92}} \quad \mathbb{G}_4^{(1,-1;c)}(A_{1u}, 1) = \frac{\sqrt{5}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g, 1)\mathbb{T}_{1,1}^{(b)}(E_u)}{4} - \frac{\sqrt{3}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g, 2)\mathbb{T}_{1,1}^{(b)}(E_u)}{4} - \frac{\sqrt{5}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g, 1)\mathbb{T}_{1,2}^{(b)}(E_u)}{4} + \frac{\sqrt{3}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g, 2)\mathbb{T}_{1,2}^{(b)}(E_u)}{4}$$

$$\boxed{\text{z93}} \quad \mathbb{G}_2^{(1,0;c)}(A_{1u}) = -\frac{\sqrt{2}\mathbb{T}_{2,1}^{(1,0;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{T}_{2,2}^{(1,0;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z94}} \quad \mathbb{G}_0^{(1,1;c)}(A_{1u}) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z126}} \quad \mathbb{Q}_4^{(c)}(A_{2g}) = \mathbb{Q}_2^{(a)}(B_{1g})\mathbb{Q}_2^{(b)}(B_{2g})$$

$$\boxed{\text{z127}} \quad \mathbb{Q}_4^{(1,-1;c)}(A_{2g}) = \mathbb{Q}_2^{(1,-1;a)}(B_{1g})\mathbb{Q}_2^{(b)}(B_{2g})$$

$$\boxed{\text{z128}} \quad \mathbb{G}_1^{(1,0;c)}(A_{2g}) = \mathbb{G}_1^{(1,0;a)}(A_{2g})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z129}} \quad \mathbb{Q}_1^{(c)}(A_{2u}) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{M}_{1,2}^{(a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z130}} \quad \mathbb{Q}_1^{(1,-1;c)}(A_{2u}) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z131}} \quad \mathbb{Q}_3^{(1,-1;c)}(A_{2u}) = -\frac{\sqrt{3}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,1)\mathbb{T}_{1,2}^{(b)}(E_u)}{4} - \frac{\sqrt{5}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,2}^{(b)}(E_u)}{4} - \frac{\sqrt{3}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,1)\mathbb{T}_{1,1}^{(b)}(E_u)}{4} - \frac{\sqrt{5}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,1}^{(b)}(E_u)}{4}$$

$$\boxed{\text{z189}} \quad \mathbb{Q}_1^{(1,0;c)}(A_{2u}) = \frac{\sqrt{2}\mathbb{T}_{2,1}^{(1,0;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{T}_{2,2}^{(1,0;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z190}} \quad \mathbb{Q}_1^{(1,1;c)}(A_{2u}) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z191}} \quad \mathbb{G}_4^{(1,-1;c)}(A_{2u}) = \frac{\sqrt{5}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,1)\mathbb{T}_{1,2}^{(b)}(E_u)}{4} - \frac{\sqrt{3}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,2}^{(b)}(E_u)}{4} + \frac{\sqrt{5}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,1)\mathbb{T}_{1,1}^{(b)}(E_u)}{4} - \frac{\sqrt{3}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,1}^{(b)}(E_u)}{4}$$

$$\boxed{\text{z192}} \quad \mathbb{Q}_2^{(c)}(B_{1g}) = \mathbb{Q}_2^{(a)}(B_{1g})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z193}} \quad \mathbb{Q}_2^{(1,-1;c)}(B_{1g}) = \mathbb{Q}_2^{(1,-1;a)}(B_{1g})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z194}} \quad \mathbb{Q}_2^{(1,0;c)}(B_{1g}) = -\mathbb{G}_1^{(1,0;a)}(A_{2g})\mathbb{Q}_2^{(b)}(B_{2g})$$

$$\boxed{\text{z195}} \quad \mathbb{Q}_3^{(1,-1;c)}(B_{1u}) = -\frac{\sqrt{2}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z196}} \quad \mathbb{Q}_3^{(1,0;c)}(B_{1u}) = \frac{\sqrt{2}\mathbb{T}_{2,1}^{(1,0;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{T}_{2,2}^{(1,0;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z197}} \quad \mathbb{G}_2^{(c)}(B_{1u}) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{M}_{1,2}^{(a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z198}} \quad \mathbb{G}_2^{(1,-1;c)}(B_{1u}, a) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z199}} \quad \mathbb{G}_2^{(1,-1;c)}(B_{1u}, b) = \frac{\sqrt{2}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g, 1)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g, 1)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z200}} \quad \mathbb{G}_2^{(1,1;c)}(B_{1u}) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z285}} \quad \mathbb{Q}_2^{(c)}(B_{2g}, a) = \mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_2^{(b)}(B_{2g})$$

$$\boxed{\text{z286}} \quad \mathbb{Q}_2^{(c)}(B_{2g}, b) = \mathbb{Q}_2^{(a)}(B_{2g})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z287}} \quad \mathbb{Q}_2^{(c)}(B_{2g}, c) = -\mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_2^{(b)}(B_{2g})$$

$$\boxed{\text{z288}} \quad \mathbb{Q}_2^{(1,-1;c)}(B_{2g}, a) = \mathbb{Q}_2^{(1,-1;a)}(B_{2g})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z289}} \quad \mathbb{Q}_2^{(1,-1;c)}(B_{2g}, b) = -\mathbb{Q}_2^{(1,-1;a)}(A_{1g})\mathbb{Q}_2^{(b)}(B_{2g})$$

$$\boxed{\text{z290}} \quad \mathbb{Q}_2^{(1,1;c)}(B_{2g}) = \mathbb{Q}_0^{(1,1;a)}(A_{1g})\mathbb{Q}_2^{(b)}(B_{2g})$$

$$\boxed{\text{z334}} \quad \mathbb{Q}_3^{(1,-1;c)}(B_{2u}) = \frac{\sqrt{30}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g, 1)\mathbb{T}_{1,2}^{(b)}(E_u)}{8} + \frac{\sqrt{2}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g, 2)\mathbb{T}_{1,2}^{(b)}(E_u)}{8} - \frac{\sqrt{30}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g, 1)\mathbb{T}_{1,1}^{(b)}(E_u)}{8} - \frac{\sqrt{2}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g, 2)\mathbb{T}_{1,1}^{(b)}(E_u)}{8}$$

$$\boxed{\text{z335}} \quad \mathbb{Q}_3^{(1,0;c)}(B_{2u}) = -\frac{\sqrt{2}\mathbb{T}_{2,1}^{(1,0;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{T}_{2,2}^{(1,0;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z336}} \quad \mathbb{G}_2^{(c)}(B_{2u}) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{M}_{1,2}^{(a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z337}} \quad \mathbb{G}_2^{(1,-1;c)}(B_{2u}, a) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z338}} \quad \mathbb{G}_2^{(1,-1;c)}(B_{2u}, b) = -\frac{\sqrt{2}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g, 1)\mathbb{T}_{1,2}^{(b)}(E_u)}{8} + \frac{\sqrt{30}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g, 2)\mathbb{T}_{1,2}^{(b)}(E_u)}{8} + \frac{\sqrt{2}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g, 1)\mathbb{T}_{1,1}^{(b)}(E_u)}{8} - \frac{\sqrt{30}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g, 2)\mathbb{T}_{1,1}^{(b)}(E_u)}{8}$$

$$\boxed{\text{z339}} \quad \mathbb{G}_2^{(1,1;c)}(B_{2u}) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z374}} \quad \mathbb{Q}_{2,1}^{(c)}(E_g, a) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z375}} \quad \mathbb{Q}_{2,2}^{(c)}(E_g, a) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z376}} \quad \mathbb{Q}_{2,1}^{(c)}(E_g, b) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_2^{(b)}(B_{2g})}{2}$$

$$\boxed{\text{z377}} \quad \mathbb{Q}_{2,2}^{(c)}(E_g, b) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_2^{(b)}(B_{2g})}{2}$$

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

$$\boxed{\text{z379}} \quad \mathbb{Q}_{2,2}^{(1,-1;c)}(E_g, a) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z418}} \quad \mathbb{Q}_{2,1}^{(1,-1;c)}(E_g, b) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_2^{(b)}(B_{2g})}{2}$$

$$\boxed{\text{z419}} \quad \mathbb{Q}_{2,2}^{(1,-1;c)}(E_g, b) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_2^{(b)}(B_{2g})}{2}$$

$$\boxed{\text{z420}} \quad \mathbb{Q}_{2,1}^{(1,0;c)}(E_g) = \frac{\sqrt{2}\mathbb{G}_{1,2}^{(1,0;a)}(E_g)\mathbb{Q}_2^{(b)}(B_{2g})}{2}$$

$$\boxed{\text{z421}} \quad \mathbb{Q}_{2,2}^{(1,0;c)}(E_g) = \frac{\sqrt{2}\mathbb{G}_{1,1}^{(1,0;a)}(E_g)\mathbb{Q}_2^{(b)}(B_{2g})}{2}$$

$$\boxed{\text{z422}} \quad \mathbb{G}_{1,1}^{(1,0;c)}(E_g) = \frac{\sqrt{2}\mathbb{G}_{1,1}^{(1,0;a)}(E_g)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z423}} \quad \mathbb{G}_{1,2}^{(1,0;c)}(E_g) = \frac{\sqrt{2}\mathbb{G}_{1,2}^{(1,0;a)}(E_g)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z495}} \quad \mathbb{Q}_{1,1}^{(c)}(E_u) = -\frac{\sqrt{2}\mathbb{M}_1^{(a)}(A_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z496}} \quad \mathbb{Q}_{1,2}^{(c)}(E_u) = \frac{\sqrt{2}\mathbb{M}_1^{(a)}(A_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z497}} \quad \mathbb{Q}_{1,1}^{(1,-1;c)}(E_u) = -\frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z498}} \quad \mathbb{Q}_{1,2}^{(1,-1;c)}(E_u) = \frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z499}} \quad \mathbb{Q}_{3,1}^{(1,-1;c)}(E_u, 1) = \frac{\sqrt{3}\mathbb{M}_3^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{4} - \frac{\sqrt{5}\mathbb{M}_3^{(1,-1;a)}(B_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{4}$$

$$\boxed{\text{z500}} \quad \mathbb{Q}_{3,2}^{(1,-1;c)}(E_u, 1) = -\frac{\sqrt{3}\mathbb{M}_3^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{4} - \frac{\sqrt{5}\mathbb{M}_3^{(1,-1;a)}(B_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{4}$$

$$\boxed{\text{z501}} \quad \mathbb{Q}_{3,1}^{(1,-1;c)}(E_u, 2) = \frac{\sqrt{165}\mathbb{M}_3^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{44} + \frac{2\sqrt{11}\mathbb{M}_3^{(1,-1;a)}(B_{1g})\mathbb{T}_{1,1}^{(b)}(E_u)}{11} + \frac{3\sqrt{11}\mathbb{M}_3^{(1,-1;a)}(B_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{44}$$

$$\boxed{\text{z502}} \quad \mathbb{Q}_{3,2}^{(1,-1;c)}(E_u, 2) = -\frac{\sqrt{165}\mathbb{M}_3^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{44} - \frac{2\sqrt{11}\mathbb{M}_3^{(1,-1;a)}(B_{1g})\mathbb{T}_{1,2}^{(b)}(E_u)}{11} + \frac{3\sqrt{11}\mathbb{M}_3^{(1,-1;a)}(B_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{44}$$

$$\boxed{\text{z503}} \quad \mathbb{Q}_{1,1}^{(1,0;c)}(E_u) = -\frac{\sqrt{14}\mathbb{T}_2^{(1,0;a)}(A_{1g})\mathbb{T}_{1,1}^{(b)}(E_u)}{14} + \frac{\sqrt{42}\mathbb{T}_2^{(1,0;a)}(B_{1g})\mathbb{T}_{1,1}^{(b)}(E_u)}{14} + \frac{\sqrt{42}\mathbb{T}_2^{(1,0;a)}(B_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{14}$$

$$\boxed{\text{z504}} \quad \mathbb{Q}_{1,2}^{(1,0;c)}(E_u) = -\frac{\sqrt{14}\mathbb{T}_2^{(1,0;a)}(A_{1g})\mathbb{T}_{1,2}^{(b)}(E_u)}{14} - \frac{\sqrt{42}\mathbb{T}_2^{(1,0;a)}(B_{1g})\mathbb{T}_{1,1}^{(b)}(E_u)}{14} + \frac{\sqrt{42}\mathbb{T}_2^{(1,0;a)}(B_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{14}$$

$$\boxed{\text{z505}} \quad \mathbb{Q}_{3,1}^{(1,0;c)}(E_u, 1) = -\frac{\sqrt{42}\mathbb{T}_2^{(1,0;a)}(A_{1g})\mathbb{T}_{1,1}^{(b)}(E_u)}{28} + \frac{3\sqrt{14}\mathbb{T}_2^{(1,0;a)}(B_{1g})\mathbb{T}_{1,1}^{(b)}(E_u)}{28} - \frac{\sqrt{14}\mathbb{T}_2^{(1,0;a)}(B_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{7}$$

$$\boxed{\text{z506}} \quad \mathbb{Q}_{3,2}^{(1,0;c)}(E_u, 1) = -\frac{\sqrt{42}\mathbb{T}_2^{(1,0;a)}(A_{1g})\mathbb{T}_{1,2}^{(b)}(E_u)}{28} - \frac{3\sqrt{14}\mathbb{T}_2^{(1,0;a)}(B_{1g})\mathbb{T}_{1,2}^{(b)}(E_u)}{28} - \frac{\sqrt{14}\mathbb{T}_2^{(1,0;a)}(B_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{7}$$

$$\boxed{\text{z507}} \quad \mathbb{Q}_{3,1}^{(1,0;c)}(E_u, 2) = -\frac{\sqrt{6}\mathbb{T}_2^{(1,0;a)}(A_{1g})\mathbb{T}_{1,1}^{(b)}(E_u)}{4} - \frac{\sqrt{2}\mathbb{T}_2^{(1,0;a)}(B_{1g})\mathbb{T}_{1,1}^{(b)}(E_u)}{4}$$

$$\boxed{\text{z508}} \quad \mathbb{Q}_{3,2}^{(1,0;c)}(E_u, 2) = -\frac{\sqrt{6}\mathbb{T}_2^{(1,0;a)}(A_{1g})\mathbb{T}_{1,2}^{(b)}(E_u)}{4} + \frac{\sqrt{2}\mathbb{T}_2^{(1,0;a)}(B_{1g})\mathbb{T}_{1,2}^{(b)}(E_u)}{4}$$

$$\boxed{\text{z509}} \quad \mathbb{Q}_{1,1}^{(1,1;c)}(E_u) = -\frac{\sqrt{2}\mathbb{M}_1^{(1,1;a)}(A_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z510}} \quad \mathbb{Q}_{1,2}^{(1,1;c)}(E_u) = \frac{\sqrt{2}\mathbb{M}_1^{(1,1;a)}(A_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z511}} \quad \mathbb{G}_{2,1}^{(1,-1;c)}(E_u) = -\frac{\sqrt{110}\mathbb{M}_3^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{22} + \frac{\sqrt{66}\mathbb{M}_3^{(1,-1;a)}(B_{1g})\mathbb{T}_{1,1}^{(b)}(E_u)}{22} - \frac{\sqrt{66}\mathbb{M}_3^{(1,-1;a)}(B_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{22}$$

$$\boxed{\text{z512}} \quad \mathbb{G}_{2,2}^{(1,-1;c)}(E_u) = \frac{\sqrt{110}\mathbb{M}_3^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{22} - \frac{\sqrt{66}\mathbb{M}_3^{(1,-1;a)}(B_{1g})\mathbb{T}_{1,2}^{(b)}(E_u)}{22} - \frac{\sqrt{66}\mathbb{M}_3^{(1,-1;a)}(B_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{22}$$

• 'A'-A' bond-cluster : A;A\_003\_1

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

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

\* wyckoff: 1a@1b

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

$$\boxed{\text{z291}} \quad \mathbb{G}_0^{(1,-1;c)}(A_{1u}) = \mathbb{M}_1^{(1,-1;a)}(A_{2g})\mathbb{T}_1^{(b)}(A_{2u})$$

$$\boxed{\text{z513}} \quad \mathbb{Q}_{1,1}^{(1,-1;c)}(E_u) = -\frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_1^{(b)}(A_{2u})}{2}$$

$$\boxed{\text{z514}} \quad \mathbb{Q}_{1,2}^{(1,-1;c)}(E_u) = -\frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_1^{(b)}(A_{2u})}{2}$$

