

# Model for “D2h1”

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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.: [ $A_g$ ,  $B_{1g}$ ,  $B_{2g}$ ,  $B_{3g}$ ,  $A_u$ ,  $B_{1u}$ ,  $B_{2u}$ ,  $B_{3u}$ ]
  - 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.: [ $A_g$ ,  $B_{1g}$ ,  $B_{2g}$ ,  $B_{3g}$ ,  $A_u$ ,  $B_{1u}$ ,  $B_{2u}$ ,  $B_{3u}$ ]
  - Spin (s): [0, 1]
- Site-cluster selection:
  - Rank: [0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11]
  - Irrep.: [ $A_g$ ,  $B_{1g}$ ,  $B_{2g}$ ,  $B_{3g}$ ,  $A_u$ ,  $B_{1u}$ ,  $B_{2u}$ ,  $B_{3u}$ ]
- Bond-cluster selection:
  - Type: [Q, G, M, T]
  - Rank: [0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11]
  - Irrep.: [ $A_g$ ,  $B_{1g}$ ,  $B_{2g}$ ,  $B_{3g}$ ,  $A_u$ ,  $B_{1u}$ ,  $B_{2u}$ ,  $B_{3u}$ ]
- 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. 47  $D_{2h}^1$   $Pmmm$  [ orthorhombic ]
- Associated point group: PG No. 47  $D_{2h}$   $mmm$  [ orthorhombic ]
- Unit cell:  
 $a = 1.00000, b = 1.20000, c = 1.50000, \alpha = 90.0, \beta = 90.0, \gamma = 90.0$
- Lattice vectors (conventional cell):  
 $\mathbf{a}_1 = [1.00000, 0.00000, 0.00000]$   
 $\mathbf{a}_2 = [0.00000, 1.20000, 0.00000]$   
 $\mathbf{a}_3 = [0.00000, 0.00000, 1.50000]$

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 — Symmetry Operation —

Table 1: Symmetry operation

	# SO	# SO	# SO	# SO	# SO
1	{1 0}	2	{2001 0}	3	{2010 0}
6	{m001 0}	7	{m010 0}	8	{m100 0}

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 — Harmonics —

Table 2: Harmonics

#	symbol	irrep.	rank	X	multiplicity	component	symmetry
1	$\mathbb{Q}_0(A_g)$	$A_g$	0	$Q, T$	-	-	1
2	$\mathbb{Q}_2(A_g, 1)$	$A_g$	2	$Q, T$	1	-	$-\frac{x^2}{2} - \frac{y^2}{2} + z^2$
3	$\mathbb{Q}_2(A_g, 2)$	$A_g$	2	$Q, T$	2	-	$\frac{\sqrt{3}(x-y)(x+y)}{2}$
4	$\mathbb{G}_3(A_g)$	$A_g$	3	$G, M$	-	-	$\sqrt{15}xyz$
5	$\mathbb{G}_0(A_u)$	$A_u$	0	$G, M$	-	-	1
6	$\mathbb{G}_2(A_u, 1)$	$A_u$	2	$G, M$	1	-	$-\frac{x^2}{2} - \frac{y^2}{2} + z^2$
7	$\mathbb{G}_2(A_u, 2)$	$A_u$	2	$G, M$	2	-	$\frac{\sqrt{3}(x-y)(x+y)}{2}$
8	$\mathbb{Q}_3(A_u)$	$A_u$	3	$Q, T$	-	-	$\sqrt{15}xyz$

continued ...

Table 2

#	symbol	irrep.	rank	X	multiplicity	component	symmetry
9	$\mathbb{G}_4(A_u, 1)$	$A_u$	4	$G, M$	1	-	$\frac{\sqrt{21}(x^4 - 3x^2y^2 - 3x^2z^2 + y^4 - 3y^2z^2 + z^4)}{6}$
10	$\mathbb{G}_1(B_{1g})$	$B_{1g}$	1	$G, M$	-	-	$z$
11	$\mathbb{Q}_2(B_{1g})$	$B_{1g}$	2	$Q, T$	-	-	$\sqrt{3}xy$
12	$\mathbb{G}_3(B_{1g}, 1)$	$B_{1g}$	3	$G, M$	1	-	$-\frac{z(3x^2 + 3y^2 - 2z^2)}{2}$
13	$\mathbb{G}_3(B_{1g}, 2)$	$B_{1g}$	3	$G, M$	2	-	$\frac{\sqrt{15}z(x-y)(x+y)}{2}$
14	$\mathbb{Q}_4(B_{1g}, 1)$	$B_{1g}$	4	$Q, T$	1	-	$\frac{\sqrt{35}xy(x-y)(x+y)}{2}$
15	$\mathbb{Q}_1(B_{1u})$	$B_{1u}$	1	$Q, T$	-	-	$z$
16	$\mathbb{G}_2(B_{1u})$	$B_{1u}$	2	$G, M$	-	-	$\sqrt{3}xy$
17	$\mathbb{Q}_3(B_{1u}, 1)$	$B_{1u}$	3	$Q, T$	1	-	$-\frac{z(3x^2 + 3y^2 - 2z^2)}{2}$
18	$\mathbb{Q}_3(B_{1u}, 2)$	$B_{1u}$	3	$Q, T$	2	-	$\frac{\sqrt{15}z(x-y)(x+y)}{2}$
19	$\mathbb{G}_4(B_{1u}, 1)$	$B_{1u}$	4	$G, M$	1	-	$\frac{\sqrt{35}xy(x-y)(x+y)}{2}$
20	$\mathbb{G}_1(B_{2g})$	$B_{2g}$	1	$G, M$	-	-	$y$
21	$\mathbb{Q}_2(B_{2g})$	$B_{2g}$	2	$Q, T$	-	-	$\sqrt{3}xz$
22	$\mathbb{G}_3(B_{2g}, 1)$	$B_{2g}$	3	$G, M$	1	-	$-\frac{y(3x^2 - 2y^2 + 3z^2)}{2}$
23	$\mathbb{G}_3(B_{2g}, 2)$	$B_{2g}$	3	$G, M$	2	-	$-\frac{\sqrt{15}y(x-z)(x+z)}{2}$
24	$\mathbb{Q}_1(B_{2u})$	$B_{2u}$	1	$Q, T$	-	-	$y$
25	$\mathbb{G}_2(B_{2u})$	$B_{2u}$	2	$G, M$	-	-	$\sqrt{3}xz$
26	$\mathbb{Q}_3(B_{2u}, 1)$	$B_{2u}$	3	$Q, T$	1	-	$-\frac{y(3x^2 - 2y^2 + 3z^2)}{2}$
27	$\mathbb{Q}_3(B_{2u}, 2)$	$B_{2u}$	3	$Q, T$	2	-	$-\frac{\sqrt{15}y(x-z)(x+z)}{2}$
28	$\mathbb{G}_1(B_{3g})$	$B_{3g}$	1	$G, M$	-	-	$x$
29	$\mathbb{Q}_2(B_{3g})$	$B_{3g}$	2	$Q, T$	-	-	$\sqrt{3}yz$

continued ...