• 'A'-A' bond-cluster : A;A\_003\_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: 1a@1b

$$\boxed{\text{z27}} \quad \mathbb{Q}_0^{(c)}(A_{1g}) = \mathbb{T}_1^{(a)}(A_{2u})\mathbb{T}_1^{(b)}(A_{2u})$$

$$\boxed{\text{z28}} \quad \mathbb{Q}_0^{(1,0;c)}(A_{1g}) = \mathbb{T}_1^{(1,0;a)}(A_{2u})\mathbb{T}_1^{(b)}(A_{2u})$$

$$\boxed{\text{z62}} \quad \mathbb{G}_2^{(1,-1;c)}(A_{1u}) = \mathbb{G}_2^{(1,-1;a)}(A_{1u})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z63}} \quad \mathbb{G}_0^{(1,1;c)}(A_{1u}) = \mathbb{G}_0^{(1,1;a)}(A_{1u})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z95}} \quad \mathbb{G}_1^{(1,-1;c)}(A_{2g}) = \mathbb{M}_2^{(1,-1;a)}(A_{1u})\mathbb{T}_1^{(b)}(A_{2u})$$

$$\boxed{\text{z132}} \quad \mathbb{G}_1^{(1,1;c)}(A_{2g}) = \mathbb{M}_0^{(1,1;a)}(A_{1u})\mathbb{T}_1^{(b)}(A_{2u})$$

$$\boxed{\text{z201}} \quad \mathbb{Q}_1^{(c)}(A_{2u}) = \mathbb{Q}_1^{(a)}(A_{2u})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z202}} \quad \mathbb{Q}_1^{(1,0;c)}(A_{2u}) = \mathbb{Q}_1^{(1,0;a)}(A_{2u})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z203}} \quad \mathbb{Q}_2^{(1,-1;c)}(B_{1g}) = \mathbb{M}_2^{(1,-1;a)}(B_{2u})\mathbb{T}_1^{(b)}(A_{2u})$$

$$\boxed{\text{z204}} \quad \mathbb{G}_2^{(1,-1;c)}(B_{1u}) = \mathbb{G}_2^{(1,-1;a)}(B_{1u})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z205}} \quad \mathbb{Q}_2^{(1,-1;c)}(B_{2g}) = -\mathbb{M}_2^{(1,-1;a)}(B_{1u})\mathbb{T}_1^{(b)}(A_{2u})$$

$$\boxed{\text{z206}} \quad \mathbb{G}_2^{(1,-1;c)}(B_{2u}) = \mathbb{G}_2^{(1,-1;a)}(B_{2u})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z292}} \quad \mathbb{Q}_{2,1}^{(c)}(E_g) = \frac{\sqrt{2}\mathbb{T}_{1,2}^{(a)}(E_u)\mathbb{T}_1^{(b)}(A_{2u})}{2}$$

$$\boxed{\text{z293}} \quad \mathbb{Q}_{2,2}^{(c)}(E_g) = \frac{\sqrt{2}\mathbb{T}_{1,1}^{(a)}(E_u)\mathbb{T}_1^{(b)}(A_{2u})}{2}$$

$$\boxed{\text{z340}} \quad \mathbb{Q}_{2,1}^{(1,-1;c)}(E_g) = \frac{\sqrt{2}\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{T}_1^{(b)}(A_{2u})}{2}$$

$$\boxed{\text{z341}} \quad \mathbb{Q}_{2,2}^{(1,-1;c)}(E_g) = \frac{\sqrt{2}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{T}_1^{(b)}(A_{2u})}{2}$$

$$\boxed{\text{z380}} \quad \mathbb{Q}_{2,1}^{(1,0;c)}(E_g) = \frac{\sqrt{2}\mathbb{T}_{1,2}^{(1,0;a)}(E_u)\mathbb{T}_1^{(b)}(A_{2u})}{2}$$

$$\boxed{\text{z424}} \quad \mathbb{Q}_{2,2}^{(1,0;c)}(E_g) = \frac{\sqrt{2}\mathbb{T}_{1,1}^{(1,0;a)}(E_u)\mathbb{T}_1^{(b)}(A_{2u})}{2}$$

$$\boxed{\text{z515}} \quad \mathbb{Q}_{1,1}^{(c)}(E_u) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z516}} \quad \mathbb{Q}_{1,2}^{(c)}(E_u) = \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z517}} \quad \mathbb{Q}_{1,1}^{(1,0;c)}(E_u) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(1,0;a)}(E_u)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z518}} \quad \mathbb{Q}_{1,2}^{(1,0;c)}(E_u) = \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(1,0;a)}(E_u)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z519}} \quad \mathbb{G}_{2,1}^{(1,-1;c)}(E_u) = \frac{\sqrt{2}\mathbb{G}_{2,1}^{(1,-1;a)}(E_u)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z520}} \quad \mathbb{G}_{2,2}^{(1,-1;c)}(E_u) = \frac{\sqrt{2}\mathbb{G}_{2,2}^{(1,-1;a)}(E_u)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

• 'A'-A' bond-cluster : A;A\_003\_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: 1a@1b

$$\boxed{\text{z29}} \quad \mathbb{Q}_0^{(c)}(A_{1g}) = \mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z30}} \quad \mathbb{Q}_2^{(c)}(A_{1g}) = \mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z31}} \quad \mathbb{Q}_2^{(1,-1;c)}(A_{1g}) = \mathbb{Q}_2^{(1,-1;a)}(A_{1g})\mathbb{Q}_0^{(b)}(A_{1g})$$

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

$$\boxed{\text{z64}} \quad \mathbb{G}_0^{(c)}(A_{1u}) = \mathbb{M}_1^{(a)}(A_{2g})\mathbb{T}_1^{(b)}(A_{2u})$$

$$\boxed{\text{z96}} \quad \mathbb{G}_0^{(1,-1;c)}(A_{1u}) = \mathbb{M}_1^{(1,-1;a)}(A_{2g})\mathbb{T}_1^{(b)}(A_{2u})$$

$$\boxed{\text{z97}} \quad \mathbb{G}_2^{(1,-1;c)}(A_{1u}) = \mathbb{M}_3^{(1,-1;a)}(A_{2g})\mathbb{T}_1^{(b)}(A_{2u})$$

$$\boxed{\text{z133}} \quad \mathbb{G}_0^{(1,1;c)}(A_{1u}) = \mathbb{M}_1^{(1,1;a)}(A_{2g})\mathbb{T}_1^{(b)}(A_{2u})$$

$$\boxed{\text{z134}} \quad \mathbb{G}_1^{(1,0;c)}(A_{2g}) = \mathbb{G}_1^{(1,0;a)}(A_{2g})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z207}} \quad \mathbb{Q}_1^{(1,0;c)}(A_{2u}) = \mathbb{T}_2^{(1,0;a)}(A_{1g})\mathbb{T}_1^{(b)}(A_{2u})$$

$$\boxed{\text{z208}} \quad \mathbb{Q}_2^{(c)}(B_{1g}) = \mathbb{Q}_2^{(a)}(B_{1g})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z209}} \quad \mathbb{Q}_2^{(1,-1;c)}(B_{1g}) = \mathbb{Q}_2^{(1,-1;a)}(B_{1g})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z210}} \quad \mathbb{Q}_3^{(1,-1;c)}(B_{1u}) = -\mathbb{M}_3^{(1,-1;a)}(B_{2g})\mathbb{T}_1^{(b)}(A_{2u})$$

$$\boxed{\text{z211}} \quad \mathbb{Q}_3^{(1,0;c)}(B_{1u}) = \mathbb{T}_2^{(1,0;a)}(B_{2g})\mathbb{T}_1^{(b)}(A_{2u})$$

$$\boxed{\text{z212}} \quad \mathbb{Q}_2^{(c)}(B_{2g}) = \mathbb{Q}_2^{(a)}(B_{2g})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z294}} \quad \mathbb{Q}_2^{(1,-1;c)}(B_{2g}) = \mathbb{Q}_2^{(1,-1;a)}(B_{2g})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z295}} \quad \mathbb{Q}_3^{(1,-1;c)}(B_{2u}) = \mathbb{M}_3^{(1,-1;a)}(B_{1g})\mathbb{T}_1^{(b)}(A_{2u})$$

$$\boxed{\text{z296}} \quad \mathbb{Q}_3^{(1,0;c)}(B_{2u}) = \mathbb{T}_2^{(1,0;a)}(B_{1g})\mathbb{T}_1^{(b)}(A_{2u})$$

$$\boxed{\text{z297}} \quad \mathbb{Q}_{2,1}^{(c)}(E_g) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z342}} \quad \mathbb{Q}_{2,2}^{(c)}(E_g) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z381}} \quad \mathbb{Q}_{2,1}^{(1,-1;c)}(E_g) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z382}} \quad \mathbb{Q}_{2,2}^{(1,-1;c)}(E_g) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z425}} \quad \mathbb{G}_{1,1}^{(1,0;c)}(E_g) = \frac{\sqrt{2}\mathbb{G}_{1,1}^{(1,0;a)}(E_g)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z426}} \quad \mathbb{G}_{1,2}^{(1,0;c)}(E_g) = \frac{\sqrt{2}\mathbb{G}_{1,2}^{(1,0;a)}(E_g)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z521}} \quad \mathbb{Q}_{1,1}^{(c)}(E_u) = -\frac{\sqrt{2}\mathbb{M}_{1,2}^{(a)}(E_g)\mathbb{T}_1^{(b)}(A_{2u})}{2}$$

$$\boxed{\text{z522}} \quad \mathbb{Q}_{1,2}^{(c)}(E_u) = -\frac{\sqrt{2}\mathbb{M}_{1,1}^{(a)}(E_g)\mathbb{T}_1^{(b)}(A_{2u})}{2}$$

$$\boxed{\text{z523}} \quad \mathbb{Q}_{1,1}^{(1,-1;c)}(E_u) = -\frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_1^{(b)}(A_{2u})}{2}$$

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

$$\boxed{\text{z525}} \quad \mathbb{Q}_{3,1}^{(1,-1;c)}(E_u, 1) = \frac{\sqrt{3}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g, 1)\mathbb{T}_1^{(b)}(A_{2u})}{4} - \frac{\sqrt{5}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g, 2)\mathbb{T}_1^{(b)}(A_{2u})}{4}$$

$$\boxed{\text{z526}} \quad \mathbb{Q}_{3,2}^{(1,-1;c)}(E_u, 1) = \frac{\sqrt{3}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g, 1)\mathbb{T}_1^{(b)}(A_{2u})}{4} - \frac{\sqrt{5}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g, 2)\mathbb{T}_1^{(b)}(A_{2u})}{4}$$

$$\boxed{\text{z527}} \quad \mathbb{Q}_{3,1}^{(1,-1;c)}(E_u, 2) = -\frac{\sqrt{5}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g, 1)\mathbb{T}_1^{(b)}(A_{2u})}{4} - \frac{\sqrt{3}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g, 2)\mathbb{T}_1^{(b)}(A_{2u})}{4}$$

$$\boxed{\text{z528}} \quad \mathbb{Q}_{3,2}^{(1,-1;c)}(E_u, 2) = -\frac{\sqrt{5}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g, 1)\mathbb{T}_1^{(b)}(A_{2u})}{4} - \frac{\sqrt{3}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g, 2)\mathbb{T}_1^{(b)}(A_{2u})}{4}$$

$$\boxed{\text{z529}} \quad \mathbb{Q}_{1,1}^{(1,0;c)}(E_u) = \frac{\sqrt{2}\mathbb{T}_{2,2}^{(1,0;a)}(E_g)\mathbb{T}_1^{(b)}(A_{2u})}{2}$$

$$\boxed{\text{z530}} \quad \mathbb{Q}_{1,2}^{(1,0;c)}(E_u) = \frac{\sqrt{2}\mathbb{T}_{2,1}^{(1,0;a)}(E_g)\mathbb{T}_1^{(b)}(A_{2u})}{2}$$

$$\boxed{\text{z531}} \quad \mathbb{Q}_{1,1}^{(1,1;c)}(E_u) = -\frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,1;a)}(E_g)\mathbb{T}_1^{(b)}(A_{2u})}{2}$$

$$\boxed{\text{z532}} \quad \mathbb{Q}_{1,2}^{(1,1;c)}(E_u) = -\frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,1;a)}(E_g)\mathbb{T}_1^{(b)}(A_{2u})}{2}$$

• 'A'-'A' bond-cluster : A;A\_004\_1

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

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

\* wyckoff: 4e@2e

$$\boxed{\text{z33}} \quad \mathbb{Q}_0^{(c)}(A_{1g}) = \mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z98}} \quad \mathbb{G}_0^{(1,-1;c)}(A_{1u}) = \frac{\sqrt{3}\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{3} - \frac{\sqrt{3}\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{3} + \frac{\sqrt{3}\mathbb{M}_1^{(1,-1;a)}(A_{2g})\mathbb{T}_1^{(b)}(A_{2u})}{3}$$

$$\boxed{\text{z213}} \quad \mathbb{G}_2^{(1,-1;c)}(A_{1u}) = -\frac{\sqrt{6}\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{6} + \frac{\sqrt{6}\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{6} + \frac{\sqrt{6}\mathbb{M}_1^{(1,-1;a)}(A_{2g})\mathbb{T}_1^{(b)}(A_{2u})}{3}$$

$$\boxed{\text{z214}} \quad \mathbb{Q}_1^{(1,-1;c)}(A_{2u}) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z298}} \quad \mathbb{Q}_2^{(c)}(B_{1g}) = \mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_2^{(b)}(B_{1g})$$

$$\boxed{\text{z299}} \quad \mathbb{Q}_3^{(1,-1;c)}(B_{1u}) = \mathbb{M}_1^{(1,-1;a)}(A_{2g})\mathbb{M}_2^{(b)}(B_{2u})$$

$$\boxed{\text{z343}} \quad \mathbb{G}_2^{(1,-1;c)}(B_{1u}) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z383}} \quad \mathbb{G}_2^{(1,-1;c)}(B_{2u}) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z384}} \quad \mathbb{Q}_{2,1}^{(c)}(E_g) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z427}} \quad \mathbb{Q}_{2,2}^{(c)}(E_g) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z533}} \quad \mathbb{Q}_{1,1}^{(1,-1;c)}(E_u, a) = -\frac{\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_1^{(b)}(A_{2u})}{2} - \frac{\mathbb{M}_1^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z534}} \quad \mathbb{Q}_{1,2}^{(1,-1;c)}(E_u, a) = -\frac{\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_1^{(b)}(A_{2u})}{2} + \frac{\mathbb{M}_1^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z535}} \quad \mathbb{Q}_{1,1}^{(1,-1;c)}(E_u, b) = -\frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{M}_2^{(b)}(B_{2u})}{2}$$

$$\boxed{\text{z536}} \quad \mathbb{Q}_{1,2}^{(1,-1;c)}(E_u, b) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{M}_2^{(b)}(B_{2u})}{2}$$

$$\boxed{\text{z537}} \quad \mathbb{G}_{2,1}^{(1,-1;c)}(E_u) = -\frac{\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_1^{(b)}(A_{2u})}{2} + \frac{\mathbb{M}_1^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z538}} \quad \mathbb{G}_{2,2}^{(1,-1;c)}(E_u) = -\frac{\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_1^{(b)}(A_{2u})}{2} - \frac{\mathbb{M}_1^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

• 'A'-'A' bond-cluster : A;A\_004\_-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: 4e@2e

$$\boxed{\text{z34}} \quad \mathbb{Q}_0^{(c)}(A_{1g}) = \frac{\sqrt{3}\mathbb{T}_{1,1}^{(a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{3} + \frac{\sqrt{3}\mathbb{T}_{1,2}^{(a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{3} + \frac{\sqrt{3}\mathbb{T}_1^{(a)}(A_{2u})\mathbb{T}_1^{(b)}(A_{2u})}{3}$$

$$\boxed{\text{z35}} \quad \mathbb{Q}_2^{(c)}(A_{1g}) = -\frac{\sqrt{6}\mathbb{T}_{1,1}^{(a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{6} - \frac{\sqrt{6}\mathbb{T}_{1,2}^{(a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{6} + \frac{\sqrt{6}\mathbb{T}_1^{(a)}(A_{2u})\mathbb{T}_1^{(b)}(A_{2u})}{3}$$

$$\boxed{\text{z36}} \quad \mathbb{Q}_0^{(1,-1;c)}(A_{1g}) = \mathbb{M}_2^{(1,-1;a)}(B_{2u})\mathbb{M}_2^{(b)}(B_{2u})$$

$$\boxed{\text{z37}} \quad \mathbb{Q}_2^{(1,-1;c)}(A_{1g}) = -\frac{\sqrt{2}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z38}} \quad \mathbb{Q}_0^{(1,0;c)}(A_{1g}) = \frac{\sqrt{3}\mathbb{T}_{1,1}^{(1,0;a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{3} + \frac{\sqrt{3}\mathbb{T}_{1,2}^{(1,0;a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{3} + \frac{\sqrt{3}\mathbb{T}_1^{(1,0;a)}(A_{2u})\mathbb{T}_1^{(b)}(A_{2u})}{3}$$

$$\boxed{\text{z39}} \quad \mathbb{Q}_2^{(1,0;c)}(A_{1g}) = -\frac{\sqrt{6}\mathbb{T}_{1,1}^{(1,0;a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{6} - \frac{\sqrt{6}\mathbb{T}_{1,2}^{(1,0;a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{6} + \frac{\sqrt{6}\mathbb{T}_1^{(1,0;a)}(A_{2u})\mathbb{T}_1^{(b)}(A_{2u})}{3}$$

$$\boxed{\text{z65}} \quad \mathbb{G}_2^{(c)}(A_{1u}) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} - \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z66}} \quad \mathbb{G}_0^{(1,-1;c)}(A_{1u}) = \frac{\sqrt{3}\mathbb{G}_{2,1}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{3} - \frac{\sqrt{3}\mathbb{G}_{2,2}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{3} + \frac{\sqrt{3}\mathbb{G}_2^{(1,-1;a)}(B_{1u})\mathbb{Q}_2^{(b)}(B_{1g})}{3}$$

$$\boxed{\text{z67}} \quad \mathbb{G}_2^{(1,-1;c)}(A_{1u}, a) = \mathbb{G}_2^{(1,-1;a)}(A_{1u})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z68}} \quad \mathbb{G}_2^{(1,-1;c)}(A_{1u}, b) = \frac{\sqrt{6}\mathbb{G}_{2,1}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{6} - \frac{\sqrt{6}\mathbb{G}_{2,2}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{6} - \frac{\sqrt{6}\mathbb{G}_2^{(1,-1;a)}(B_{1u})\mathbb{Q}_2^{(b)}(B_{1g})}{3}$$

$$\boxed{\text{z69}} \quad \mathbb{G}_2^{(1,0;c)}(A_{1u}) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(1,0;a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} - \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(1,0;a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$$