Table 2

#	symbol	irrep.	rank	X	multiplicity	component	symmetry
30	$\mathbb{G}_3(B_{3g}, 1)$	$B_{3g}$	3	$G, M$	1	-	$\frac{x(2x^2 - 3y^2 - 3z^2)}{2}$
31	$\mathbb{G}_3(B_{3g}, 2)$	$B_{3g}$	3	$G, M$	2	-	$\frac{\sqrt{15}x(y-z)(y+z)}{2}$
32	$\mathbb{Q}_1(B_{3u})$	$B_{3u}$	1	$Q, T$	-	-	$x$
33	$\mathbb{G}_2(B_{3u})$	$B_{3u}$	2	$G, M$	-	-	$\sqrt{3}yz$
34	$\mathbb{Q}_3(B_{3u}, 1)$	$B_{3u}$	3	$Q, T$	1	-	$\frac{x(2x^2 - 3y^2 - 3z^2)}{2}$
35	$\mathbb{Q}_3(B_{3u}, 2)$	$B_{3u}$	3	$Q, T$	2	-	$\frac{\sqrt{15}x(y-z)(y+z)}{2}$

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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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348 (all 348) SAMBs

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

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

- '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

[z157]  $\mathbb{G}_2^{(1,-1;c)}(A_u, 1) = \mathbb{G}_2^{(1,-1;a)}(A_u, 1)\mathbb{Q}_0^{(s)}(A_g)$

[z158]  $\mathbb{G}_2^{(1,-1;c)}(A_u, 2) = \mathbb{G}_2^{(1,-1;a)}(A_u, 2)\mathbb{Q}_0^{(s)}(A_g)$

[z159]  $\mathbb{G}_0^{(1,1;c)}(A_u) = \mathbb{G}_0^{(1,1;a)}(A_u)\mathbb{Q}_0^{(s)}(A_g)$

[z210]  $\mathbb{Q}_1^{(c)}(B_{1u}) = \mathbb{Q}_1^{(a)}(B_{1u})\mathbb{Q}_0^{(s)}(A_g)$

$$\boxed{\text{z211}} \quad \mathbb{Q}_1^{(1,0;c)}(B_{1u}) = \mathbb{Q}_1^{(1,0;a)}(B_{1u})\mathbb{Q}_0^{(s)}(A_g)$$

$$\boxed{\text{z212}} \quad \mathbb{G}_2^{(1,-1;c)}(B_{1u}) = \mathbb{G}_2^{(1,-1;a)}(B_{1u})\mathbb{Q}_0^{(s)}(A_g)$$

$$\boxed{\text{z259}} \quad \mathbb{Q}_1^{(c)}(B_{2u}) = \mathbb{Q}_1^{(a)}(B_{2u})\mathbb{Q}_0^{(s)}(A_g)$$

$$\boxed{\text{z260}} \quad \mathbb{Q}_1^{(1,0;c)}(B_{2u}) = \mathbb{Q}_1^{(1,0;a)}(B_{2u})\mathbb{Q}_0^{(s)}(A_g)$$

$$\boxed{\text{z261}} \quad \mathbb{G}_2^{(1,-1;c)}(B_{2u}) = \mathbb{G}_2^{(1,-1;a)}(B_{2u})\mathbb{Q}_0^{(s)}(A_g)$$

$$\boxed{\text{z304}} \quad \mathbb{Q}_1^{(c)}(B_{3u}) = \mathbb{Q}_1^{(a)}(B_{3u})\mathbb{Q}_0^{(s)}(A_g)$$

$$\boxed{\text{z305}} \quad \mathbb{Q}_1^{(1,0;c)}(B_{3u}) = \mathbb{Q}_1^{(1,0;a)}(B_{3u})\mathbb{Q}_0^{(s)}(A_g)$$

$$\boxed{\text{z306}} \quad \mathbb{G}_2^{(1,-1;c)}(B_{3u}) = \mathbb{G}_2^{(1,-1;a)}(B_{3u})\mathbb{Q}_0^{(s)}(A_g)$$

• 'A' site-cluster : A

- \* bra:  $\langle p_x, \uparrow |, \langle p_x, \downarrow |, \langle p_y, \uparrow |, \langle p_y, \downarrow |, \langle p_z, \uparrow |, \langle p_z, \downarrow |$
- \* ket:  $|p_x, \uparrow \rangle, |p_x, \downarrow \rangle, |p_y, \uparrow \rangle, |p_y, \downarrow \rangle, |p_z, \uparrow \rangle, |p_z, \downarrow \rangle$
- \* wyckoff: 1a

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

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

$$\boxed{\text{z4}} \quad \mathbb{Q}_2^{(c)}(A_g, 2) = \mathbb{Q}_2^{(a)}(A_g, 2)\mathbb{Q}_0^{(s)}(A_g)$$

$$\boxed{\text{z5}} \quad \mathbb{Q}_2^{(1,-1;c)}(A_g, 1) = \mathbb{Q}_2^{(1,-1;a)}(A_g, 1)\mathbb{Q}_0^{(s)}(A_g)$$

$$\boxed{\text{z6}} \quad \mathbb{Q}_2^{(1,-1;c)}(A_g, 2) = \mathbb{Q}_2^{(1,-1;a)}(A_g, 2)\mathbb{Q}_0^{(s)}(A_g)$$

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

$$\boxed{\text{z54}} \quad \mathbb{Q}_2^{(c)}(B_{1g}) = \mathbb{Q}_2^{(a)}(B_{1g})\mathbb{Q}_0^{(s)}(A_g)$$

$$\boxed{\text{z55}} \quad \mathbb{Q}_2^{(1,-1;c)}(B_{1g}) = \mathbb{Q}_2^{(1,-1;a)}(B_{1g})\mathbb{Q}_0^{(s)}(A_g)$$

$$\boxed{\text{z56}} \quad \mathbb{G}_1^{(1,0;c)}(B_{1g}) = \mathbb{G}_1^{(1,0;a)}(B_{1g})\mathbb{Q}_0^{(s)}(A_g)$$

$$\boxed{\text{z91}} \quad \mathbb{Q}_2^{(c)}(B_{2g}) = \mathbb{Q}_2^{(a)}(B_{2g})\mathbb{Q}_0^{(s)}(A_g)$$

$$\boxed{\text{z92}} \quad \mathbb{Q}_2^{(1,-1;c)}(B_{2g}) = \mathbb{Q}_2^{(1,-1;a)}(B_{2g})\mathbb{Q}_0^{(s)}(A_g)$$

$$\boxed{\text{z93}} \quad \mathbb{G}_1^{(1,0;c)}(B_{2g}) = \mathbb{G}_1^{(1,0;a)}(B_{2g})\mathbb{Q}_0^{(s)}(A_g)$$

$$\boxed{\text{z124}} \quad \mathbb{Q}_2^{(c)}(B_{3g}) = \mathbb{Q}_2^{(a)}(B_{3g})\mathbb{Q}_0^{(s)}(A_g)$$

$$\boxed{\text{z125}} \quad \mathbb{Q}_2^{(1,-1;c)}(B_{3g}) = \mathbb{Q}_2^{(1,-1;a)}(B_{3g})\mathbb{Q}_0^{(s)}(A_g)$$

$$\boxed{\text{z126}} \quad \mathbb{G}_1^{(1,0;c)}(B_{3g}) = \mathbb{G}_1^{(1,0;a)}(B_{3g})\mathbb{Q}_0^{(s)}(A_g)$$