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

$$\boxed{\text{z99}} \quad \mathbb{Q}_4^{(1,-1;c)}(A_{2g}) = \mathbb{M}_2^{(1,-1;a)}(B_{1u})\mathbb{M}_2^{(b)}(B_{2u})$$

$$\boxed{\text{z100}} \quad \mathbb{G}_1^{(c)}(A_{2g}) = \frac{\sqrt{2}\mathbb{T}_{1,1}^{(a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{T}_{1,2}^{(a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z101}} \quad \mathbb{G}_1^{(1,-1;c)}(A_{2g}) = \frac{\sqrt{30}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{10} - \frac{\sqrt{30}\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{10} + \frac{\sqrt{10}\mathbb{M}_2^{(1,-1;a)}(A_{1u})\mathbb{T}_1^{(b)}(A_{2u})}{5}$$

$$\boxed{\text{z102}} \quad \mathbb{G}_3^{(1,-1;c)}(A_{2g}) = -\frac{\sqrt{5}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{5} + \frac{\sqrt{5}\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{5} + \frac{\sqrt{15}\mathbb{M}_2^{(1,-1;a)}(A_{1u})\mathbb{T}_1^{(b)}(A_{2u})}{5}$$

$$\boxed{\text{z103}} \quad \mathbb{G}_1^{(1,0;c)}(A_{2g}) = \frac{\sqrt{2}\mathbb{T}_{1,1}^{(1,0;a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{T}_{1,2}^{(1,0;a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z104}} \quad \mathbb{G}_1^{(1,1;c)}(A_{2g}) = \mathbb{M}_0^{(1,1;a)}(A_{1u})\mathbb{T}_1^{(b)}(A_{2u})$$

$$\boxed{\text{z135}} \quad \mathbb{Q}_1^{(c)}(A_{2u}, a) = \mathbb{Q}_1^{(a)}(A_{2u})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z136}} \quad \mathbb{Q}_1^{(c)}(A_{2u}, b) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2} + \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z137}} \quad \mathbb{Q}_1^{(1,-1;c)}(A_{2u}) = -\frac{\sqrt{6}\mathbb{G}_{2,1}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{6} - \frac{\sqrt{6}\mathbb{G}_{2,2}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{6} - \frac{\sqrt{6}\mathbb{G}_2^{(1,-1;a)}(B_{2u})\mathbb{Q}_2^{(b)}(B_{1g})}{3}$$

$$\boxed{\text{z138}} \quad \mathbb{Q}_3^{(1,-1;c)}(A_{2u}) = -\frac{\sqrt{3}\mathbb{G}_{2,1}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{3} - \frac{\sqrt{3}\mathbb{G}_{2,2}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{3} + \frac{\sqrt{3}\mathbb{G}_2^{(1,-1;a)}(B_{2u})\mathbb{Q}_2^{(b)}(B_{1g})}{3}$$

$$\boxed{\text{z139}} \quad \mathbb{Q}_1^{(1,0;c)}(A_{2u}, a) = \mathbb{Q}_1^{(1,0;a)}(A_{2u})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z140}} \quad \mathbb{Q}_1^{(1,0;c)}(A_{2u}, b) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(1,0;a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2} + \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(1,0;a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z215}} \quad \mathbb{Q}_2^{(c)}(B_{1g}, a) = \frac{\sqrt{2}\mathbb{T}_{1,1}^{(a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{T}_{1,2}^{(a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z216}} \quad \mathbb{Q}_2^{(c)}(B_{1g}, b) = -\mathbb{T}_1^{(a)}(A_{2u})\mathbb{M}_2^{(b)}(B_{2u})$$

$$\boxed{\text{z217}} \quad \mathbb{Q}_2^{(1,-1;c)}(B_{1g}) = -\frac{\sqrt{6}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{6} + \frac{\sqrt{6}\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{6} + \frac{\sqrt{6}\mathbb{M}_2^{(1,-1;a)}(B_{2u})\mathbb{T}_1^{(b)}(A_{2u})}{3}$$

$$\boxed{\text{z218}} \quad \mathbb{Q}_2^{(1,0;c)}(B_{1g}, a) = \frac{\sqrt{2}\mathbb{T}_{1,1}^{(1,0;a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{T}_{1,2}^{(1,0;a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z219}} \quad \mathbb{Q}_2^{(1,0;c)}(B_{1g}, b) = -\mathbb{T}_1^{(1,0;a)}(A_{2u})\mathbb{M}_2^{(b)}(B_{2u})$$

$$\boxed{\text{z220}} \quad \mathbb{G}_3^{(1,-1;c)}(B_{1g}) = \frac{\sqrt{3}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{3} - \frac{\sqrt{3}\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{3} + \frac{\sqrt{3}\mathbb{M}_2^{(1,-1;a)}(B_{2u})\mathbb{T}_1^{(b)}(A_{2u})}{3}$$

$$\boxed{\text{z221}} \quad \mathbb{Q}_3^{(c)}(B_{1u}) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} + \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z222}} \quad \mathbb{Q}_3^{(1,-1;c)}(B_{1u}) = \mathbb{G}_2^{(1,-1;a)}(A_{1u})\mathbb{Q}_2^{(b)}(B_{1g})$$

$$\boxed{\text{z223}} \quad \mathbb{Q}_3^{(1,0;c)}(B_{1u}) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(1,0;a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} + \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(1,0;a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z224}} \quad \mathbb{G}_2^{(1,-1;c)}(B_{1u}, a) = \mathbb{G}_2^{(1,-1;a)}(B_{1u})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z225}} \quad \mathbb{G}_2^{(1,-1;c)}(B_{1u}, b) = -\frac{\sqrt{2}\mathbb{G}_{2,1}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} - \frac{\sqrt{2}\mathbb{G}_{2,2}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z226}} \quad \mathbb{G}_2^{(1,1;c)}(B_{1u}) = \mathbb{G}_0^{(1,1;a)}(A_{1u})\mathbb{Q}_2^{(b)}(B_{1g})$$

$$\boxed{\text{z227}} \quad \mathbb{Q}_2^{(c)}(B_{2g}) = \frac{\sqrt{2}\mathbb{T}_{1,1}^{(a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{T}_{1,2}^{(a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z228}} \quad \mathbb{Q}_2^{(1,-1;c)}(B_{2g}, a) = -\frac{\sqrt{6}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{6} - \frac{\sqrt{6}\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{6} - \frac{\sqrt{6}\mathbb{M}_2^{(1,-1;a)}(B_{1u})\mathbb{T}_1^{(b)}(A_{2u})}{3}$$

$$\boxed{\text{z229}} \quad \mathbb{Q}_2^{(1,-1;c)}(B_{2g}, b) = -\mathbb{M}_2^{(1,-1;a)}(A_{1u})\mathbb{M}_2^{(b)}(B_{2u})$$

$$\boxed{\text{z230}} \quad \mathbb{Q}_2^{(1,0;c)}(B_{2g}) = \frac{\sqrt{2}\mathbb{T}_{1,1}^{(1,0;a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{T}_{1,2}^{(1,0;a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z231}} \quad \mathbb{Q}_2^{(1,1;c)}(B_{2g}) = \mathbb{M}_0^{(1,1;a)}(A_{1u})\mathbb{M}_2^{(b)}(B_{2u})$$

$$\boxed{\text{z232}} \quad \mathbb{G}_3^{(1,-1;c)}(B_{2g}) = -\frac{\sqrt{3}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{3} - \frac{\sqrt{3}\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{3} + \frac{\sqrt{3}\mathbb{M}_2^{(1,-1;a)}(B_{1u})\mathbb{T}_1^{(b)}(A_{2u})}{3}$$

$$\boxed{\text{z233}} \quad \mathbb{Q}_3^{(c)}(B_{2u}) = \frac{\sqrt{3}\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{3} - \frac{\sqrt{3}\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{3} + \frac{\sqrt{3}\mathbb{Q}_1^{(a)}(A_{2u})\mathbb{Q}_2^{(b)}(B_{1g})}{3}$$

$$\boxed{\text{z234}} \quad \mathbb{Q}_3^{(1,0;c)}(B_{2u}) = \frac{\sqrt{3}\mathbb{Q}_{1,1}^{(1,0;a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{3} - \frac{\sqrt{3}\mathbb{Q}_{1,2}^{(1,0;a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{3} + \frac{\sqrt{3}\mathbb{Q}_1^{(1,0;a)}(A_{2u})\mathbb{Q}_2^{(b)}(B_{1g})}{3}$$

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

$$\boxed{\text{z236}} \quad \mathbb{G}_2^{(1,-1;c)}(B_{2u}, a) = \mathbb{G}_2^{(1,-1;a)}(B_{2u})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z237}} \quad \mathbb{G}_2^{(1,-1;c)}(B_{2u}, b) = \frac{\sqrt{2}\mathbb{G}_{2,1}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2} - \frac{\sqrt{2}\mathbb{G}_{2,2}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z238}} \quad \mathbb{G}_2^{(1,0;c)}(B_{2u}) = -\frac{\sqrt{6}\mathbb{Q}_{1,1}^{(1,0;a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{6} + \frac{\sqrt{6}\mathbb{Q}_{1,2}^{(1,0;a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{6} + \frac{\sqrt{6}\mathbb{Q}_1^{(1,0;a)}(A_{2u})\mathbb{Q}_2^{(b)}(B_{1g})}{3}$$

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

$$\boxed{\text{z301}} \quad \mathbb{Q}_{2,2}^{(c)}(E_g, a) = \frac{\mathbb{T}_{1,1}^{(a)}(E_u)\mathbb{T}_1^{(b)}(A_{2u})}{2} + \frac{\mathbb{T}_1^{(a)}(A_{2u})\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z302}} \quad \mathbb{Q}_{2,1}^{(c)}(E_g, b) = -\frac{\sqrt{2}\mathbb{T}_{1,2}^{(a)}(E_u)\mathbb{M}_2^{(b)}(B_{2u})}{2}$$

$$\boxed{\text{z303}} \quad \mathbb{Q}_{2,2}^{(c)}(E_g, b) = \frac{\sqrt{2}\mathbb{T}_{1,1}^{(a)}(E_u)\mathbb{M}_2^{(b)}(B_{2u})}{2}$$

$$\boxed{\text{z304}} \quad \mathbb{Q}_{2,1}^{(1,-1;c)}(E_g, a) = \frac{\sqrt{3}\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{T}_1^{(b)}(A_{2u})}{6} + \frac{\mathbb{M}_2^{(1,-1;a)}(A_{1u})\mathbb{T}_{1,1}^{(b)}(E_u)}{2} + \frac{\sqrt{3}\mathbb{M}_2^{(1,-1;a)}(B_{1u})\mathbb{T}_{1,1}^{(b)}(E_u)}{6} + \frac{\sqrt{3}\mathbb{M}_2^{(1,-1;a)}(B_{2u})\mathbb{T}_{1,2}^{(b)}(E_u)}{6}$$

$$\boxed{\text{z305}} \quad \mathbb{Q}_{2,2}^{(1,-1;c)}(E_g, a) = \frac{\sqrt{3}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{T}_1^{(b)}(A_{2u})}{6} - \frac{\mathbb{M}_2^{(1,-1;a)}(A_{1u})\mathbb{T}_{1,2}^{(b)}(E_u)}{2} + \frac{\sqrt{3}\mathbb{M}_2^{(1,-1;a)}(B_{1u})\mathbb{T}_{1,2}^{(b)}(E_u)}{6} - \frac{\sqrt{3}\mathbb{M}_2^{(1,-1;a)}(B_{2u})\mathbb{T}_{1,1}^{(b)}(E_u)}{6}$$

$$\boxed{\text{z344}} \quad \mathbb{Q}_{2,1}^{(1,-1;c)}(E_g, b) = -\frac{\sqrt{2}\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{M}_2^{(b)}(B_{2u})}{2}$$

$$\boxed{\text{z345}} \quad \mathbb{Q}_{2,2}^{(1,-1;c)}(E_g, b) = \frac{\sqrt{2}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{M}_2^{(b)}(B_{2u})}{2}$$

$$\boxed{\text{z346}} \quad \mathbb{Q}_{2,1}^{(1,0;c)}(E_g, a) = \frac{\mathbb{T}_{1,2}^{(1,0;a)}(E_u)\mathbb{T}_1^{(b)}(A_{2u})}{2} + \frac{\mathbb{T}_1^{(1,0;a)}(A_{2u})\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z347}} \quad \mathbb{Q}_{2,2}^{(1,0;c)}(E_g, a) = \frac{\mathbb{T}_{1,1}^{(1,0;a)}(E_u)\mathbb{T}_1^{(b)}(A_{2u})}{2} + \frac{\mathbb{T}_1^{(1,0;a)}(A_{2u})\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z348}} \quad \mathbb{Q}_{2,1}^{(1,0;c)}(E_g, b) = -\frac{\sqrt{2}\mathbb{T}_{1,2}^{(1,0;a)}(E_u)\mathbb{M}_2^{(b)}(B_{2u})}{2}$$

$$\boxed{\text{z349}} \quad \mathbb{Q}_{2,2}^{(1,0;c)}(E_g, b) = \frac{\sqrt{2}\mathbb{T}_{1,1}^{(1,0;a)}(E_u)\mathbb{M}_2^{(b)}(B_{2u})}{2}$$

$$\boxed{\text{z385}} \quad \mathbb{G}_{1,1}^{(c)}(E_g) = \frac{\mathbb{T}_{1,2}^{(a)}(E_u)\mathbb{T}_1^{(b)}(A_{2u})}{2} - \frac{\mathbb{T}_1^{(a)}(A_{2u})\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z386}} \quad \mathbb{G}_{1,2}^{(c)}(E_g) = \frac{\mathbb{T}_{1,1}^{(a)}(E_u)\mathbb{T}_1^{(b)}(A_{2u})}{2} - \frac{\mathbb{T}_1^{(a)}(A_{2u})\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z387}} \quad \mathbb{G}_{1,1}^{(1,-1;c)}(E_g) = -\frac{\sqrt{15}\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{T}_1^{(b)}(A_{2u})}{10} - \frac{\sqrt{5}\mathbb{M}_2^{(1,-1;a)}(A_{1u})\mathbb{T}_{1,1}^{(b)}(E_u)}{10} + \frac{\sqrt{15}\mathbb{M}_2^{(1,-1;a)}(B_{1u})\mathbb{T}_{1,1}^{(b)}(E_u)}{10} + \frac{\sqrt{15}\mathbb{M}_2^{(1,-1;a)}(B_{2u})\mathbb{T}_{1,2}^{(b)}(E_u)}{10}$$

$$\boxed{\text{z388}} \quad \mathbb{G}_{1,2}^{(1,-1;c)}(E_g) = -\frac{\sqrt{15}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{T}_1^{(b)}(A_{2u})}{10} + \frac{\sqrt{5}\mathbb{M}_2^{(1,-1;a)}(A_{1u})\mathbb{T}_{1,2}^{(b)}(E_u)}{10} + \frac{\sqrt{15}\mathbb{M}_2^{(1,-1;a)}(B_{1u})\mathbb{T}_{1,2}^{(b)}(E_u)}{10} - \frac{\sqrt{15}\mathbb{M}_2^{(1,-1;a)}(B_{2u})\mathbb{T}_{1,1}^{(b)}(E_u)}{10}$$

$$\boxed{\text{z389}} \quad \mathbb{G}_{3,1}^{(1,-1;c)}(E_g, 1) = \frac{\sqrt{10}\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{T}_1^{(b)}(A_{2u})}{10} - \frac{\sqrt{30}\mathbb{M}_2^{(1,-1;a)}(A_{1u})\mathbb{T}_{1,1}^{(b)}(E_u)}{20} + \frac{3\sqrt{10}\mathbb{M}_2^{(1,-1;a)}(B_{1u})\mathbb{T}_{1,1}^{(b)}(E_u)}{20} - \frac{\sqrt{10}\mathbb{M}_2^{(1,-1;a)}(B_{2u})\mathbb{T}_{1,2}^{(b)}(E_u)}{10}$$

$$\boxed{\text{z390}} \quad \mathbb{G}_{3,2}^{(1,-1;c)}(E_g, 1) = \frac{\sqrt{10}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{T}_1^{(b)}(A_{2u})}{10} + \frac{\sqrt{30}\mathbb{M}_2^{(1,-1;a)}(A_{1u})\mathbb{T}_{1,2}^{(b)}(E_u)}{20} + \frac{3\sqrt{10}\mathbb{M}_2^{(1,-1;a)}(B_{1u})\mathbb{T}_{1,2}^{(b)}(E_u)}{20} + \frac{\sqrt{10}\mathbb{M}_2^{(1,-1;a)}(B_{2u})\mathbb{T}_{1,1}^{(b)}(E_u)}{10}$$

$$\boxed{\text{z428}} \quad \mathbb{G}_{3,1}^{(1,-1;c)}(E_g, 2) = \frac{\sqrt{6}\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{T}_1^{(b)}(A_{2u})}{6} - \frac{\sqrt{2}\mathbb{M}_2^{(1,-1;a)}(A_{1u})\mathbb{T}_{1,1}^{(b)}(E_u)}{4} - \frac{\sqrt{6}\mathbb{M}_2^{(1,-1;a)}(B_{1u})\mathbb{T}_{1,1}^{(b)}(E_u)}{12} + \frac{\sqrt{6}\mathbb{M}_2^{(1,-1;a)}(B_{2u})\mathbb{T}_{1,2}^{(b)}(E_u)}{6}$$

$$\boxed{\text{z429}} \quad \mathbb{G}_{3,2}^{(1,-1;c)}(E_g, 2) = \frac{\sqrt{6}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{T}_1^{(b)}(A_{2u})}{6} + \frac{\sqrt{2}\mathbb{M}_2^{(1,-1;a)}(A_{1u})\mathbb{T}_{1,2}^{(b)}(E_u)}{4} - \frac{\sqrt{6}\mathbb{M}_2^{(1,-1;a)}(B_{1u})\mathbb{T}_{1,2}^{(b)}(E_u)}{12} - \frac{\sqrt{6}\mathbb{M}_2^{(1,-1;a)}(B_{2u})\mathbb{T}_{1,1}^{(b)}(E_u)}{6}$$

$$\boxed{\text{z430}} \quad \mathbb{G}_{1,1}^{(1,0;c)}(E_g) = \frac{\mathbb{T}_{1,2}^{(1,0;a)}(E_u)\mathbb{T}_1^{(b)}(A_{2u})}{2} - \frac{\mathbb{T}_1^{(1,0;a)}(A_{2u})\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z431}} \quad \mathbb{G}_{1,2}^{(1,0;c)}(E_g) = \frac{\mathbb{T}_{1,1}^{(1,0;a)}(E_u)\mathbb{T}_1^{(b)}(A_{2u})}{2} - \frac{\mathbb{T}_1^{(1,0;a)}(A_{2u})\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z432}} \quad \mathbb{G}_{1,1}^{(1,1;c)}(E_g) = \frac{\sqrt{2}\mathbb{M}_0^{(1,1;a)}(A_{1u})\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z433}} \quad \mathbb{G}_{1,2}^{(1,1;c)}(E_g) = -\frac{\sqrt{2}\mathbb{M}_0^{(1,1;a)}(A_{1u})\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z539}} \quad \mathbb{Q}_{1,1}^{(c)}(E_u, a) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z540}} \quad \mathbb{Q}_{1,2}^{(c)}(E_u, a) = \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z541}} \quad \mathbb{Q}_{1,1}^{(c)}(E_u, b) = \frac{\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_2^{(b)}(B_{1g})}{2} + \frac{\mathbb{Q}_1^{(a)}(A_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z542}} \quad \mathbb{Q}_{1,2}^{(c)}(E_u, b) = -\frac{\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_2^{(b)}(B_{1g})}{2} + \frac{\mathbb{Q}_1^{(a)}(A_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z543}} \quad \mathbb{Q}_{3,1}^{(c)}(E_u, 1) = \frac{\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_2^{(b)}(B_{1g})}{2} - \frac{\mathbb{Q}_1^{(a)}(A_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z544}} \quad \mathbb{Q}_{3,2}^{(c)}(E_u, 1) = -\frac{\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_2^{(b)}(B_{1g})}{2} - \frac{\mathbb{Q}_1^{(a)}(A_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z545}} \quad \mathbb{Q}_{1,1}^{(1,-1;c)}(E_u) = \frac{\sqrt{3}\mathbb{G}_{2,1}^{(1,-1;a)}(E_u)\mathbb{Q}_2^{(b)}(B_{1g})}{6} - \frac{\mathbb{G}_2^{(1,-1;a)}(A_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} - \frac{\sqrt{3}\mathbb{G}_2^{(1,-1;a)}(B_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{6} + \frac{\sqrt{3}\mathbb{G}_2^{(1,-1;a)}(B_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{6}$$

$$\boxed{\text{z546}} \quad \mathbb{Q}_{1,2}^{(1,-1;c)}(E_u) = -\frac{\sqrt{3}\mathbb{G}_{2,2}^{(1,-1;a)}(E_u)\mathbb{Q}_2^{(b)}(B_{1g})}{6} + \frac{\mathbb{G}_2^{(1,-1;a)}(A_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2} - \frac{\sqrt{3}\mathbb{G}_2^{(1,-1;a)}(B_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{6} - \frac{\sqrt{3}\mathbb{G}_2^{(1,-1;a)}(B_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{6}$$

$$\boxed{\text{z547}} \quad \mathbb{Q}_{3,1}^{(1,-1;c)}(E_u, 1) = -\frac{\sqrt{15}\mathbb{G}_{2,1}^{(1,-1;a)}(E_u)\mathbb{Q}_2^{(b)}(B_{1g})}{30} + \frac{\sqrt{5}\mathbb{G}_2^{(1,-1;a)}(A_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{10} + \frac{\sqrt{15}\mathbb{G}_2^{(1,-1;a)}(B_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{30} + \frac{\sqrt{15}\mathbb{G}_2^{(1,-1;a)}(B_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{6}$$

$$\boxed{\text{z548}} \quad \mathbb{Q}_{3,2}^{(1,-1;c)}(E_u, 1) = \frac{\sqrt{15}\mathbb{G}_{2,2}^{(1,-1;a)}(E_u)\mathbb{Q}_2^{(b)}(B_{1g})}{30} - \frac{\sqrt{5}\mathbb{G}_2^{(1,-1;a)}(A_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{10} + \frac{\sqrt{15}\mathbb{G}_2^{(1,-1;a)}(B_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{30} - \frac{\sqrt{15}\mathbb{G}_2^{(1,-1;a)}(B_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{6}$$

$$\boxed{\text{z549}} \quad \mathbb{Q}_{3,1}^{(1,-1;c)}(E_u, 2) = \frac{\sqrt{15}\mathbb{G}_{2,1}^{(1,-1;a)}(E_u)\mathbb{Q}_2^{(b)}(B_{1g})}{10} + \frac{\sqrt{5}\mathbb{G}_2^{(1,-1;a)}(A_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{5} - \frac{\sqrt{15}\mathbb{G}_2^{(1,-1;a)}(B_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{10}$$

$$\boxed{\text{z550}} \quad \mathbb{Q}_{3,2}^{(1,-1;c)}(E_u, 2) = -\frac{\sqrt{15}\mathbb{G}_{2,2}^{(1,-1;a)}(E_u)\mathbb{Q}_2^{(b)}(B_{1g})}{10} - \frac{\sqrt{5}\mathbb{G}_2^{(1,-1;a)}(A_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{5} - \frac{\sqrt{15}\mathbb{G}_2^{(1,-1;a)}(B_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{10}$$

$$\boxed{\text{z551}} \quad \mathbb{Q}_{1,1}^{(1,0;c)}(E_u, a) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(1,0;a)}(E_u)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z552}} \quad \mathbb{Q}_{1,2}^{(1,0;c)}(E_u, a) = \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(1,0;a)}(E_u)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z553}} \quad \mathbb{Q}_{1,1}^{(1,0;c)}(E_u, b) = \frac{\mathbb{Q}_{1,1}^{(1,0;a)}(E_u)\mathbb{Q}_2^{(b)}(B_{1g})}{2} + \frac{\mathbb{Q}_1^{(1,0;a)}(A_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z554}} \quad \mathbb{Q}_{1,2}^{(1,0;c)}(E_u, b) = -\frac{\mathbb{Q}_{1,2}^{(1,0;a)}(E_u)\mathbb{Q}_2^{(b)}(B_{1g})}{2} + \frac{\mathbb{Q}_1^{(1,0;a)}(A_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z555}} \quad \mathbb{Q}_{3,1}^{(1,0;c)}(E_u, 1) = \frac{\mathbb{Q}_{1,1}^{(1,0;a)}(E_u)\mathbb{Q}_2^{(b)}(B_{1g})}{2} - \frac{\mathbb{Q}_1^{(1,0;a)}(A_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z556}} \quad \mathbb{Q}_{3,2}^{(1,0;c)}(E_u, 1) = -\frac{\mathbb{Q}_{1,2}^{(1,0;a)}(E_u)\mathbb{Q}_2^{(b)}(B_{1g})}{2} - \frac{\mathbb{Q}_1^{(1,0;a)}(A_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z557}} \quad \mathbb{G}_{2,1}^{(1,-1;c)}(E_u, a) = \frac{\sqrt{2}\mathbb{G}_{2,1}^{(1,-1;a)}(E_u)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z558}} \quad \mathbb{G}_{2,2}^{(1,-1;c)}(E_u, a) = \frac{\sqrt{2}\mathbb{G}_{2,2}^{(1,-1;a)}(E_u)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z559}} \quad \mathbb{G}_{2,1}^{(1,-1;c)}(E_u, b) = -\frac{\mathbb{G}_{2,1}^{(1,-1;a)}(E_u)\mathbb{Q}_2^{(b)}(B_{1g})}{2} - \frac{\mathbb{G}_2^{(1,-1;a)}(B_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z560}} \quad \mathbb{G}_{2,2}^{(1,-1;c)}(E_u, b) = \frac{\mathbb{G}_{2,2}^{(1,-1;a)}(E_u)\mathbb{Q}_2^{(b)}(B_{1g})}{2} - \frac{\mathbb{G}_2^{(1,-1;a)}(B_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z561}} \quad \mathbb{G}_{2,1}^{(1,1;c)}(E_u) = \frac{\sqrt{2}\mathbb{G}_0^{(1,1;a)}(A_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z562}} \quad \mathbb{G}_{2,2}^{(1,1;c)}(E_u) = -\frac{\sqrt{2}\mathbb{G}_0^{(1,1;a)}(A_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$$

• 'A'-'A' bond-cluster : A\_A\_004\_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: 4e@2e

$$\boxed{\text{z40}} \quad \mathbb{Q}_0^{(c)}(A_{1g}, a) = \mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z41}} \quad \mathbb{Q}_0^{(c)}(A_{1g}, b) = \frac{\sqrt{3}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(E_g)}{3} + \frac{\sqrt{3}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(E_g)}{3} + \frac{\sqrt{3}\mathbb{Q}_2^{(a)}(B_{1g})\mathbb{Q}_2^{(b)}(B_{1g})}{3}$$

$$\boxed{\text{z42}} \quad \mathbb{Q}_2^{(c)}(A_{1g}, a) = \mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z43}} \quad \mathbb{Q}_2^{(c)}(A_{1g}, b) = \frac{\sqrt{6}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(E_g)}{6} + \frac{\sqrt{6}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(E_g)}{6} - \frac{\sqrt{6}\mathbb{Q}_2^{(a)}(B_{1g})\mathbb{Q}_2^{(b)}(B_{1g})}{3}$$

$$\boxed{\text{z44}} \quad \mathbb{Q}_0^{(1,-1;c)}(A_{1g}) = \frac{\sqrt{3}\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(E_g)}{3} + \frac{\sqrt{3}\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(E_g)}{3} + \frac{\sqrt{3}\mathbb{Q}_2^{(1,-1;a)}(B_{1g})\mathbb{Q}_2^{(b)}(B_{1g})}{3}$$

$$\boxed{\text{z45}} \quad \mathbb{Q}_2^{(1,-1;c)}(A_{1g}, a) = \mathbb{Q}_2^{(1,-1;a)}(A_{1g})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z46}} \quad \mathbb{Q}_2^{(1,-1;c)}(A_{1g}, b) = \frac{\sqrt{6}\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(E_g)}{6} + \frac{\sqrt{6}\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(E_g)}{6} - \frac{\sqrt{6}\mathbb{Q}_2^{(1,-1;a)}(B_{1g})\mathbb{Q}_2^{(b)}(B_{1g})}{3}$$

$$\boxed{\text{z47}} \quad \mathbb{Q}_2^{(1,0;c)}(A_{1g}) = \frac{\sqrt{2}\mathbb{G}_{1,1}^{(1,0;a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} + \frac{\sqrt{2}\mathbb{G}_{1,2}^{(1,0;a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z48}} \quad \mathbb{Q}_0^{(1,1;c)}(A_{1g}) = \mathbb{Q}_0^{(1,1;a)}(A_{1g})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z71}} \quad \mathbb{Q}_5^{(1,-1;c)}(A_{1u}) = \mathbb{M}_3^{(1,-1;a)}(B_{2g})\mathbb{M}_2^{(b)}(B_{2u})$$

$$\boxed{\text{z72}} \quad \mathbb{G}_0^{(c)}(A_{1u}) = \frac{\sqrt{3}\mathbb{M}_{1,1}^{(a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{3} - \frac{\sqrt{3}\mathbb{M}_{1,2}^{(a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{3} + \frac{\sqrt{3}\mathbb{M}_1^{(a)}(A_{2g})\mathbb{T}_1^{(b)}(A_{2u})}{3}$$

$$\boxed{\text{z73}} \quad \mathbb{G}_2^{(c)}(A_{1u}) = -\frac{\sqrt{6}\mathbb{M}_{1,1}^{(a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{6} + \frac{\sqrt{6}\mathbb{M}_{1,2}^{(a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{6} + \frac{\sqrt{6}\mathbb{M}_1^{(a)}(A_{2g})\mathbb{T}_1^{(b)}(A_{2u})}{3}$$

$$\boxed{\text{z74}} \quad \mathbb{G}_0^{(1,-1;c)}(A_{1u}) = \frac{\sqrt{3}\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{3} - \frac{\sqrt{3}\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{3} + \frac{\sqrt{3}\mathbb{M}_1^{(1,-1;a)}(A_{2g})\mathbb{T}_1^{(b)}(A_{2u})}{3}$$

$$\boxed{\text{z75}} \quad \mathbb{G}_2^{(1,-1;c)}(A_{1u}, a) = -\frac{\sqrt{6}\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{6} + \frac{\sqrt{6}\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{6} + \frac{\sqrt{6}\mathbb{M}_1^{(1,-1;a)}(A_{2g})\mathbb{T}_1^{(b)}(A_{2u})}{3}$$

$$\boxed{\text{z76}} \quad \mathbb{G}_2^{(1,-1;c)}(A_{1u}, b) = -\frac{\sqrt{21}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g, 1)\mathbb{T}_{1,1}^{(b)}(E_u)}{14} - \frac{\sqrt{35}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g, 2)\mathbb{T}_{1,1}^{(b)}(E_u)}{14} + \frac{\sqrt{21}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g, 1)\mathbb{T}_{1,2}^{(b)}(E_u)}{14} + \frac{\sqrt{35}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g, 2)\mathbb{T}_{1,2}^{(b)}(E_u)}{14} + \frac{\sqrt{21}\mathbb{M}_3^{(1,-1;a)}(A_{2g})\mathbb{T}_1^{(b)}(A_{2u})}{7}$$

$$\boxed{\text{z105}} \quad \mathbb{G}_4^{(1,-1;c)}(A_{1u}, 1) = \frac{\sqrt{3}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g, 1)\mathbb{T}_{1,1}^{(b)}(E_u)}{3} - \frac{\sqrt{3}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g, 1)\mathbb{T}_{1,2}^{(b)}(E_u)}{3} + \frac{\sqrt{3}\mathbb{M}_3^{(1,-1;a)}(A_{2g})\mathbb{T}_1^{(b)}(A_{2u})}{3}$$

$$\begin{aligned} \boxed{\text{z106}} \quad \mathbb{G}_4^{(1,-1;c)}(A_{1u}, 2) &= -\frac{\sqrt{105}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g, 1)\mathbb{T}_{1,1}^{(b)}(E_u)}{42} + \frac{3\sqrt{7}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g, 2)\mathbb{T}_{1,1}^{(b)}(E_u)}{14} + \frac{\sqrt{105}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g, 1)\mathbb{T}_{1,2}^{(b)}(E_u)}{42} \\ &\quad - \frac{3\sqrt{7}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g, 2)\mathbb{T}_{1,2}^{(b)}(E_u)}{14} + \frac{\sqrt{105}\mathbb{M}_3^{(1,-1;a)}(A_{2g})\mathbb{T}_1^{(b)}(A_{2u})}{21} \end{aligned}$$

$$\boxed{\text{z107}} \quad \mathbb{G}_0^{(1,0;c)}(A_{1u}) = \mathbb{T}_2^{(1,0;a)}(B_{2g})\mathbb{M}_2^{(b)}(B_{2u})$$