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

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

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

\* wyckoff: **1c@1b**

$$\boxed{\text{z8}} \quad \mathbb{Q}_0^{(c)}(A_g) = \mathbb{Q}_0^{(a)}(A_g)\mathbb{Q}_0^{(b)}(A_g)$$

$$\boxed{\text{z160}} \quad \mathbb{G}_0^{(1,-1;c)}(A_u) = \mathbb{M}_1^{(1,-1;a)}(B_{3g})\mathbb{T}_1^{(b)}(B_{3u})$$

$$\boxed{\text{z213}} \quad \mathbb{Q}_1^{(1,-1;c)}(B_{1u}) = -\mathbb{M}_1^{(1,-1;a)}(B_{2g})\mathbb{T}_1^{(b)}(B_{3u})$$

$$\boxed{\text{z262}} \quad \mathbb{Q}_1^{(1,-1;c)}(B_{2u}) = \mathbb{M}_1^{(1,-1;a)}(B_{1g})\mathbb{T}_1^{(b)}(B_{3u})$$

• '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: **1c@1b**

$$\boxed{\text{z9}} \quad \mathbb{Q}_0^{(c)}(A_g) = \mathbb{T}_1^{(a)}(B_{3u})\mathbb{T}_1^{(b)}(B_{3u})$$

$$\boxed{\text{z10}} \quad \mathbb{Q}_2^{(1,-1;c)}(A_g, 1) = -\mathbb{M}_2^{(1,-1;a)}(B_{3u})\mathbb{T}_1^{(b)}(B_{3u})$$

$$\boxed{\text{z11}} \quad \mathbb{Q}_0^{(1,0;c)}(A_g) = \mathbb{T}_1^{(1,0;a)}(B_{3u})\mathbb{T}_1^{(b)}(B_{3u})$$

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

$$\boxed{\text{z58}} \quad \mathbb{G}_2^{(1,-1;c)}(A_u, 2) = \mathbb{G}_2^{(1,-1;a)}(A_u, 2)\mathbb{Q}_0^{(b)}(A_g)$$

$$\boxed{\text{z59}} \quad \mathbb{G}_0^{(1,1;c)}(A_u) = \mathbb{G}_0^{(1,1;a)}(A_u)\mathbb{Q}_0^{(b)}(A_g)$$

$$\boxed{\text{z94}} \quad \mathbb{Q}_2^{(c)}(B_{1g}) = \mathbb{T}_1^{(a)}(B_{2u})\mathbb{T}_1^{(b)}(B_{3u})$$

$$\boxed{\text{z95}} \quad \mathbb{Q}_2^{(1,-1;c)}(B_{1g}) = \mathbb{M}_2^{(1,-1;a)}(B_{2u})\mathbb{T}_1^{(b)}(B_{3u})$$

$$\boxed{\text{z96}} \quad \mathbb{Q}_2^{(1,0;c)}(B_{1g}) = \mathbb{T}_1^{(1,0;a)}(B_{2u})\mathbb{T}_1^{(b)}(B_{3u})$$

$$\boxed{\text{z127}} \quad \mathbb{Q}_1^{(c)}(B_{1u}) = \mathbb{Q}_1^{(a)}(B_{1u})\mathbb{Q}_0^{(b)}(A_g)$$

$$\boxed{\text{z128}} \quad \mathbb{Q}_1^{(1,0;c)}(B_{1u}) = \mathbb{Q}_1^{(1,0;a)}(B_{1u})\mathbb{Q}_0^{(b)}(A_g)$$

$$\boxed{\text{z129}} \quad \mathbb{G}_2^{(1,-1;c)}(B_{1u}) = \mathbb{G}_2^{(1,-1;a)}(B_{1u})\mathbb{Q}_0^{(b)}(A_g)$$

$$\boxed{\text{z161}} \quad \mathbb{Q}_2^{(c)}(B_{2g}) = \mathbb{T}_1^{(a)}(B_{1u})\mathbb{T}_1^{(b)}(B_{3u})$$

$$\boxed{\text{z162}} \quad \mathbb{Q}_2^{(1,-1;c)}(B_{2g}) = -\mathbb{M}_2^{(1,-1;a)}(B_{1u})\mathbb{T}_1^{(b)}(B_{3u})$$

$$\boxed{\text{z163}} \quad \mathbb{Q}_2^{(1,0;c)}(B_{2g}) = \mathbb{T}_1^{(1,0;a)}(B_{1u})\mathbb{T}_1^{(b)}(B_{3u})$$

$$\boxed{\text{z214}} \quad \mathbb{Q}_1^{(c)}(B_{2u}) = \mathbb{Q}_1^{(a)}(B_{2u})\mathbb{Q}_0^{(b)}(A_g)$$

$$\boxed{\text{z215}} \quad \mathbb{Q}_1^{(1,0;c)}(B_{2u}) = \mathbb{Q}_1^{(1,0;a)}(B_{2u})\mathbb{Q}_0^{(b)}(A_g)$$

$$\boxed{\text{z216}} \quad \mathbb{G}_2^{(1,-1;c)}(B_{2u}) = \mathbb{G}_2^{(1,-1;a)}(B_{2u})\mathbb{Q}_0^{(b)}(A_g)$$

$$\boxed{\text{z263}} \quad \mathbb{Q}_2^{(1,-1;c)}(B_{3g}) = \frac{\sqrt{3}\mathbb{M}_2^{(1,-1;a)}(A_u, 1)\mathbb{T}_1^{(b)}(B_{3u})}{2} + \frac{\mathbb{M}_2^{(1,-1;a)}(A_u, 2)\mathbb{T}_1^{(b)}(B_{3u})}{2}$$

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

$$\boxed{\text{z265}} \quad \mathbb{G}_1^{(1,1;c)}(B_{3g}) = \mathbb{M}_0^{(1,1;a)}(A_u)\mathbb{T}_1^{(b)}(B_{3u})$$

$$\boxed{\text{z307}} \quad \mathbb{Q}_1^{(c)}(B_{3u}) = \mathbb{Q}_1^{(a)}(B_{3u})\mathbb{Q}_0^{(b)}(A_g)$$

$$\boxed{\text{z308}} \quad \mathbb{Q}_1^{(1,0;c)}(B_{3u}) = \mathbb{Q}_1^{(1,0;a)}(B_{3u})\mathbb{Q}_0^{(b)}(A_g)$$

$$\boxed{\text{z309}} \quad \mathbb{G}_2^{(1,-1;c)}(B_{3u}) = \mathbb{G}_2^{(1,-1;a)}(B_{3u})\mathbb{Q}_0^{(b)}(A_g)$$