$$\boxed{\text{z108}} \quad \mathbb{G}_2^{(1,0;c)}(A_{1u}) = -\frac{\sqrt{2}\mathbb{T}_{2,1}^{(1,0;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{T}_{2,2}^{(1,0;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z109}} \quad \mathbb{G}_0^{(1,1;c)}(A_{1u}) = \frac{\sqrt{3}\mathbb{M}_{1,1}^{(1,1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{3} - \frac{\sqrt{3}\mathbb{M}_{1,2}^{(1,1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{3} + \frac{\sqrt{3}\mathbb{M}_1^{(1,1;a)}(A_{2g})\mathbb{T}_1^{(b)}(A_{2u})}{3}$$

$$\boxed{\text{z110}} \quad \mathbb{G}_2^{(1,1;c)}(A_{1u}) = -\frac{\sqrt{6}\mathbb{M}_{1,1}^{(1,1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{6} + \frac{\sqrt{6}\mathbb{M}_{1,2}^{(1,1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{6} + \frac{\sqrt{6}\mathbb{M}_1^{(1,1;a)}(A_{2g})\mathbb{T}_1^{(b)}(A_{2u})}{3}$$

$$\boxed{\text{z111}} \quad \mathbb{Q}_4^{(c)}(A_{2g}) = \mathbb{Q}_2^{(a)}(B_{2g})\mathbb{Q}_2^{(b)}(B_{1g})$$

$$\boxed{\text{z112}} \quad \mathbb{Q}_4^{(1,-1;c)}(A_{2g}) = \mathbb{Q}_2^{(1,-1;a)}(B_{2g})\mathbb{Q}_2^{(b)}(B_{1g})$$

$$\boxed{\text{z113}} \quad \mathbb{G}_1^{(c)}(A_{2g}) = -\frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2} + \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z141}} \quad \mathbb{G}_1^{(1,-1;c)}(A_{2g}) = -\frac{\sqrt{2}\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2} + \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z142}} \quad \mathbb{G}_1^{(1,0;c)}(A_{2g}, a) = \mathbb{G}_1^{(1,0;a)}(A_{2g})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z143}} \quad \mathbb{G}_1^{(1,0;c)}(A_{2g}, b) = \frac{\sqrt{2}\mathbb{G}_{1,1}^{(1,0;a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2} - \frac{\sqrt{2}\mathbb{G}_{1,2}^{(1,0;a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z144}} \quad \mathbb{Q}_1^{(c)}(A_{2u}) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{M}_{1,2}^{(a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z145}} \quad \mathbb{Q}_1^{(1,-1;c)}(A_{2u}, a) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z146}} \quad \mathbb{Q}_1^{(1,-1;c)}(A_{2u}, b) = \mathbb{M}_3^{(1,-1;a)}(B_{1g})\mathbb{M}_2^{(b)}(B_{2u})$$

$$\boxed{\text{z239}} \quad \mathbb{Q}_3^{(1,-1;c)}(A_{2u}) = -\frac{\sqrt{3}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g, 1)\mathbb{T}_{1,2}^{(b)}(E_u)}{4} - \frac{\sqrt{5}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g, 2)\mathbb{T}_{1,2}^{(b)}(E_u)}{4} - \frac{\sqrt{3}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g, 1)\mathbb{T}_{1,1}^{(b)}(E_u)}{4} - \frac{\sqrt{5}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g, 2)\mathbb{T}_{1,1}^{(b)}(E_u)}{4}$$

$$\boxed{\text{z240}} \quad \mathbb{Q}_1^{(1,0;c)}(A_{2u}, a) = \frac{\sqrt{30}\mathbb{T}_{2,1}^{(1,0;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{10} + \frac{\sqrt{30}\mathbb{T}_{2,2}^{(1,0;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{10} + \frac{\sqrt{10}\mathbb{T}_2^{(1,0;a)}(A_{1g})\mathbb{T}_1^{(b)}(A_{2u})}{5}$$

$$\boxed{\text{z241}} \quad \mathbb{Q}_1^{(1,0;c)}(A_{2u}, b) = \mathbb{T}_2^{(1,0;a)}(B_{1g})\mathbb{M}_2^{(b)}(B_{2u})$$

$$\boxed{\text{z242}} \quad \mathbb{Q}_3^{(1,0;c)}(A_{2u}) = -\frac{\sqrt{5}\mathbb{T}_{2,1}^{(1,0;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{5} - \frac{\sqrt{5}\mathbb{T}_{2,2}^{(1,0;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{5} + \frac{\sqrt{15}\mathbb{T}_2^{(1,0;a)}(A_{1g})\mathbb{T}_1^{(b)}(A_{2u})}{5}$$

$$\boxed{\text{z243}} \quad \mathbb{Q}_1^{(1,1;c)}(A_{2u}) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z244}} \quad \mathbb{G}_4^{(1,-1;c)}(A_{2u}) = \frac{\sqrt{5}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,1)\mathbb{T}_{1,2}^{(b)}(E_u)}{4} - \frac{\sqrt{3}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,2}^{(b)}(E_u)}{4} + \frac{\sqrt{5}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,1)\mathbb{T}_{1,1}^{(b)}(E_u)}{4} - \frac{\sqrt{3}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,1}^{(b)}(E_u)}{4}$$

$$\boxed{\text{z245}} \quad \mathbb{Q}_2^{(c)}(B_{1g}, a) = \mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_2^{(b)}(B_{1g})$$

$$\boxed{\text{z246}} \quad \mathbb{Q}_2^{(c)}(B_{1g}, b) = \mathbb{Q}_2^{(a)}(B_{1g})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z247}} \quad \mathbb{Q}_2^{(c)}(B_{1g}, c) = -\frac{\sqrt{30}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(E_g)}{10} + \frac{\sqrt{30}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(E_g)}{10} - \frac{\sqrt{10}\mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_2^{(b)}(B_{1g})}{5}$$

$$\boxed{\text{z248}} \quad \mathbb{Q}_4^{(c)}(B_{1g}) = \frac{\sqrt{5}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(E_g)}{5} - \frac{\sqrt{5}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(E_g)}{5} - \frac{\sqrt{15}\mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_2^{(b)}(B_{1g})}{5}$$

$$\boxed{\text{z249}} \quad \mathbb{Q}_2^{(1,-1;c)}(B_{1g}, a) = \mathbb{Q}_2^{(1,-1;a)}(B_{1g})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z250}} \quad \mathbb{Q}_2^{(1,-1;c)}(B_{1g}, b) = -\frac{\sqrt{30}\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(E_g)}{10} + \frac{\sqrt{30}\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(E_g)}{10} - \frac{\sqrt{10}\mathbb{Q}_2^{(1,-1;a)}(A_{1g})\mathbb{Q}_2^{(b)}(B_{1g})}{5}$$

$$\boxed{\text{z251}} \quad \mathbb{Q}_4^{(1,-1;c)}(B_{1g}) = \frac{\sqrt{5}\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(E_g)}{5} - \frac{\sqrt{5}\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(E_g)}{5} - \frac{\sqrt{15}\mathbb{Q}_2^{(1,-1;a)}(A_{1g})\mathbb{Q}_2^{(b)}(B_{1g})}{5}$$

$$\boxed{\text{z252}} \quad \mathbb{Q}_2^{(1,0;c)}(B_{1g}) = \frac{\sqrt{2}\mathbb{G}_{1,1}^{(1,0;a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} - \frac{\sqrt{2}\mathbb{G}_{1,2}^{(1,0;a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z253}} \quad \mathbb{Q}_2^{(1,1;c)}(B_{1g}) = \mathbb{Q}_0^{(1,1;a)}(A_{1g})\mathbb{Q}_2^{(b)}(B_{1g})$$

$$\boxed{\text{z254}} \quad \mathbb{Q}_3^{(c)}(B_{1u}) = \mathbb{M}_1^{(a)}(A_{2g})\mathbb{M}_2^{(b)}(B_{2u})$$

$$\boxed{\text{z255}} \quad \mathbb{Q}_3^{(1,-1;c)}(B_{1u}, a) = \mathbb{M}_1^{(1,-1;a)}(A_{2g})\mathbb{M}_2^{(b)}(B_{2u})$$

$$\boxed{\text{z256}} \quad \mathbb{Q}_3^{(1,-1;c)}(B_{1u}, b) = -\frac{\sqrt{3}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,1}^{(b)}(E_u)}{3} - \frac{\sqrt{3}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,2}^{(b)}(E_u)}{3} - \frac{\sqrt{3}\mathbb{M}_3^{(1,-1;a)}(B_{2g})\mathbb{T}_1^{(b)}(A_{2u})}{3}$$

$$\boxed{\text{z257}} \quad \mathbb{Q}_3^{(1,-1;c)}(B_{1u}, c) = -\mathbb{M}_3^{(1,-1;a)}(A_{2g})\mathbb{M}_2^{(b)}(B_{2u})$$

$$\boxed{\text{z258}} \quad \mathbb{Q}_3^{(1,0;c)}(B_{1u}) = \frac{\sqrt{3}\mathbb{T}_{2,1}^{(1,0;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{3} + \frac{\sqrt{3}\mathbb{T}_{2,2}^{(1,0;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{3} + \frac{\sqrt{3}\mathbb{T}_2^{(1,0;a)}(B_{2g})\mathbb{T}_1^{(b)}(A_{2u})}{3}$$

$$\boxed{\text{z259}} \quad \mathbb{Q}_3^{(1,1;c)}(B_{1u}) = \mathbb{M}_1^{(1,1;a)}(A_{2g})\mathbb{M}_2^{(b)}(B_{2u})$$

$$\boxed{\text{z260}} \quad \mathbb{G}_2^{(c)}(B_{1u}) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{M}_{1,2}^{(a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z261}} \quad \mathbb{G}_2^{(1,-1;c)}(B_{1u}, a) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z262}} \quad \mathbb{G}_2^{(1,-1;c)}(B_{1u}, b) = \frac{3\sqrt{7}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g, 1)\mathbb{T}_{1,1}^{(b)}(E_u)}{14} - \frac{\sqrt{105}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g, 2)\mathbb{T}_{1,1}^{(b)}(E_u)}{42} + \frac{3\sqrt{7}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g, 1)\mathbb{T}_{1,2}^{(b)}(E_u)}{14} \\ - \frac{\sqrt{105}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g, 2)\mathbb{T}_{1,2}^{(b)}(E_u)}{42} + \frac{\sqrt{105}\mathbb{M}_3^{(1,-1;a)}(B_{2g})\mathbb{T}_1^{(b)}(A_{2u})}{21}$$

$$\boxed{\text{z263}} \quad \mathbb{G}_4^{(1,-1;c)}(B_{1u}) = \frac{\sqrt{35}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g, 1)\mathbb{T}_{1,1}^{(b)}(E_u)}{14} + \frac{\sqrt{21}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g, 2)\mathbb{T}_{1,1}^{(b)}(E_u)}{14} + \frac{\sqrt{35}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g, 1)\mathbb{T}_{1,2}^{(b)}(E_u)}{14} + \frac{\sqrt{21}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g, 2)\mathbb{T}_{1,2}^{(b)}(E_u)}{14} - \frac{\sqrt{21}\mathbb{M}_3^{(1,-1;a)}(B_{2g})\mathbb{T}_1^{(b)}(A_{2u})}{7}$$

$$\boxed{\text{z264}} \quad \mathbb{G}_2^{(1,0;c)}(B_{1u}) = -\frac{\sqrt{6}\mathbb{T}_{2,1}^{(1,0;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{6} - \frac{\sqrt{6}\mathbb{T}_{2,2}^{(1,0;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{6} + \frac{\sqrt{6}\mathbb{T}_2^{(1,0;a)}(B_{2g})\mathbb{T}_1^{(b)}(A_{2u})}{3}$$

$$\boxed{\text{z265}} \quad \mathbb{G}_2^{(1,1;c)}(B_{1u}) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z266}} \quad \mathbb{Q}_2^{(c)}(B_{2g}, a) = \mathbb{Q}_2^{(a)}(B_{2g})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z267}} \quad \mathbb{Q}_2^{(c)}(B_{2g}, b) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2} + \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z268}} \quad \mathbb{Q}_2^{(1,-1;c)}(B_{2g}, a) = \mathbb{Q}_2^{(1,-1;a)}(B_{2g})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z306}} \quad \mathbb{Q}_2^{(1,-1;c)}(B_{2g}, b) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2} + \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z307}} \quad \mathbb{Q}_2^{(1,0;c)}(B_{2g}) = -\frac{\sqrt{6}\mathbb{G}_{1,1}^{(1,0;a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(E_g)}{6} - \frac{\sqrt{6}\mathbb{G}_{1,2}^{(1,0;a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(E_g)}{6} + \frac{\sqrt{6}\mathbb{G}_1^{(1,0;a)}(A_{2g})\mathbb{Q}_2^{(b)}(B_{1g})}{3}$$

$$\boxed{\text{z308}} \quad \mathbb{G}_3^{(1,0;c)}(B_{2g}) = \frac{\sqrt{3}\mathbb{G}_{1,1}^{(1,0;a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(E_g)}{3} + \frac{\sqrt{3}\mathbb{G}_{1,2}^{(1,0;a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(E_g)}{3} + \frac{\sqrt{3}\mathbb{G}_1^{(1,0;a)}(A_{2g})\mathbb{Q}_2^{(b)}(B_{1g})}{3}$$

$$\boxed{\text{z309}} \quad \mathbb{Q}_3^{(1,-1;c)}(B_{2u}) = \frac{\sqrt{5}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,1)\mathbb{T}_{1,2}^{(b)}(E_u)}{4} + \frac{\sqrt{3}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,2}^{(b)}(E_u)}{12} - \frac{\sqrt{5}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,1)\mathbb{T}_{1,1}^{(b)}(E_u)}{4} - \frac{\sqrt{3}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,1}^{(b)}(E_u)}{12} + \frac{\sqrt{3}\mathbb{M}_3^{(1,-1;a)}(B_{1g})\mathbb{T}_1^{(b)}(A_{2u})}{3}$$

$$\boxed{\text{z310}} \quad \mathbb{Q}_3^{(1,0;c)}(B_{2u}, a) = -\frac{\sqrt{3}\mathbb{T}_{2,1}^{(1,0;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{3} + \frac{\sqrt{3}\mathbb{T}_{2,2}^{(1,0;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{3} + \frac{\sqrt{3}\mathbb{T}_2^{(1,0;a)}(B_{1g})\mathbb{T}_1^{(b)}(A_{2u})}{3}$$

$$\boxed{\text{z311}} \quad \mathbb{Q}_3^{(1,0;c)}(B_{2u}, b) = -\mathbb{T}_2^{(1,0;a)}(A_{1g})\mathbb{M}_2^{(b)}(B_{2u})$$

$$\boxed{\text{z312}} \quad \mathbb{G}_2^{(c)}(B_{2u}) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{M}_{1,2}^{(a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z313}} \quad \mathbb{G}_2^{(1,-1;c)}(B_{2u}, a) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z314}} \quad \mathbb{G}_2^{(1,-1;c)}(B_{2u}, b) = -\frac{\sqrt{7}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,1)\mathbb{T}_{1,2}^{(b)}(E_u)}{7} + \frac{\sqrt{105}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,2}^{(b)}(E_u)}{21} + \frac{\sqrt{7}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,1)\mathbb{T}_{1,1}^{(b)}(E_u)}{7} \\ - \frac{\sqrt{105}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,1}^{(b)}(E_u)}{21} + \frac{\sqrt{105}\mathbb{M}_3^{(1,-1;a)}(B_{1g})\mathbb{T}_1^{(b)}(A_{2u})}{21}$$

$$\boxed{\text{z315}} \quad \mathbb{G}_4^{(1,-1;c)}(B_{2u}) = -\frac{\sqrt{35}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,1)\mathbb{T}_{1,2}^{(b)}(E_u)}{28} - \frac{3\sqrt{21}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,2}^{(b)}(E_u)}{28} + \frac{\sqrt{35}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,1)\mathbb{T}_{1,1}^{(b)}(E_u)}{28} + \frac{3\sqrt{21}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,1}^{(b)}(E_u)}{28} + \frac{\sqrt{21}\mathbb{M}_3^{(1,-1;a)}(B_{1g})\mathbb{T}_1^{(b)}(A_{2u})}{7}$$

$$\boxed{\text{z316}} \quad \mathbb{G}_2^{(1,0;c)}(B_{2u}) = -\frac{\sqrt{6}\mathbb{T}_{2,1}^{(1,0;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{6} + \frac{\sqrt{6}\mathbb{T}_{2,2}^{(1,0;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{6} - \frac{\sqrt{6}\mathbb{T}_2^{(1,0;a)}(B_{1g})\mathbb{T}_1^{(b)}(A_{2u})}{3}$$

$$\boxed{\text{z317}} \quad \mathbb{G}_2^{(1,1;c)}(B_{2u}) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z350}} \quad \mathbb{Q}_{2,1}^{(c)}(E_g, a) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z351}} \quad \mathbb{Q}_{2,2}^{(c)}(E_g, a) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z352}} \quad \mathbb{Q}_{2,1}^{(c)}(E_g, b) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z353}} \quad \mathbb{Q}_{2,2}^{(c)}(E_g, b) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z354}} \quad \mathbb{Q}_{2,1}^{(c)}(E_g, c) = -\frac{\sqrt{15}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_2^{(b)}(B_{1g})}{10} + \frac{\sqrt{5}\mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{10} - \frac{\sqrt{15}\mathbb{Q}_2^{(a)}(B_{1g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{10} + \frac{\sqrt{15}\mathbb{Q}_2^{(a)}(B_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{10}$$