• '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: **1c@1b**

$$\boxed{\text{z12}} \quad \mathbb{Q}_0^{(c)}(A_g) = \mathbb{Q}_0^{(a)}(A_g)\mathbb{Q}_0^{(b)}(A_g)$$

$$\boxed{\text{z13}} \quad \mathbb{Q}_2^{(c)}(A_g, 1) = \mathbb{Q}_2^{(a)}(A_g, 1)\mathbb{Q}_0^{(b)}(A_g)$$

$$\boxed{\text{z14}} \quad \mathbb{Q}_2^{(c)}(A_g, 2) = \mathbb{Q}_2^{(a)}(A_g, 2)\mathbb{Q}_0^{(b)}(A_g)$$

$$\boxed{\text{z15}} \quad \mathbb{Q}_2^{(1,-1;c)}(A_g, 1) = \mathbb{Q}_2^{(1,-1;a)}(A_g, 1)\mathbb{Q}_0^{(b)}(A_g)$$

$$\boxed{\text{z16}} \quad \mathbb{Q}_2^{(1,-1;c)}(A_g, 2) = \mathbb{Q}_2^{(1,-1;a)}(A_g, 2)\mathbb{Q}_0^{(b)}(A_g)$$

$$\boxed{\text{z17}} \quad \mathbb{Q}_0^{(1,1;c)}(A_g) = \mathbb{Q}_0^{(1,1;a)}(A_g)\mathbb{Q}_0^{(b)}(A_g)$$

$$\boxed{\text{z60}} \quad \mathbb{Q}_3^{(1,-1;c)}(A_u) = -\mathbb{M}_3^{(1,-1;a)}(B_{3g}, 2)\mathbb{T}_1^{(b)}(B_{3u})$$

$$\boxed{\text{z61}} \quad \mathbb{Q}_3^{(1,0;c)}(A_u) = \mathbb{T}_2^{(1,0;a)}(B_{3g})\mathbb{T}_1^{(b)}(B_{3u})$$

$$\boxed{\text{z62}} \quad \mathbb{G}_0^{(c)}(A_u) = \mathbb{M}_1^{(a)}(B_{3g})\mathbb{T}_1^{(b)}(B_{3u})$$

$$\boxed{\text{z97}} \quad \mathbb{G}_0^{(1,-1;c)}(A_u) = \mathbb{M}_1^{(1,-1;a)}(B_{3g})\mathbb{T}_1^{(b)}(B_{3u})$$

$$\boxed{\text{z98}} \quad \mathbb{G}_2^{(1,-1;c)}(A_u, 1) = -\mathbb{M}_3^{(1,-1;a)}(B_{3g}, 1)\mathbb{T}_1^{(b)}(B_{3u})$$

$$\boxed{\text{z99}} \quad \mathbb{G}_0^{(1,1;c)}(A_u) = \mathbb{M}_1^{(1,1;a)}(B_{3g})\mathbb{T}_1^{(b)}(B_{3u})$$

$$\boxed{\text{z130}} \quad \mathbb{Q}_2^{(c)}(B_{1g}) = \mathbb{Q}_2^{(a)}(B_{1g})\mathbb{Q}_0^{(b)}(A_g)$$

$$\boxed{\text{z131}} \quad \mathbb{Q}_2^{(1,-1;c)}(B_{1g}) = \mathbb{Q}_2^{(1,-1;a)}(B_{1g})\mathbb{Q}_0^{(b)}(A_g)$$

$$\boxed{\text{z132}} \quad \mathbb{G}_1^{(1,0;c)}(B_{1g}) = \mathbb{G}_1^{(1,0;a)}(B_{1g})\mathbb{Q}_0^{(b)}(A_g)$$

$$\boxed{\text{z164}} \quad \mathbb{Q}_1^{(c)}(B_{1u}) = -\mathbb{M}_1^{(a)}(B_{2g})\mathbb{T}_1^{(b)}(B_{3u})$$

$$\boxed{\text{z165}} \quad \mathbb{Q}_1^{(1,-1;c)}(B_{1u}) = -\mathbb{M}_1^{(1,-1;a)}(B_{2g})\mathbb{T}_1^{(b)}(B_{3u})$$

$$\boxed{\text{z166}} \quad \mathbb{Q}_3^{(1,-1;c)}(B_{1u}, 1) = \frac{\sqrt{6}\mathbb{M}_3^{(1,-1;a)}(B_{2g}, 1)\mathbb{T}_1^{(b)}(B_{3u})}{4} - \frac{\sqrt{10}\mathbb{M}_3^{(1,-1;a)}(B_{2g}, 2)\mathbb{T}_1^{(b)}(B_{3u})}{4}$$

$$\boxed{\text{z167}} \quad \mathbb{Q}_3^{(1,-1;c)}(B_{1u}, 2) = \frac{\sqrt{10}\mathbb{M}_3^{(1,-1;a)}(B_{2g}, 1)\mathbb{T}_1^{(b)}(B_{3u})}{4} + \frac{\sqrt{6}\mathbb{M}_3^{(1,-1;a)}(B_{2g}, 2)\mathbb{T}_1^{(b)}(B_{3u})}{4}$$

$$\boxed{\text{z168}} \quad \mathbb{Q}_1^{(1,0;c)}(B_{1u}) = \mathbb{T}_2^{(1,0;a)}(B_{2g})\mathbb{T}_1^{(b)}(B_{3u})$$

$$\boxed{\text{z169}} \quad \mathbb{Q}_1^{(1,1;c)}(B_{1u}) = -\mathbb{M}_1^{(1,1;a)}(B_{2g})\mathbb{T}_1^{(b)}(B_{3u})$$

$$\boxed{\text{z217}} \quad \mathbb{Q}_2^{(c)}(B_{2g}) = \mathbb{Q}_2^{(a)}(B_{2g})\mathbb{Q}_0^{(b)}(A_g)$$

$$\boxed{\text{z218}} \quad \mathbb{Q}_2^{(1,-1;c)}(B_{2g}) = \mathbb{Q}_2^{(1,-1;a)}(B_{2g})\mathbb{Q}_0^{(b)}(A_g)$$

$$\boxed{\text{z219}} \quad \mathbb{G}_1^{(1,0;c)}(B_{2g}) = \mathbb{G}_1^{(1,0;a)}(B_{2g})\mathbb{Q}_0^{(b)}(A_g)$$

$$\boxed{\text{z220}} \quad \mathbb{Q}_1^{(c)}(B_{2u}) = \mathbb{M}_1^{(a)}(B_{1g})\mathbb{T}_1^{(b)}(B_{3u})$$

$$\boxed{\text{z221}} \quad \mathbb{Q}_1^{(1,-1;c)}(B_{2u}) = \mathbb{M}_1^{(1,-1;a)}(B_{1g})\mathbb{T}_1^{(b)}(B_{3u})$$

$$\boxed{\text{z222}} \quad \mathbb{Q}_3^{(1,-1;c)}(B_{2u}, 1) = -\frac{\sqrt{6}\mathbb{M}_3^{(1,-1;a)}(B_{1g}, 1)\mathbb{T}_1^{(b)}(B_{3u})}{4} - \frac{\sqrt{10}\mathbb{M}_3^{(1,-1;a)}(B_{1g}, 2)\mathbb{T}_1^{(b)}(B_{3u})}{4}$$

$$\boxed{\text{z266}} \quad \mathbb{Q}_3^{(1,-1;c)}(B_{2u}, 2) = \frac{\sqrt{10}\mathbb{M}_3^{(1,-1;a)}(B_{1g}, 1)\mathbb{T}_1^{(b)}(B_{3u})}{4} - \frac{\sqrt{6}\mathbb{M}_3^{(1,-1;a)}(B_{1g}, 2)\mathbb{T}_1^{(b)}(B_{3u})}{4}$$

$$\boxed{\text{z267}} \quad \mathbb{Q}_1^{(1,0;c)}(B_{2u}) = \mathbb{T}_2^{(1,0;a)}(B_{1g})\mathbb{T}_1^{(b)}(B_{3u})$$

$$\boxed{\text{z268}} \quad \mathbb{Q}_1^{(1,1;c)}(B_{2u}) = \mathbb{M}_1^{(1,1;a)}(B_{1g})\mathbb{T}_1^{(b)}(B_{3u})$$

$$\boxed{\text{z269}} \quad \mathbb{Q}_2^{(c)}(B_{3g}) = \mathbb{Q}_2^{(a)}(B_{3g})\mathbb{Q}_0^{(b)}(A_g)$$

$$\boxed{\text{z270}} \quad \mathbb{Q}_2^{(1,-1;c)}(B_{3g}) = \mathbb{Q}_2^{(1,-1;a)}(B_{3g})\mathbb{Q}_0^{(b)}(A_g)$$

$$\boxed{\text{z271}} \quad \mathbb{G}_1^{(1,0;c)}(B_{3g}) = \mathbb{G}_1^{(1,0;a)}(B_{3g})\mathbb{Q}_0^{(b)}(A_g)$$

$$\boxed{\text{z310}} \quad \mathbb{Q}_3^{(1,-1;c)}(B_{3u}, 2) = \mathbb{M}_3^{(1,-1;a)}(A_g)\mathbb{T}_1^{(b)}(B_{3u})$$

$$\boxed{\text{z311}} \quad \mathbb{Q}_1^{(1,0;c)}(B_{3u}) = -\frac{\mathbb{T}_2^{(1,0;a)}(A_g, 1)\mathbb{T}_1^{(b)}(B_{3u})}{2} + \frac{\sqrt{3}\mathbb{T}_2^{(1,0;a)}(A_g, 2)\mathbb{T}_1^{(b)}(B_{3u})}{2}$$

$$\boxed{\text{z312}} \quad \mathbb{Q}_3^{(1,0;c)}(B_{3u}, 2) = -\frac{\sqrt{3}\mathbb{T}_2^{(1,0;a)}(A_g, 1)\mathbb{T}_1^{(b)}(B_{3u})}{2} - \frac{\mathbb{T}_2^{(1,0;a)}(A_g, 2)\mathbb{T}_1^{(b)}(B_{3u})}{2}$$

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

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

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

\* wyckoff: **1b@1e**

$$\boxed{\text{z18}} \quad \mathbb{Q}_0^{(c)}(A_g) = \mathbb{Q}_0^{(a)}(A_g)\mathbb{Q}_0^{(b)}(A_g)$$

$$\boxed{\text{z170}} \quad \mathbb{G}_0^{(1,-1;c)}(A_u) = \mathbb{M}_1^{(1,-1;a)}(B_{2g})\mathbb{T}_1^{(b)}(B_{2u})$$

$$\boxed{\text{z223}} \quad \mathbb{Q}_1^{(1,-1;c)}(B_{1u}) = \mathbb{M}_1^{(1,-1;a)}(B_{3g})\mathbb{T}_1^{(b)}(B_{2u})$$

$$\boxed{\text{z313}} \quad \mathbb{Q}_1^{(1,-1;c)}(B_{3u}) = -\mathbb{M}_1^{(1,-1;a)}(B_{1g})\mathbb{T}_1^{(b)}(B_{2u})$$

• '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: **1b@1e**

$$\boxed{\text{z19}} \quad \mathbb{Q}_0^{(c)}(A_g) = \mathbb{T}_1^{(a)}(B_{2u})\mathbb{T}_1^{(b)}(B_{2u})$$

$$\boxed{\text{z20}} \quad \mathbb{Q}_2^{(1,-1;c)}(A_g, 1) = \mathbb{M}_2^{(1,-1;a)}(B_{2u})\mathbb{T}_1^{(b)}(B_{2u})$$

$$\boxed{\text{z21}} \quad \mathbb{Q}_0^{(1,0;c)}(A_g) = \mathbb{T}_1^{(1,0;a)}(B_{2u})\mathbb{T}_1^{(b)}(B_{2u})$$

$$\boxed{\text{z63}} \quad \mathbb{G}_2^{(1,-1;c)}(A_u, 1) = \mathbb{G}_2^{(1,-1;a)}(A_u, 1)\mathbb{Q}_0^{(b)}(A_g)$$

$$\boxed{\text{z64}} \quad \mathbb{G}_2^{(1,-1;c)}(A_u, 2) = \mathbb{G}_2^{(1,-1;a)}(A_u, 2)\mathbb{Q}_0^{(b)}(A_g)$$

$$\boxed{\text{z65}} \quad \mathbb{G}_0^{(1,1;c)}(A_u) = \mathbb{G}_0^{(1,1;a)}(A_u)\mathbb{Q}_0^{(b)}(A_g)$$

$$\boxed{\text{z100}} \quad \mathbb{Q}_2^{(c)}(B_{1g}) = \mathbb{T}_1^{(a)}(B_{3u})\mathbb{T}_1^{(b)}(B_{2u})$$

$$\boxed{\text{z101}} \quad \mathbb{Q}_2^{(1,-1;c)}(B_{1g}) = -\mathbb{M}_2^{(1,-1;a)}(B_{3u})\mathbb{T}_1^{(b)}(B_{2u})$$

$$\boxed{\text{z102}} \quad \mathbb{Q}_2^{(1,0;c)}(B_{1g}) = \mathbb{T}_1^{(1,0;a)}(B_{3u})\mathbb{T}_1^{(b)}(B_{2u})$$