$$\boxed{\text{z355}} \quad \mathbb{Q}_{2,2}^{(c)}(E_g, c) = \frac{\sqrt{15}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_2^{(b)}(B_{1g})}{10} + \frac{\sqrt{5}\mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{10} + \frac{\sqrt{15}\mathbb{Q}_2^{(a)}(B_{1g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{10} + \frac{\sqrt{15}\mathbb{Q}_2^{(a)}(B_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{10}$$

$$\boxed{\text{z356}} \quad \mathbb{Q}_{4,1}^{(c)}(E_g, 1) = -\frac{7\sqrt{235}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_2^{(b)}(B_{1g})}{470} - \frac{11\sqrt{705}\mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{470} - \frac{7\sqrt{235}\mathbb{Q}_2^{(a)}(B_{1g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{470} - \frac{3\sqrt{235}\mathbb{Q}_2^{(a)}(B_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{470}$$

$$\boxed{\text{z357}} \quad \mathbb{Q}_{4,2}^{(c)}(E_g, 1) = \frac{7\sqrt{235}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_2^{(b)}(B_{1g})}{470} - \frac{11\sqrt{705}\mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{470} + \frac{7\sqrt{235}\mathbb{Q}_2^{(a)}(B_{1g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{470} - \frac{3\sqrt{235}\mathbb{Q}_2^{(a)}(B_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{470}$$

$$\boxed{\text{z358}} \quad \mathbb{Q}_{4,1}^{(c)}(E_g, 2) = \frac{3\sqrt{47}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_2^{(b)}(B_{1g})}{94} - \frac{\sqrt{141}\mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{47} + \frac{3\sqrt{47}\mathbb{Q}_2^{(a)}(B_{1g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{94} + \frac{4\sqrt{47}\mathbb{Q}_2^{(a)}(B_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{47}$$

$$\boxed{\text{z391}} \quad \mathbb{Q}_{4,2}^{(c)}(E_g, 2) = -\frac{3\sqrt{47}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_2^{(b)}(B_{1g})}{94} - \frac{\sqrt{141}\mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{47} - \frac{3\sqrt{47}\mathbb{Q}_2^{(a)}(B_{1g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{94} + \frac{4\sqrt{47}\mathbb{Q}_2^{(a)}(B_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{47}$$

$$\boxed{\text{z392}} \quad \mathbb{Q}_{2,1}^{(1,-1;c)}(E_g, a) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z393}} \quad \mathbb{Q}_{2,2}^{(1,-1;c)}(E_g, a) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z394}} \quad \mathbb{Q}_{2,1}^{(1,-1;c)}(E_g, b) = -\frac{\sqrt{15}\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_2^{(b)}(B_{1g})}{10} + \frac{\sqrt{5}\mathbb{Q}_2^{(1,-1;a)}(A_{1g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{10} - \frac{\sqrt{15}\mathbb{Q}_2^{(1,-1;a)}(B_{1g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{10} + \frac{\sqrt{15}\mathbb{Q}_2^{(1,-1;a)}(B_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{10}$$

$$\boxed{\text{z395}} \quad \mathbb{Q}_{2,2}^{(1,-1;c)}(E_g, b) = \frac{\sqrt{15}\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_2^{(b)}(B_{1g})}{10} + \frac{\sqrt{5}\mathbb{Q}_2^{(1,-1;a)}(A_{1g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{10} + \frac{\sqrt{15}\mathbb{Q}_2^{(1,-1;a)}(B_{1g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{10} + \frac{\sqrt{15}\mathbb{Q}_2^{(1,-1;a)}(B_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{10}$$

$$\boxed{\text{z396}} \quad \mathbb{Q}_{4,1}^{(1,-1;c)}(E_g, 1) = -\frac{7\sqrt{235}\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_2^{(b)}(B_{1g})}{470} - \frac{11\sqrt{705}\mathbb{Q}_2^{(1,-1;a)}(A_{1g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{470} - \frac{7\sqrt{235}\mathbb{Q}_2^{(1,-1;a)}(B_{1g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{470} - \frac{3\sqrt{235}\mathbb{Q}_2^{(1,-1;a)}(B_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{470}$$

$$\boxed{\text{z397}} \quad \mathbb{Q}_{4,2}^{(1,-1;c)}(E_g, 1) = \frac{7\sqrt{235}\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_2^{(b)}(B_{1g})}{470} - \frac{11\sqrt{705}\mathbb{Q}_2^{(1,-1;a)}(A_{1g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{470} + \frac{7\sqrt{235}\mathbb{Q}_2^{(1,-1;a)}(B_{1g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{470} - \frac{3\sqrt{235}\mathbb{Q}_2^{(1,-1;a)}(B_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{470}$$

$$\boxed{\text{z398}} \quad \mathbb{Q}_{4,1}^{(1,-1;c)}(E_g, 2) = \frac{3\sqrt{47}\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_2^{(b)}(B_{1g})}{94} - \frac{\sqrt{141}\mathbb{Q}_2^{(1,-1;a)}(A_{1g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{47} + \frac{3\sqrt{47}\mathbb{Q}_2^{(1,-1;a)}(B_{1g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{94} + \frac{4\sqrt{47}\mathbb{Q}_2^{(1,-1;a)}(B_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{47}$$

$$\boxed{\text{z399}} \quad \mathbb{Q}_{4,2}^{(1,-1;c)}(E_g, 2) = -\frac{3\sqrt{47}\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_2^{(b)}(B_{1g})}{94} - \frac{\sqrt{141}\mathbb{Q}_2^{(1,-1;a)}(A_{1g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{47} - \frac{3\sqrt{47}\mathbb{Q}_2^{(1,-1;a)}(B_{1g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{94} + \frac{4\sqrt{47}\mathbb{Q}_2^{(1,-1;a)}(B_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{47}$$

$$\boxed{\text{z400}} \quad \mathbb{Q}_{2,1}^{(1,0;c)}(E_g) = -\frac{\mathbb{G}_{1,1}^{(1,0;a)}(E_g)\mathbb{Q}_2^{(b)}(B_{1g})}{2} + \frac{\mathbb{G}_1^{(1,0;a)}(A_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z401}} \quad \mathbb{Q}_{2,2}^{(1,0;c)}(E_g) = \frac{\mathbb{G}_{1,2}^{(1,0;a)}(E_g)\mathbb{Q}_2^{(b)}(B_{1g})}{2} - \frac{\mathbb{G}_1^{(1,0;a)}(A_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z402}} \quad \mathbb{Q}_{2,1}^{(1,1;c)}(E_g) = \frac{\sqrt{2}\mathbb{Q}_0^{(1,1;a)}(A_{1g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$$

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

$$\boxed{\text{z435}} \quad \mathbb{G}_{1,1}^{(c)}(E_g) = \frac{\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_2^{(b)}(B_{1g})}{2} - \frac{\mathbb{Q}_2^{(a)}(B_{1g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z436}} \quad \mathbb{G}_{1,2}^{(c)}(E_g) = -\frac{\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_2^{(b)}(B_{1g})}{2} + \frac{\mathbb{Q}_2^{(a)}(B_{1g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z437}} \quad \mathbb{G}_{1,1}^{(1,-1;c)}(E_g) = \frac{\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_2^{(b)}(B_{1g})}{2} - \frac{\mathbb{Q}_2^{(1,-1;a)}(B_{1g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z438}} \quad \mathbb{G}_{1,2}^{(1,-1;c)}(E_g) = -\frac{\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_2^{(b)}(B_{1g})}{2} + \frac{\mathbb{Q}_2^{(1,-1;a)}(B_{1g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z439}} \quad \mathbb{G}_{1,1}^{(1,0;c)}(E_g, a) = \frac{\sqrt{2}\mathbb{G}_{1,1}^{(1,0;a)}(E_g)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z440}} \quad \mathbb{G}_{1,2}^{(1,0;c)}(E_g, a) = \frac{\sqrt{2}\mathbb{G}_{1,2}^{(1,0;a)}(E_g)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z441}} \quad \mathbb{G}_{1,1}^{(1,0;c)}(E_g, b) = \frac{\mathbb{G}_{1,1}^{(1,0;a)}(E_g)\mathbb{Q}_2^{(b)}(B_{1g})}{2} + \frac{\mathbb{G}_1^{(1,0;a)}(A_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z442}} \quad \mathbb{G}_{1,2}^{(1,0;c)}(E_g, b) = -\frac{\mathbb{G}_{1,2}^{(1,0;a)}(E_g)\mathbb{Q}_2^{(b)}(B_{1g})}{2} - \frac{\mathbb{G}_1^{(1,0;a)}(A_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z563}} \quad \mathbb{Q}_{1,1}^{(c)}(E_u, a) = -\frac{\mathbb{M}_{1,2}^{(a)}(E_g)\mathbb{T}_1^{(b)}(A_{2u})}{2} - \frac{\mathbb{M}_1^{(a)}(A_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z564}} \quad \mathbb{Q}_{1,2}^{(c)}(E_u, a) = -\frac{\mathbb{M}_{1,1}^{(a)}(E_g)\mathbb{T}_1^{(b)}(A_{2u})}{2} + \frac{\mathbb{M}_1^{(a)}(A_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z565}} \quad \mathbb{Q}_{1,1}^{(c)}(E_u, b) = -\frac{\sqrt{2}\mathbb{M}_{1,2}^{(a)}(E_g)\mathbb{M}_2^{(b)}(B_{2u})}{2}$$

$$\boxed{\text{z566}} \quad \mathbb{Q}_{1,2}^{(c)}(E_u, b) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(a)}(E_g)\mathbb{M}_2^{(b)}(B_{2u})}{2}$$

$$\boxed{\text{z567}} \quad \mathbb{Q}_{1,1}^{(1,-1;c)}(E_u, a) = -\frac{\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_1^{(b)}(A_{2u})}{2} - \frac{\mathbb{M}_1^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z568}} \quad \mathbb{Q}_{1,2}^{(1,-1;c)}(E_u, a) = -\frac{\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_1^{(b)}(A_{2u})}{2} + \frac{\mathbb{M}_1^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z569}} \quad \mathbb{Q}_{1,1}^{(1,-1;c)}(E_u, b) = -\frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{M}_2^{(b)}(B_{2u})}{2}$$

$$\boxed{\text{z570}} \quad \mathbb{Q}_{1,2}^{(1,-1;c)}(E_u, b) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{M}_2^{(b)}(B_{2u})}{2}$$

$$\boxed{\text{z571}} \quad \mathbb{Q}_{1,1}^{(1,-1;c)}(E_u, c) = \frac{\sqrt{3}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g, 1)\mathbb{M}_2^{(b)}(B_{2u})}{4} - \frac{\sqrt{5}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g, 2)\mathbb{M}_2^{(b)}(B_{2u})}{4}$$

$$\boxed{\text{z572}} \quad \mathbb{Q}_{1,2}^{(1,-1;c)}(E_u, c) = -\frac{\sqrt{3}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g, 1)\mathbb{M}_2^{(b)}(B_{2u})}{4} + \frac{\sqrt{5}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g, 2)\mathbb{M}_2^{(b)}(B_{2u})}{4}$$

$$\boxed{\text{z573}} \quad \mathbb{Q}_{3,1}^{(1,-1;c)}(E_u, 1) = \frac{\sqrt{6}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g, 1)\mathbb{T}_1^{(b)}(A_{2u})}{8} - \frac{\sqrt{10}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g, 2)\mathbb{T}_1^{(b)}(A_{2u})}{8} + \frac{\sqrt{6}\mathbb{M}_3^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{8} - \frac{\sqrt{10}\mathbb{M}_3^{(1,-1;a)}(B_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{8}$$

$$\boxed{\text{z574}} \quad \mathbb{Q}_{3,2}^{(1,-1;c)}(E_u, 1) = \frac{\sqrt{6}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g, 1)\mathbb{T}_1^{(b)}(A_{2u})}{8} - \frac{\sqrt{10}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g, 2)\mathbb{T}_1^{(b)}(A_{2u})}{8} - \frac{\sqrt{6}\mathbb{M}_3^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{8} - \frac{\sqrt{10}\mathbb{M}_3^{(1,-1;a)}(B_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{8}$$

$$\boxed{\text{z575}} \quad \mathbb{Q}_{3,1}^{(1,-1;c)}(E_u, 2a) = -\frac{\sqrt{10}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g, 1)\mathbb{T}_1^{(b)}(A_{2u})}{8} + \frac{\sqrt{6}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g, 2)\mathbb{T}_1^{(b)}(A_{2u})}{24} + \frac{\sqrt{10}\mathbb{M}_3^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{8} + \frac{\sqrt{6}\mathbb{M}_3^{(1,-1;a)}(B_{1g})\mathbb{T}_{1,1}^{(b)}(E_u)}{6} - \frac{\sqrt{6}\mathbb{M}_3^{(1,-1;a)}(B_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{24}$$

$$\boxed{\text{z576}} \quad \mathbb{Q}_{3,2}^{(1,-1;c)}(E_u, 2a) = -\frac{\sqrt{10}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g, 1)\mathbb{T}_1^{(b)}(A_{2u})}{8} + \frac{\sqrt{6}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g, 2)\mathbb{T}_1^{(b)}(A_{2u})}{24} - \frac{\sqrt{10}\mathbb{M}_3^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{8} - \frac{\sqrt{6}\mathbb{M}_3^{(1,-1;a)}(B_{1g})\mathbb{T}_{1,2}^{(b)}(E_u)}{6} - \frac{\sqrt{6}\mathbb{M}_3^{(1,-1;a)}(B_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{24}$$

$$\boxed{\text{z577}} \quad \mathbb{Q}_{3,1}^{(1,-1;c)}(E_u, 2b) = -\frac{\sqrt{5}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g, 1)\mathbb{M}_2^{(b)}(B_{2u})}{4} - \frac{\sqrt{3}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g, 2)\mathbb{M}_2^{(b)}(B_{2u})}{4}$$

$$\boxed{\text{z578}} \quad \mathbb{Q}_{3,2}^{(1,-1;c)}(E_u, 2b) = \frac{\sqrt{5}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g, 1)\mathbb{M}_2^{(b)}(B_{2u})}{4} + \frac{\sqrt{3}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g, 2)\mathbb{M}_2^{(b)}(B_{2u})}{4}$$

$$\boxed{\text{z579}} \quad \mathbb{Q}_{1,1}^{(1,0;c)}(E_u, a) = \frac{\sqrt{15}\mathbb{T}_{2,2}^{(1,0;a)}(E_g)\mathbb{T}_1^{(b)}(A_{2u})}{10} - \frac{\sqrt{5}\mathbb{T}_2^{(1,0;a)}(A_{1g})\mathbb{T}_{1,1}^{(b)}(E_u)}{10} + \frac{\sqrt{15}\mathbb{T}_2^{(1,0;a)}(B_{1g})\mathbb{T}_{1,1}^{(b)}(E_u)}{10} + \frac{\sqrt{15}\mathbb{T}_2^{(1,0;a)}(B_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{10}$$

$$\boxed{\text{z580}} \quad \mathbb{Q}_{1,2}^{(1,0;c)}(E_u, a) = \frac{\sqrt{15}\mathbb{T}_{2,1}^{(1,0;a)}(E_g)\mathbb{T}_1^{(b)}(A_{2u})}{10} - \frac{\sqrt{5}\mathbb{T}_2^{(1,0;a)}(A_{1g})\mathbb{T}_{1,2}^{(b)}(E_u)}{10} - \frac{\sqrt{15}\mathbb{T}_2^{(1,0;a)}(B_{1g})\mathbb{T}_{1,2}^{(b)}(E_u)}{10} + \frac{\sqrt{15}\mathbb{T}_2^{(1,0;a)}(B_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{10}$$

$$\boxed{\text{z581}} \quad \mathbb{Q}_{1,1}^{(1,0;c)}(E_u, b) = -\frac{\sqrt{2}\mathbb{T}_{2,2}^{(1,0;a)}(E_g)\mathbb{M}_2^{(b)}(B_{2u})}{2}$$

$$\boxed{\text{z582}} \quad \mathbb{Q}_{1,2}^{(1,0;c)}(E_u, b) = \frac{\sqrt{2}\mathbb{T}_{2,1}^{(1,0;a)}(E_g)\mathbb{M}_2^{(b)}(B_{2u})}{2}$$

$$\boxed{\text{z583}} \quad \mathbb{Q}_{3,1}^{(1,0;c)}(E_u, 1) = -\frac{\sqrt{10}\mathbb{T}_{2,2}^{(1,0;a)}(E_g)\mathbb{T}_1^{(b)}(A_{2u})}{10} - \frac{\sqrt{30}\mathbb{T}_2^{(1,0;a)}(A_{1g})\mathbb{T}_{1,1}^{(b)}(E_u)}{20} + \frac{3\sqrt{10}\mathbb{T}_2^{(1,0;a)}(B_{1g})\mathbb{T}_{1,1}^{(b)}(E_u)}{20} - \frac{\sqrt{10}\mathbb{T}_2^{(1,0;a)}(B_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{10}$$