$$\boxed{\text{z133}} \quad \mathbb{Q}_1^{(c)}(B_{1u}) = \mathbb{Q}_1^{(a)}(B_{1u})\mathbb{Q}_0^{(b)}(A_g)$$

$$\boxed{\text{z134}} \quad \mathbb{Q}_1^{(1,0;c)}(B_{1u}) = \mathbb{Q}_1^{(1,0;a)}(B_{1u})\mathbb{Q}_0^{(b)}(A_g)$$

$$\boxed{\text{z135}} \quad \mathbb{G}_2^{(1,-1;c)}(B_{1u}) = \mathbb{G}_2^{(1,-1;a)}(B_{1u})\mathbb{Q}_0^{(b)}(A_g)$$

$$\boxed{\text{z171}} \quad \mathbb{Q}_2^{(1,-1;c)}(B_{2g}) = -\frac{\sqrt{3}\mathbb{M}_2^{(1,-1;a)}(A_u, 1)\mathbb{T}_1^{(b)}(B_{2u})}{2} + \frac{\mathbb{M}_2^{(1,-1;a)}(A_u, 2)\mathbb{T}_1^{(b)}(B_{2u})}{2}$$

$$\boxed{\text{z172}} \quad \mathbb{G}_1^{(1,-1;c)}(B_{2g}) = -\frac{\mathbb{M}_2^{(1,-1;a)}(A_u, 1)\mathbb{T}_1^{(b)}(B_{2u})}{2} - \frac{\sqrt{3}\mathbb{M}_2^{(1,-1;a)}(A_u, 2)\mathbb{T}_1^{(b)}(B_{2u})}{2}$$

$$\boxed{\text{z173}} \quad \mathbb{G}_1^{(1,1;c)}(B_{2g}) = \mathbb{M}_0^{(1,1;a)}(A_u)\mathbb{T}_1^{(b)}(B_{2u})$$

$$\boxed{\text{z224}} \quad \mathbb{Q}_1^{(c)}(B_{2u}) = \mathbb{Q}_1^{(a)}(B_{2u})\mathbb{Q}_0^{(b)}(A_g)$$

$$\boxed{\text{z225}} \quad \mathbb{Q}_1^{(1,0;c)}(B_{2u}) = \mathbb{Q}_1^{(1,0;a)}(B_{2u})\mathbb{Q}_0^{(b)}(A_g)$$

$$\boxed{\text{z226}} \quad \mathbb{G}_2^{(1,-1;c)}(B_{2u}) = \mathbb{G}_2^{(1,-1;a)}(B_{2u})\mathbb{Q}_0^{(b)}(A_g)$$

$$\boxed{\text{z272}} \quad \mathbb{Q}_2^{(c)}(B_{3g}) = \mathbb{T}_1^{(a)}(B_{1u})\mathbb{T}_1^{(b)}(B_{2u})$$

$$\boxed{\text{z273}} \quad \mathbb{Q}_2^{(1,-1;c)}(B_{3g}) = \mathbb{M}_2^{(1,-1;a)}(B_{1u})\mathbb{T}_1^{(b)}(B_{2u})$$

$$\boxed{\text{z274}} \quad \mathbb{Q}_2^{(1,0;c)}(B_{3g}) = \mathbb{T}_1^{(1,0;a)}(B_{1u})\mathbb{T}_1^{(b)}(B_{2u})$$

$$\boxed{\text{z314}} \quad \mathbb{Q}_1^{(c)}(B_{3u}) = \mathbb{Q}_1^{(a)}(B_{3u})\mathbb{Q}_0^{(b)}(A_g)$$

$$\boxed{\text{z315}} \quad \mathbb{Q}_1^{(1,0;c)}(B_{3u}) = \mathbb{Q}_1^{(1,0;a)}(B_{3u})\mathbb{Q}_0^{(b)}(A_g)$$

$$\boxed{\text{z316}} \quad \mathbb{G}_2^{(1,-1;c)}(B_{3u}) = \mathbb{G}_2^{(1,-1;a)}(B_{3u})\mathbb{Q}_0^{(b)}(A_g)$$

• '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: **1b@1e**

$$\boxed{\text{z22}} \quad \mathbb{Q}_0^{(c)}(A_g) = \mathbb{Q}_0^{(a)}(A_g)\mathbb{Q}_0^{(b)}(A_g)$$

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

$$\boxed{\text{z24}} \quad \mathbb{Q}_2^{(c)}(A_g, 2) = \mathbb{Q}_2^{(a)}(A_g, 2)\mathbb{Q}_0^{(b)}(A_g)$$

$$\boxed{\text{z25}} \quad \mathbb{Q}_2^{(1,-1;c)}(A_g, 1) = \mathbb{Q}_2^{(1,-1;a)}(A_g, 1)\mathbb{Q}_0^{(b)}(A_g)$$

$$\boxed{\text{z26}} \quad \mathbb{Q}_2^{(1,-1;c)}(A_g, 2) = \mathbb{Q}_2^{(1,-1;a)}(A_g, 2)\mathbb{Q}_0^{(b)}(A_g)$$

$$\boxed{\text{z27}} \quad \mathbb{Q}_0^{(1,1;c)}(A_g) = \mathbb{Q}_0^{(1,1;a)}(A_g)\mathbb{Q}_0^{(b)}(A_g)$$

$$\boxed{\text{z66}} \quad \mathbb{Q}_3^{(1,-1;c)}(A_u) = -\mathbb{M}_3^{(1,-1;a)}(B_{2g}, 2)\mathbb{T}_1^{(b)}(B_{2u})$$

$$\boxed{\text{z67}} \quad \mathbb{Q}_3^{(1,0;c)}(A_u) = \mathbb{T}_2^{(1,0;a)}(B_{2g})\mathbb{T}_1^{(b)}(B_{2u})$$

$$\boxed{\text{z68}} \quad \mathbb{G}_0^{(c)}(A_u) = \mathbb{M}_1^{(a)}(B_{2g})\mathbb{T}_1^{(b)}(B_{2u})$$

$$\boxed{\text{z103}} \quad \mathbb{G}_0^{(1,-1;c)}(A_u) = \mathbb{M}_1^{(1,-1;a)}(B_{2g})\mathbb{T}_1^{(b)}(B_{2u})$$

$$\boxed{\text{z104}} \quad \mathbb{G}_2^{(1,-1;c)}(A_u, 1) = -\mathbb{M}_3^{(1,-1;a)}(B_{2g}, 1)\mathbb{T}_1^{(b)}(B_{2u})$$

$$\boxed{\text{z105}} \quad \mathbb{G}_0^{(1,1;c)}(A_u) = \mathbb{M}_1^{(1,1;a)}(B_{2g})\mathbb{T}_1^{(b)}(B_{2u})$$

$$\boxed{\text{z136}} \quad \mathbb{Q}_2^{(c)}(B_{1g}) = \mathbb{Q}_2^{(a)}(B_{1g})\mathbb{Q}_0^{(b)}(A_g)$$

$$\boxed{\text{z137}} \quad \mathbb{Q}_2^{(1,-1;c)}(B_{1g}) = \mathbb{Q}_2^{(1,-1;a)}(B_{1g})\mathbb{Q}_0^{(b)}(A_g)$$

$$\boxed{\text{z138}} \quad \mathbb{G}_1^{(1,0;c)}(B_{1g}) = \mathbb{G}_1^{(1,0;a)}(B_{1g})\mathbb{Q}_0^{(b)}(A_g)$$

$$\boxed{\text{z174}} \quad \mathbb{Q}_1^{(c)}(B_{1u}) = \mathbb{M}_1^{(a)}(B_{3g})\mathbb{T}_1^{(b)}(B_{2u})$$

$$\boxed{\text{z175}} \quad \mathbb{Q}_1^{(1,-1;c)}(B_{1u}) = \mathbb{M}_1^{(1,-1;a)}(B_{3g})\mathbb{T}_1^{(b)}(B_{2u})$$

$$\boxed{\text{z176}} \quad \mathbb{Q}_3^{(1,-1;c)}(B_{1u}, 1) = -\frac{\sqrt{6}\mathbb{M}_3^{(1,-1;a)}(B_{3g}, 1)\mathbb{T}_1^{(b)}(B_{2u})}{4} - \frac{\sqrt{10}\mathbb{M}_3^{(1,-1;a)}(B_{3g}, 2)\mathbb{T}_1^{(b)}(B_{2u})}{4}$$

$$\boxed{\text{z177}} \quad \mathbb{Q}_3^{(1,-1;c)}(B_{1u}, 2) = \frac{\sqrt{10}\mathbb{M}_3^{(1,-1;a)}(B_{3g}, 1)\mathbb{T}_1^{(b)}(B_{2u})}{4} - \frac{\sqrt{6}\mathbb{M}_3^{(1,-1;a)}(B_{3g}, 2)\mathbb{T}_1^{(b)}(B_{2u})}{4}$$

$$\boxed{\text{z178}} \quad \mathbb{Q}_1^{(1,0;c)}(B_{1u}) = \mathbb{T}_2^{(1,0;a)}(B_{3g})\mathbb{T}_1^{(b)}(B_{2u})$$

$$\boxed{\text{z179}} \quad \mathbb{Q}_1^{(1,1;c)}(B_{1u}) = \mathbb{M}_1^{(1,1;a)}(B_{3g})\mathbb{T}_1^{(b)}(B_{2u})$$

$$\boxed{\text{z227}} \quad \mathbb{Q}_2^{(c)}(B_{2g}) = \mathbb{Q}_2^{(a)}(B_{2g})\mathbb{Q}_0^{(b)}(A_g)$$

$$\boxed{\text{z228}} \quad \mathbb{Q}_2^{(1,-1;c)}(B_{2g}) = \mathbb{Q}_2^{(1,-1;a)}(B_{2g})\mathbb{Q}_0^{(b)}(A_g)$$

$$\boxed{\text{z229}} \quad \mathbb{G}_1^{(1,0;c)}(B_{2g}) = \mathbb{G}_1^{(1,0;a)}(B_{2g})\mathbb{Q}_0^{(b)}(A_g)$$

$$\boxed{\text{z230}} \quad \mathbb{Q}_3^{(1,-1;c)}(B_{2u}, 2) = \mathbb{M}_3^{(1,-1;a)}(A_g)\mathbb{T}_1^{(b)}(B_{2u})$$

$$\boxed{\text{z231}} \quad \mathbb{Q}_1^{(1,0;c)}(B_{2u}) = -\frac{\mathbb{T}_2^{(1,0;a)}(A_g, 1)\mathbb{T}_1^{(b)}(B_{2u})}{2} - \frac{\sqrt{3}\mathbb{T}_2^{(1,0;a)}(A_g, 2)\mathbb{T}_1^{(b)}(B_{2u})}{2}$$

$$\boxed{\text{z232}} \quad \mathbb{Q}_3^{(1,0;c)}(B_{2u}, 2) = \frac{\sqrt{3}\mathbb{T}_2^{(1,0;a)}(A_g, 1)\mathbb{T}_1^{(b)}(B_{2u})}{2} - \frac{\mathbb{T}_2^{(1,0;a)}(A_g, 2)\mathbb{T}_1^{(b)}(B_{2u})}{2}$$

$$\boxed{\text{z275}} \quad \mathbb{Q}_2^{(c)}(B_{3g}) = \mathbb{Q}_2^{(a)}(B_{3g})\mathbb{Q}_0^{(b)}(A_g)$$

$$\boxed{\text{z276}} \quad \mathbb{Q}_2^{(1,-1;c)}(B_{3g}) = \mathbb{Q}_2^{(1,-1;a)}(B_{3g})\mathbb{Q}_0^{(b)}(A_g)$$

$$\boxed{\text{z277}} \quad \mathbb{G}_1^{(1,0;c)}(B_{3g}) = \mathbb{G}_1^{(1,0;a)}(B_{3g})\mathbb{Q}_0^{(b)}(A_g)$$

$$\boxed{\text{z317}} \quad \mathbb{Q}_1^{(c)}(B_{3u}) = -\mathbb{M}_1^{(a)}(B_{1g})\mathbb{T}_1^{(b)}(B_{2u})$$

$$\boxed{\text{z318}} \quad \mathbb{Q}_1^{(1,-1;c)}(B_{3u}) = -\mathbb{M}_1^{(1,-1;a)}(B_{1g})\mathbb{T}_1^{(b)}(B_{2u})$$

$$\boxed{\text{z319}} \quad \mathbb{Q}_3^{(1,-1;c)}(B_{3u}, 1) = \frac{\sqrt{6}\mathbb{M}_3^{(1,-1;a)}(B_{1g}, 1)\mathbb{T}_1^{(b)}(B_{2u})}{4} - \frac{\sqrt{10}\mathbb{M}_3^{(1,-1;a)}(B_{1g}, 2)\mathbb{T}_1^{(b)}(B_{2u})}{4}$$

$$\boxed{\text{z320}} \quad \mathbb{Q}_3^{(1,-1;c)}(B_{3u}, 2) = \frac{\sqrt{10}\mathbb{M}_3^{(1,-1;a)}(B_{1g}, 1)\mathbb{T}_1^{(b)}(B_{2u})}{4} + \frac{\sqrt{6}\mathbb{M}_3^{(1,-1;a)}(B_{1g}, 2)\mathbb{T}_1^{(b)}(B_{2u})}{4}$$

$$\boxed{\text{z321}} \quad \mathbb{Q}_1^{(1,0;c)}(B_{3u}) = \mathbb{T}_2^{(1,0;a)}(B_{1g})\mathbb{T}_1^{(b)}(B_{2u})$$

$$\boxed{\text{z322}} \quad \mathbb{Q}_1^{(1,1;c)}(B_{3u}) = -\mathbb{M}_1^{(1,1;a)}(B_{1g})\mathbb{T}_1^{(b)}(B_{2u})$$