$$\boxed{\text{z584}} \quad \mathbb{Q}_{3,2}^{(1,0;c)}(E_u, 1) = -\frac{\sqrt{10}\mathbb{T}_{2,1}^{(1,0;a)}(E_g)\mathbb{T}_1^{(b)}(A_{2u})}{10} - \frac{\sqrt{30}\mathbb{T}_2^{(1,0;a)}(A_{1g})\mathbb{T}_{1,2}^{(b)}(E_u)}{20} - \frac{3\sqrt{10}\mathbb{T}_2^{(1,0;a)}(B_{1g})\mathbb{T}_{1,2}^{(b)}(E_u)}{20} - \frac{\sqrt{10}\mathbb{T}_2^{(1,0;a)}(B_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{10}$$

$$\boxed{\text{z585}} \quad \mathbb{Q}_{3,1}^{(1,0;c)}(E_u, 2) = -\frac{\sqrt{6}\mathbb{T}_{2,2}^{(1,0;a)}(E_g)\mathbb{T}_1^{(b)}(A_{2u})}{6} - \frac{\sqrt{2}\mathbb{T}_2^{(1,0;a)}(A_{1g})\mathbb{T}_{1,1}^{(b)}(E_u)}{4} - \frac{\sqrt{6}\mathbb{T}_2^{(1,0;a)}(B_{1g})\mathbb{T}_{1,1}^{(b)}(E_u)}{12} + \frac{\sqrt{6}\mathbb{T}_2^{(1,0;a)}(B_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{6}$$

$$\boxed{\text{z586}} \quad \mathbb{Q}_{3,2}^{(1,0;c)}(E_u, 2) = -\frac{\sqrt{6}\mathbb{T}_{2,1}^{(1,0;a)}(E_g)\mathbb{T}_1^{(b)}(A_{2u})}{6} - \frac{\sqrt{2}\mathbb{T}_2^{(1,0;a)}(A_{1g})\mathbb{T}_{1,2}^{(b)}(E_u)}{4} + \frac{\sqrt{6}\mathbb{T}_2^{(1,0;a)}(B_{1g})\mathbb{T}_{1,2}^{(b)}(E_u)}{12} + \frac{\sqrt{6}\mathbb{T}_2^{(1,0;a)}(B_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{6}$$

$$\boxed{\text{z587}} \quad \mathbb{Q}_{1,1}^{(1,1;c)}(E_u, a) = -\frac{\mathbb{M}_{1,2}^{(1,1;a)}(E_g)\mathbb{T}_1^{(b)}(A_{2u})}{2} - \frac{\mathbb{M}_1^{(1,1;a)}(A_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z588}} \quad \mathbb{Q}_{1,2}^{(1,1;c)}(E_u, a) = -\frac{\mathbb{M}_{1,1}^{(1,1;a)}(E_g)\mathbb{T}_1^{(b)}(A_{2u})}{2} + \frac{\mathbb{M}_1^{(1,1;a)}(A_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z589}} \quad \mathbb{Q}_{1,1}^{(1,1;c)}(E_u, b) = -\frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,1;a)}(E_g)\mathbb{M}_2^{(b)}(B_{2u})}{2}$$

$$\boxed{\text{z590}} \quad \mathbb{Q}_{1,2}^{(1,1;c)}(E_u, b) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,1;a)}(E_g)\mathbb{M}_2^{(b)}(B_{2u})}{2}$$

$$\boxed{\text{z591}} \quad \mathbb{G}_{2,1}^{(c)}(E_u) = -\frac{\mathbb{M}_{1,2}^{(a)}(E_g)\mathbb{T}_1^{(b)}(A_{2u})}{2} + \frac{\mathbb{M}_1^{(a)}(A_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z592}} \quad \mathbb{G}_{2,2}^{(c)}(E_u) = -\frac{\mathbb{M}_{1,1}^{(a)}(E_g)\mathbb{T}_1^{(b)}(A_{2u})}{2} - \frac{\mathbb{M}_1^{(a)}(A_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z593}} \quad \mathbb{G}_{2,1}^{(1,-1;c)}(E_u, a) = -\frac{\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_1^{(b)}(A_{2u})}{2} + \frac{\mathbb{M}_1^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z594}} \quad \mathbb{G}_{2,2}^{(1,-1;c)}(E_u, a) = -\frac{\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_1^{(b)}(A_{2u})}{2} - \frac{\mathbb{M}_1^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z595}} \quad \mathbb{G}_{2,1}^{(1,-1;c)}(E_u, b) = \frac{\sqrt{14}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g, 1)\mathbb{T}_1^{(b)}(A_{2u})}{14} + \frac{\sqrt{210}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g, 2)\mathbb{T}_1^{(b)}(A_{2u})}{42} - \frac{\sqrt{14}\mathbb{M}_3^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{14} + \frac{\sqrt{210}\mathbb{M}_3^{(1,-1;a)}(B_{1g})\mathbb{T}_{1,1}^{(b)}(E_u)}{42} - \frac{\sqrt{210}\mathbb{M}_3^{(1,-1;a)}(B_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{42}$$

$$\boxed{\text{z596}} \quad \mathbb{G}_{2,2}^{(1,-1;c)}(E_u, b) = \frac{\sqrt{14}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g, 1)\mathbb{T}_1^{(b)}(A_{2u})}{14} + \frac{\sqrt{210}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g, 2)\mathbb{T}_1^{(b)}(A_{2u})}{42} + \frac{\sqrt{14}\mathbb{M}_3^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{14} - \frac{\sqrt{210}\mathbb{M}_3^{(1,-1;a)}(B_{1g})\mathbb{T}_{1,2}^{(b)}(E_u)}{42} - \frac{\sqrt{210}\mathbb{M}_3^{(1,-1;a)}(B_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{42}$$

$$\boxed{\text{z597}} \quad \mathbb{G}_{4,1}^{(1,-1;c)}(E_u, 1) = -\frac{\sqrt{10}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g, 1)\mathbb{T}_1^{(b)}(A_{2u})}{8} - \frac{\sqrt{6}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g, 2)\mathbb{T}_1^{(b)}(A_{2u})}{8} - \frac{\sqrt{10}\mathbb{M}_3^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{8} - \frac{\sqrt{6}\mathbb{M}_3^{(1,-1;a)}(B_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{8}$$

$$\boxed{\text{z598}} \quad \mathbb{G}_{4,2}^{(1,-1;c)}(E_u, 1) = -\frac{\sqrt{10}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g, 1)\mathbb{T}_1^{(b)}(A_{2u})}{8} - \frac{\sqrt{6}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g, 2)\mathbb{T}_1^{(b)}(A_{2u})}{8} + \frac{\sqrt{10}\mathbb{M}_3^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{8} - \frac{\sqrt{6}\mathbb{M}_3^{(1,-1;a)}(B_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{8}$$

$$\boxed{\text{z599}} \quad \mathbb{G}_{4,1}^{(1,-1;c)}(E_u, 2) = \frac{\sqrt{70}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g, 1)\mathbb{T}_1^{(b)}(A_{2u})}{56} - \frac{3\sqrt{42}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g, 2)\mathbb{T}_1^{(b)}(A_{2u})}{56} - \frac{\sqrt{70}\mathbb{M}_3^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{56} + \frac{\sqrt{42}\mathbb{M}_3^{(1,-1;a)}(B_{1g})\mathbb{T}_{1,1}^{(b)}(E_u)}{14} + \frac{3\sqrt{42}\mathbb{M}_3^{(1,-1;a)}(B_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{56}$$

$$\boxed{\text{z600}} \quad \mathbb{G}_{4,2}^{(1,-1;c)}(E_u, 2) = \frac{\sqrt{70}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g, 1)\mathbb{T}_1^{(b)}(A_{2u})}{56} - \frac{3\sqrt{42}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g, 2)\mathbb{T}_1^{(b)}(A_{2u})}{56} + \frac{\sqrt{70}\mathbb{M}_3^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{56} - \frac{\sqrt{42}\mathbb{M}_3^{(1,-1;a)}(B_{1g})\mathbb{T}_{1,2}^{(b)}(E_u)}{14} + \frac{3\sqrt{42}\mathbb{M}_3^{(1,-1;a)}(B_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{56}$$

$$\boxed{\text{z601}} \quad \mathbb{G}_{2,1}^{(1,0;c)}(E_u) = -\frac{\sqrt{3}\mathbb{T}_{2,2}^{(1,0;a)}(E_g)\mathbb{T}_1^{(b)}(A_{2u})}{6} + \frac{\mathbb{T}_2^{(1,0;a)}(A_{1g})\mathbb{T}_{1,1}^{(b)}(E_u)}{2} + \frac{\sqrt{3}\mathbb{T}_2^{(1,0;a)}(B_{1g})\mathbb{T}_{1,1}^{(b)}(E_u)}{6} + \frac{\sqrt{3}\mathbb{T}_2^{(1,0;a)}(B_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{6}$$

$$\boxed{\text{z602}} \quad \mathbb{G}_{2,2}^{(1,0;c)}(E_u) = -\frac{\sqrt{3}\mathbb{T}_{2,1}^{(1,0;a)}(E_g)\mathbb{T}_1^{(b)}(A_{2u})}{6} + \frac{\mathbb{T}_2^{(1,0;a)}(A_{1g})\mathbb{T}_{1,2}^{(b)}(E_u)}{2} - \frac{\sqrt{3}\mathbb{T}_2^{(1,0;a)}(B_{1g})\mathbb{T}_{1,2}^{(b)}(E_u)}{6} + \frac{\sqrt{3}\mathbb{T}_2^{(1,0;a)}(B_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{6}$$

$$\boxed{\text{z603}} \quad \mathbb{G}_{2,1}^{(1,1;c)}(E_u) = -\frac{\mathbb{M}_{1,2}^{(1,1;a)}(E_g)\mathbb{T}_1^{(b)}(A_{2u})}{2} + \frac{\mathbb{M}_1^{(1,1;a)}(A_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z604}} \quad \mathbb{G}_{2,2}^{(1,1;c)}(E_u) = -\frac{\mathbb{M}_{1,1}^{(1,1;a)}(E_g)\mathbb{T}_1^{(b)}(A_{2u})}{2} - \frac{\mathbb{M}_1^{(1,1;a)}(A_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

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

$$\boxed{x1} \quad Q_0^{(a)}(A_{1g}) = \begin{bmatrix} \frac{\sqrt{2}}{2} & 0 \\ 0 & \frac{\sqrt{2}}{2} \end{bmatrix}$$

$$\boxed{x2} \quad M_1^{(1,-1;a)}(A_{2g}) = \begin{bmatrix} \frac{\sqrt{2}}{2} & 0 \\ 0 & -\frac{\sqrt{2}}{2} \end{bmatrix}$$

$$\boxed{x3} \quad M_{1,1}^{(1,-1;a)}(E_g) = \begin{bmatrix} 0 & \frac{\sqrt{2}}{2} \\ \frac{\sqrt{2}}{2} & 0 \end{bmatrix}$$

$$\boxed{x4} \quad M_{1,2}^{(1,-1;a)}(E_g) = \begin{bmatrix} 0 & \frac{\sqrt{2}i}{2} \\ -\frac{\sqrt{2}i}{2} & 0 \end{bmatrix}$$

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

$$\boxed{x5} \quad Q_1^{(a)}(A_{2u}) = \begin{bmatrix} 0 & 0 & 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{2} \end{bmatrix}$$

$$\boxed{x6} \quad Q_{1,1}^{(a)}(E_u) = \begin{bmatrix} \frac{1}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{x7} \quad Q_{1,2}^{(a)}(E_u) = \begin{bmatrix} 0 & 0 & \frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2} & 0 & 0 \end{bmatrix}$$

$$\boxed{x8} \quad Q_1^{(1,0;a)}(A_{2u}) = \begin{bmatrix} 0 & -\frac{\sqrt{2}}{4} & 0 & \frac{\sqrt{2}i}{4} & 0 & 0 \\ \frac{\sqrt{2}}{4} & 0 & \frac{\sqrt{2}i}{4} & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{x9} \quad Q_{1,1}^{(1,0;a)}(E_u) = \begin{bmatrix} 0 & 0 & -\frac{\sqrt{2}i}{4} & 0 & 0 & \frac{\sqrt{2}}{4} \\ 0 & 0 & 0 & \frac{\sqrt{2}i}{4} & -\frac{\sqrt{2}}{4} & 0 \end{bmatrix}$$

$$\boxed{x10} \quad Q_{1,2}^{(1,0;a)}(E_u) = \begin{bmatrix} \frac{\sqrt{2}i}{4} & 0 & 0 & 0 & 0 & -\frac{\sqrt{2}i}{4} \\ 0 & -\frac{\sqrt{2}i}{4} & 0 & 0 & -\frac{\sqrt{2}i}{4} & 0 \end{bmatrix}$$

$$\boxed{x11} \quad \mathbb{G}_2^{(1,-1;a)}(A_{1u}) = \begin{bmatrix} 0 & -\frac{\sqrt{6}i}{12} & 0 & -\frac{\sqrt{6}}{12} & \frac{\sqrt{6}i}{6} & 0 \\ -\frac{\sqrt{6}i}{12} & 0 & \frac{\sqrt{6}}{12} & 0 & 0 & -\frac{\sqrt{6}i}{6} \end{bmatrix}$$

$$\boxed{x12} \quad \mathbb{G}_2^{(1,-1;a)}(B_{1u}) = \begin{bmatrix} 0 & \frac{\sqrt{2}i}{4} & 0 & -\frac{\sqrt{2}}{4} & 0 & 0 \\ \frac{\sqrt{2}i}{4} & 0 & \frac{\sqrt{2}}{4} & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{x13} \quad \mathbb{G}_2^{(1,-1;a)}(B_{2u}) = \begin{bmatrix} 0 & \frac{\sqrt{2}}{4} & 0 & \frac{\sqrt{2}i}{4} & 0 & 0 \\ -\frac{\sqrt{2}}{4} & 0 & \frac{\sqrt{2}i}{4} & 0 & 0 & 0 \end{bmatrix}$$

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

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

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

$$\boxed{x17} \quad \mathbb{M}_2^{(1,-1;a)}(A_{1u}) = \begin{bmatrix} 0 & -\frac{\sqrt{6}}{12} & 0 & \frac{\sqrt{6}i}{12} & \frac{\sqrt{6}}{6} & 0 \\ -\frac{\sqrt{6}}{12} & 0 & -\frac{\sqrt{6}i}{12} & 0 & 0 & -\frac{\sqrt{6}}{6} \end{bmatrix}$$

$$\boxed{x18} \quad \mathbb{M}_2^{(1,-1;a)}(B_{1u}) = \begin{bmatrix} 0 & \frac{\sqrt{2}}{4} & 0 & \frac{\sqrt{2}i}{4} & 0 & 0 \\ \frac{\sqrt{2}}{4} & 0 & -\frac{\sqrt{2}i}{4} & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{x19} \quad \mathbb{M}_2^{(1,-1;a)}(B_{2u}) = \begin{bmatrix} 0 & -\frac{\sqrt{2}i}{4} & 0 & \frac{\sqrt{2}}{4} & 0 & 0 \\ \frac{\sqrt{2}i}{4} & 0 & \frac{\sqrt{2}}{4} & 0 & 0 & 0 \end{bmatrix}$$

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

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

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

$$\boxed{x23} \quad \mathbb{T}_1^{(a)}(A_{2u}) = \begin{bmatrix} 0 & 0 & 0 & 0 & \frac{i}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{i}{2} \end{bmatrix}$$

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

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

$$\boxed{x26} \quad \mathbb{T}_1^{(1,0;a)}(A_{2u}) = \begin{bmatrix} 0 & \frac{\sqrt{2}i}{4} & 0 & \frac{\sqrt{2}}{4} & 0 & 0 \\ -\frac{\sqrt{2}i}{4} & 0 & \frac{\sqrt{2}}{4} & 0 & 0 & 0 \end{bmatrix}$$

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

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

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

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

$$\boxed{x30} \quad \mathbb{Q}_2^{(a)}(A_{1g}) = \begin{bmatrix} -\frac{\sqrt{3}}{6} & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{3}}{6} & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{3}}{6} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{3}}{6} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{3}}{3} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{3}}{3} \end{bmatrix}$$

$$\boxed{x31} \quad \mathbb{Q}_2^{(a)}(B_{1g}) = \begin{bmatrix} \frac{1}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{1}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{x32} \quad \mathbb{Q}_2^{(a)}(B_{2g}) = \begin{bmatrix} 0 & 0 & \frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2} & 0 & 0 \\ \frac{1}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

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

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

$$\boxed{x35} \quad \mathbb{Q}_2^{(1,-1;a)}(A_{1g}) = \begin{bmatrix} 0 & 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 & -\frac{\sqrt{6}}{12} \\ 0 & 0 & 0 & \frac{\sqrt{6}i}{6} & \frac{\sqrt{6}}{12} & 0 \\ \frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 & \frac{\sqrt{6}i}{12} \\ 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 & \frac{\sqrt{6}i}{12} & 0 \\ 0 & \frac{\sqrt{6}}{12} & 0 & -\frac{\sqrt{6}i}{12} & 0 & 0 \\ -\frac{\sqrt{6}}{12} & 0 & -\frac{\sqrt{6}i}{12} & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{x36} \quad \mathbb{Q}_2^{(1,-1;a)}(B_{1g}) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{2}}{4} \\ 0 & 0 & 0 & 0 & \frac{\sqrt{2}}{4} & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{2}i}{4} \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{2}i}{4} & 0 \\ 0 & \frac{\sqrt{2}}{4} & 0 & \frac{\sqrt{2}i}{4} & 0 & 0 \\ -\frac{\sqrt{2}}{4} & 0 & \frac{\sqrt{2}i}{4} & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{x37} \quad \mathbb{Q}_2^{(1,-1;a)}(B_{2g}) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{2}i}{4} \\ 0 & 0 & 0 & 0 & \frac{\sqrt{2}i}{4} & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{2}}{4} \\ 0 & 0 & 0 & 0 & \frac{\sqrt{2}}{4} & 0 \\ 0 & -\frac{\sqrt{2}i}{4} & 0 & \frac{\sqrt{2}}{4} & 0 & 0 \\ -\frac{\sqrt{2}i}{4} & 0 & -\frac{\sqrt{2}}{4} & 0 & 0 & 0 \end{bmatrix}$$

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

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

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

$$\boxed{x41} \quad \mathbb{G}_1^{(1,0;a)}(A_{2g}) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{2}i}{4} \\ 0 & 0 & 0 & 0 & \frac{\sqrt{2}i}{4} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{2}}{4} \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{2}}{4} & 0 \\ 0 & -\frac{\sqrt{2}i}{4} & 0 & -\frac{\sqrt{2}}{4} & 0 & 0 \\ -\frac{\sqrt{2}i}{4} & 0 & \frac{\sqrt{2}}{4} & 0 & 0 & 0 \end{bmatrix}$$

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

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

$$\boxed{x44} \quad \mathbb{M}_1^{(a)}(A_{2g}) = \begin{bmatrix} 0 & 0 & -\frac{i}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{i}{2} & 0 & 0 \\ \frac{i}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{i}{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

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

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

$$\boxed{x47} \quad \mathbb{M}_1^{(1,-1;a)}(A_{2g}) = \begin{bmatrix} \frac{\sqrt{6}}{6} & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{6}}{6} & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{6}}{6} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{6}}{6} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{6}}{6} & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{6}}{6} \end{bmatrix}$$

$$\boxed{x48} \quad \mathbb{M}_3^{(1,-1;a)}(A_{2g}) = \begin{bmatrix} -\frac{\sqrt{5}}{10} & 0 & 0 & 0 & 0 & -\frac{\sqrt{5}}{10} \\ 0 & \frac{\sqrt{5}}{10} & 0 & 0 & -\frac{\sqrt{5}}{10} & 0 \\ 0 & 0 & -\frac{\sqrt{5}}{10} & 0 & 0 & \frac{\sqrt{5}i}{10} \\ 0 & 0 & 0 & \frac{\sqrt{5}}{10} & -\frac{\sqrt{5}i}{10} & 0 \\ 0 & -\frac{\sqrt{5}}{10} & 0 & \frac{\sqrt{5}i}{10} & \frac{\sqrt{5}}{5} & 0 \\ -\frac{\sqrt{5}}{10} & 0 & -\frac{\sqrt{5}i}{10} & 0 & 0 & -\frac{\sqrt{5}}{5} \end{bmatrix}$$

$$\boxed{x49} \quad \mathbb{M}_3^{(1,-1;a)}(B_{1g}) = \begin{bmatrix} 0 & 0 & \frac{\sqrt{3}}{6} & 0 & 0 & -\frac{\sqrt{3}i}{6} \\ 0 & 0 & 0 & -\frac{\sqrt{3}}{6} & \frac{\sqrt{3}i}{6} & 0 \\ \frac{\sqrt{3}}{6} & 0 & 0 & 0 & 0 & \frac{\sqrt{3}}{6} \\ 0 & -\frac{\sqrt{3}}{6} & 0 & 0 & \frac{\sqrt{3}}{6} & 0 \\ 0 & -\frac{\sqrt{3}i}{6} & 0 & \frac{\sqrt{3}}{6} & 0 & 0 \\ \frac{\sqrt{3}i}{6} & 0 & \frac{\sqrt{3}}{6} & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{x50} \quad \mathbb{M}_3^{(1,-1;a)}(B_{2g}) = \begin{bmatrix} \frac{\sqrt{3}}{6} & 0 & 0 & 0 & 0 & \frac{\sqrt{3}}{6} \\ 0 & -\frac{\sqrt{3}}{6} & 0 & 0 & \frac{\sqrt{3}}{6} & 0 \\ 0 & 0 & -\frac{\sqrt{3}}{6} & 0 & 0 & \frac{\sqrt{3}i}{6} \\ 0 & 0 & 0 & \frac{\sqrt{3}}{6} & -\frac{\sqrt{3}i}{6} & 0 \\ 0 & \frac{\sqrt{3}}{6} & 0 & \frac{\sqrt{3}i}{6} & 0 & 0 \\ \frac{\sqrt{3}}{6} & 0 & -\frac{\sqrt{3}i}{6} & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{x51} \quad \mathbb{M}_{1,1}^{(1,-1;a)}(E_g) = \begin{bmatrix} 0 & \frac{\sqrt{6}}{6} & 0 & 0 & 0 & 0 \\ \frac{\sqrt{6}}{6} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{6}}{6} & 0 & 0 \\ 0 & 0 & \frac{\sqrt{6}}{6} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{6}}{6} \\ 0 & 0 & 0 & 0 & \frac{\sqrt{6}}{6} & 0 \end{bmatrix}$$

$$\boxed{x52} \quad \mathbb{M}_{1,2}^{(1,-1;a)}(E_g) = \begin{bmatrix} 0 & \frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 \\ -\frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{6}i}{6} & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{6}i}{6} \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{6}i}{6} & 0 \end{bmatrix}$$

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

$$\boxed{x54} \quad \mathbb{M}_{3,2}^{(1,-1;a)}(E_g, 1) = \begin{bmatrix} 0 & -\frac{\sqrt{5}i}{10} & 0 & \frac{\sqrt{5}}{10} & 0 & 0 \\ \frac{\sqrt{5}i}{10} & 0 & \frac{\sqrt{5}}{10} & 0 & 0 & 0 \\ 0 & \frac{\sqrt{5}}{10} & 0 & \frac{\sqrt{5}i}{5} & \frac{\sqrt{5}}{10} & 0 \\ \frac{\sqrt{5}}{10} & 0 & -\frac{\sqrt{5}i}{5} & 0 & 0 & -\frac{\sqrt{5}}{10} \\ 0 & 0 & \frac{\sqrt{5}}{10} & 0 & 0 & -\frac{\sqrt{5}i}{10} \\ 0 & 0 & 0 & -\frac{\sqrt{5}}{10} & \frac{\sqrt{5}i}{10} & 0 \end{bmatrix}$$

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

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

$$\boxed{x57} \quad \mathbb{M}_1^{(1,1;a)}(A_{2g}) = \begin{bmatrix} -\frac{\sqrt{30}}{30} & 0 & 0 & 0 & 0 & \frac{\sqrt{30}}{20} \\ 0 & \frac{\sqrt{30}}{30} & 0 & 0 & \frac{\sqrt{30}}{20} & 0 \\ 0 & 0 & -\frac{\sqrt{30}}{30} & 0 & 0 & -\frac{\sqrt{30}i}{20} \\ 0 & 0 & 0 & \frac{\sqrt{30}}{30} & \frac{\sqrt{30}i}{20} & 0 \\ 0 & \frac{\sqrt{30}}{20} & 0 & -\frac{\sqrt{30}i}{20} & \frac{\sqrt{30}}{15} & 0 \\ \frac{\sqrt{30}}{20} & 0 & \frac{\sqrt{30}i}{20} & 0 & 0 & -\frac{\sqrt{30}}{15} \end{bmatrix}$$

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

$$\boxed{x59} \quad \mathbb{M}_{1,2}^{(1,1;a)}(E_g) = \begin{bmatrix} 0 & -\frac{\sqrt{30}i}{30} & 0 & -\frac{\sqrt{30}}{20} & 0 & 0 \\ \frac{\sqrt{30}i}{30} & 0 & -\frac{\sqrt{30}}{20} & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{30}}{20} & 0 & \frac{\sqrt{30}i}{15} & -\frac{\sqrt{30}}{20} & 0 \\ -\frac{\sqrt{30}}{20} & 0 & -\frac{\sqrt{30}i}{20} & 0 & 0 & \frac{\sqrt{30}}{20} \\ 0 & 0 & -\frac{\sqrt{30}}{20} & 0 & 0 & -\frac{\sqrt{30}i}{30} \\ 0 & 0 & 0 & \frac{\sqrt{30}}{20} & \frac{\sqrt{30}i}{30} & 0 \end{bmatrix}$$

$$\boxed{x60} \quad \mathbb{T}_2^{(1,0;a)}(A_{1g}) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{2}i}{4} \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{2}i}{4} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{2}}{4} \\ 0 & 0 & 0 & 0 & \frac{\sqrt{2}}{4} & 0 \\ 0 & \frac{\sqrt{2}i}{4} & 0 & \frac{\sqrt{2}}{4} & 0 & 0 \\ -\frac{\sqrt{2}i}{4} & 0 & \frac{\sqrt{2}}{4} & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{x61} \quad \mathbb{T}_2^{(1,0;a)}(B_{1g}) = \begin{bmatrix} 0 & 0 & -\frac{\sqrt{6}}{6} & 0 & 0 & -\frac{\sqrt{6}i}{12} \\ 0 & 0 & 0 & \frac{\sqrt{6}}{6} & \frac{\sqrt{6}i}{12} & 0 \\ -\frac{\sqrt{6}}{6} & 0 & 0 & 0 & 0 & \frac{\sqrt{6}}{12} \\ 0 & \frac{\sqrt{6}}{6} & 0 & 0 & \frac{\sqrt{6}}{12} & 0 \\ 0 & -\frac{\sqrt{6}i}{12} & 0 & \frac{\sqrt{6}}{12} & 0 & 0 \\ \frac{\sqrt{6}i}{12} & 0 & \frac{\sqrt{6}}{12} & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{x62} \quad \mathbb{T}_2^{(1,0;a)}(B_{2g}) = \begin{bmatrix} \frac{\sqrt{6}}{6} & 0 & 0 & 0 & 0 & -\frac{\sqrt{6}}{12} \\ 0 & -\frac{\sqrt{6}}{6} & 0 & 0 & -\frac{\sqrt{6}}{12} & 0 \\ 0 & 0 & -\frac{\sqrt{6}}{6} & 0 & 0 & -\frac{\sqrt{6}i}{12} \\ 0 & 0 & 0 & \frac{\sqrt{6}}{6} & \frac{\sqrt{6}i}{12} & 0 \\ 0 & -\frac{\sqrt{6}}{12} & 0 & -\frac{\sqrt{6}i}{12} & 0 & 0 \\ -\frac{\sqrt{6}}{12} & 0 & \frac{\sqrt{6}i}{12} & 0 & 0 & 0 \end{bmatrix}$$

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

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

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### Cluster SAMB

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- Site cluster

\*\* Wyckoff: **1a**

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

- Bond cluster

\*\* Wyckoff: **1a@1b**

$$\boxed{y2} \quad \mathbb{Q}_0^{(s)}(A_{1g}) = [1]$$

$$\boxed{y3} \quad \mathbb{T}_1^{(s)}(A_{2u}) = [i]$$

\*\* Wyckoff: **2b@2f**

$$\boxed{y4} \quad \mathbb{Q}_0^{(s)}(A_{1g}) = \left[ \frac{\sqrt{2}}{2}, \frac{\sqrt{2}}{2} \right]$$

$$\boxed{y5} \quad \mathbb{Q}_2^{(s)}(B_{1g}) = \left[ \frac{\sqrt{2}}{2}, -\frac{\sqrt{2}}{2} \right]$$

$$\boxed{y6} \quad \mathbb{T}_{1,1}^{(s)}(E_u) = [0, -i]$$

$$\boxed{y7} \quad \mathbb{T}_{1,2}^{(s)}(E_u) = [i, 0]$$

\*\* Wyckoff: **2c@1c**

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

$$\boxed{y9} \quad \mathbb{Q}_2^{(s)}(B_{2g}) = \left[ \frac{\sqrt{2}}{2}, -\frac{\sqrt{2}}{2} \right]$$

$$\boxed{y10} \quad \mathbb{T}_{1,1}^{(s)}(E_u) = \left[ \frac{\sqrt{2}i}{2}, -\frac{\sqrt{2}i}{2} \right]$$

$$\boxed{y11} \quad \mathbb{T}_{1,2}^{(s)}(E_u) = \left[ \frac{\sqrt{2}i}{2}, \frac{\sqrt{2}i}{2} \right]$$

\*\* Wyckoff: 4e@2e

$$\boxed{y12} \quad \mathbb{Q}_0^{(s)}(A_{1g}) = \left[ \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \right]$$

$$\boxed{y13} \quad \mathbb{T}_1^{(s)}(A_{2u}) = \left[ \frac{i}{2}, \frac{i}{2}, \frac{i}{2}, \frac{i}{2} \right]$$

$$\boxed{y14} \quad \mathbb{Q}_2^{(s)}(B_{1g}) = \left[ \frac{1}{2}, \frac{1}{2}, -\frac{1}{2}, -\frac{1}{2} \right]$$

$$\boxed{y15} \quad \mathbb{M}_2^{(s)}(B_{2u}) = \left[ \frac{i}{2}, \frac{i}{2}, -\frac{i}{2}, -\frac{i}{2} \right]$$

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

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

$$\boxed{y18} \quad \mathbb{T}_{1,1}^{(s)}(E_u) = \left[ 0, 0, -\frac{\sqrt{2}i}{2}, \frac{\sqrt{2}i}{2} \right]$$

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

Table 5: Orbital of each site

#	site	orbital
1	A	$ 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	A	A	[1,2,3,4]	[s,p]	[s,p]

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### — Site in Unit Cell —

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

Table 7: 'A' (#1) site cluster (1a), 4/mmm

SL	position ( $s$ )	mapping
1	[ 0.00000, 0.00000, 0.00000]	[1,2,3,4,5,6,7,8,9,10,11,12,13,14,15,16]

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### — 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 (**2b@2f**), ND,  $|\mathbf{v}|=1.0$  (cartesian)

SL	vector ( $\mathbf{v}$ )	center ( $\mathbf{c}$ )	mapping	head	tail	$\mathbf{R}$ (primitive)
1	[ 0.00000, 1.00000, 0.00000]	[ 0.00000, 0.50000, 0.00000]	[1,-2,5,-6,-9,10,-13,14]	(1,1)	(1,1)	[0,-1,0]
2	[-1.00000, 0.00000, 0.00000]	[ 0.50000, 0.00000, 0.00000]	[3,-4,-7,8,-11,12,15,-16]	(1,1)	(1,1)	[1,0,0]

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

SL	vector ( $\mathbf{v}$ )	center ( $\mathbf{c}$ )	mapping	head	tail	$\mathbf{R}$ (primitive)
1	[-1.00000,-1.00000, 0.00000]	[ 0.50000, 0.50000, 0.00000]	[1,-2,7,-8,-9,10,-15,16]	(1,1)	(1,1)	[1,1,0]
2	[ 1.00000,-1.00000, 0.00000]	[ 0.50000, 0.50000, 0.00000]	[3,-4,5,-6,-11,12,-13,14]	(1,1)	(1,1)	[-1,1,0]

Table 10: 3-th 'A'-'A' [1] (#3) bond cluster (**1a@1b**), ND,  $|\mathbf{v}|=1.5$  (cartesian)

SL	vector ( $\mathbf{v}$ )	center ( $\mathbf{c}$ )	mapping	head	tail	$\mathbf{R}$ (primitive)
1	[ 0.00000, 0.00000,-1.00000]	[ 0.00000, 0.00000, 0.50000]	[1,2,3,4,-5,-6,-7,-8,-9,-10,-11,-12,13,14,15,16]	(1,1)	(1,1)	[0,0,1]

Table 11: 4-th 'A'-A' [1] (#4) bond cluster ( $4e02e$ ), ND,  $|\mathbf{v}| = 1.80278$  (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, -6, -9, 14]	(1,1)	(1,1)	[0, -1, 1]
2	[ 0.00000, -1.00000, -1.00000]	[ 0.00000, 0.50000, 0.50000]	[2, -5, -10, 13]	(1,1)	(1,1)	[0, 1, 1]
3	[-1.00000, 0.00000, -1.00000]	[ 0.50000, 0.00000, 0.50000]	[3, -7, -11, 15]	(1,1)	(1,1)	[1, 0, 1]
4	[ 1.00000, 0.00000, -1.00000]	[ 0.50000, 0.00000, 0.50000]	[4, -8, -12, 16]	(1,1)	(1,1)	[-1, 0, 1]