• 'A'-'A' bond-cluster : **A;A\_003\_1**

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

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

\* wyckoff: **1a@1c**

$$\boxed{\text{z28}} \quad \mathbb{Q}_0^{(c)}(A_g) = \mathbb{Q}_0^{(a)}(A_g)\mathbb{Q}_0^{(b)}(A_g)$$

$$\boxed{\text{z180}} \quad \mathbb{G}_0^{(1,-1;c)}(A_u) = \mathbb{M}_1^{(1,-1;a)}(B_{1g})\mathbb{T}_1^{(b)}(B_{1u})$$

$$\boxed{\text{z278}} \quad \mathbb{Q}_1^{(1,-1;c)}(B_{2u}) = -\mathbb{M}_1^{(1,-1;a)}(B_{3g})\mathbb{T}_1^{(b)}(B_{1u})$$

$$\boxed{\text{z323}} \quad \mathbb{Q}_1^{(1,-1;c)}(B_{3u}) = \mathbb{M}_1^{(1,-1;a)}(B_{2g})\mathbb{T}_1^{(b)}(B_{1u})$$

• '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@1c**

$$\boxed{\text{z29}} \quad \mathbb{Q}_0^{(c)}(A_g) = \mathbb{T}_1^{(a)}(B_{1u})\mathbb{T}_1^{(b)}(B_{1u})$$

$$\boxed{\text{z30}} \quad \mathbb{Q}_2^{(1,-1;c)}(A_g, 2) = \mathbb{M}_2^{(1,-1;a)}(B_{1u})\mathbb{T}_1^{(b)}(B_{1u})$$

$$\boxed{\text{z31}} \quad \mathbb{Q}_0^{(1,0;c)}(A_g) = \mathbb{T}_1^{(1,0;a)}(B_{1u})\mathbb{T}_1^{(b)}(B_{1u})$$

$$\boxed{\text{z69}} \quad \mathbb{G}_2^{(1,-1;c)}(A_u, 1) = \mathbb{G}_2^{(1,-1;a)}(A_u, 1)\mathbb{Q}_0^{(b)}(A_g)$$

$$\boxed{\text{z70}} \quad \mathbb{G}_2^{(1,-1;c)}(A_u, 2) = \mathbb{G}_2^{(1,-1;a)}(A_u, 2)\mathbb{Q}_0^{(b)}(A_g)$$

$$\boxed{\text{z71}} \quad \mathbb{G}_0^{(1,1;c)}(A_u) = \mathbb{G}_0^{(1,1;a)}(A_u)\mathbb{Q}_0^{(b)}(A_g)$$

$$\boxed{\text{z106}} \quad \mathbb{Q}_2^{(1,-1;c)}(B_{1g}) = -\mathbb{M}_2^{(1,-1;a)}(A_u, 2)\mathbb{T}_1^{(b)}(B_{1u})$$

$$\boxed{\text{z107}} \quad \mathbb{G}_1^{(1,-1;c)}(B_{1g}) = \mathbb{M}_2^{(1,-1;a)}(A_u, 1)\mathbb{T}_1^{(b)}(B_{1u})$$

$$\boxed{\text{z108}} \quad \mathbb{G}_1^{(1,1;c)}(B_{1g}) = \mathbb{M}_0^{(1,1;a)}(A_u)\mathbb{T}_1^{(b)}(B_{1u})$$

$$\boxed{\text{z139}} \quad \mathbb{Q}_1^{(c)}(B_{1u}) = \mathbb{Q}_1^{(a)}(B_{1u})\mathbb{Q}_0^{(b)}(A_g)$$

$$\boxed{\text{z140}} \quad \mathbb{Q}_1^{(1,0;c)}(B_{1u}) = \mathbb{Q}_1^{(1,0;a)}(B_{1u})\mathbb{Q}_0^{(b)}(A_g)$$

$$\boxed{\text{z141}} \quad \mathbb{G}_2^{(1,-1;c)}(B_{1u}) = \mathbb{G}_2^{(1,-1;a)}(B_{1u})\mathbb{Q}_0^{(b)}(A_g)$$

$$\boxed{\text{z181}} \quad \mathbb{Q}_2^{(c)}(B_{2g}) = \mathbb{T}_1^{(a)}(B_{3u})\mathbb{T}_1^{(b)}(B_{1u})$$

$$\boxed{\text{z182}} \quad \mathbb{Q}_2^{(1,-1;c)}(B_{2g}) = \mathbb{M}_2^{(1,-1;a)}(B_{3u})\mathbb{T}_1^{(b)}(B_{1u})$$

$$\boxed{\text{z183}} \quad \mathbb{Q}_2^{(1,0;c)}(B_{2g}) = \mathbb{T}_1^{(1,0;a)}(B_{3u})\mathbb{T}_1^{(b)}(B_{1u})$$

$$\boxed{\text{z233}} \quad \mathbb{Q}_1^{(c)}(B_{2u}) = \mathbb{Q}_1^{(a)}(B_{2u})\mathbb{Q}_0^{(b)}(A_g)$$

$$\boxed{\text{z234}} \quad \mathbb{Q}_1^{(1,0;c)}(B_{2u}) = \mathbb{Q}_1^{(1,0;a)}(B_{2u})\mathbb{Q}_0^{(b)}(A_g)$$

$$\boxed{\text{z235}} \quad \mathbb{G}_2^{(1,-1;c)}(B_{2u}) = \mathbb{G}_2^{(1,-1;a)}(B_{2u})\mathbb{Q}_0^{(b)}(A_g)$$

$$\boxed{\text{z279}} \quad \mathbb{Q}_2^{(c)}(B_{3g}) = \mathbb{T}_1^{(a)}(B_{2u})\mathbb{T}_1^{(b)}(B_{1u})$$

$$\boxed{\text{z280}} \quad \mathbb{Q}_2^{(1,-1;c)}(B_{3g}) = -\mathbb{M}_2^{(1,-1;a)}(B_{2u})\mathbb{T}_1^{(b)}(B_{1u})$$

$$\boxed{\text{z281}} \quad \mathbb{Q}_2^{(1,0;c)}(B_{3g}) = \mathbb{T}_1^{(1,0;a)}(B_{2u})\mathbb{T}_1^{(b)}(B_{1u})$$

$$\boxed{\text{z324}} \quad \mathbb{Q}_1^{(c)}(B_{3u}) = \mathbb{Q}_1^{(a)}(B_{3u})\mathbb{Q}_0^{(b)}(A_g)$$

$$\boxed{\text{z325}} \quad \mathbb{Q}_1^{(1,0;c)}(B_{3u}) = \mathbb{Q}_1^{(1,0;a)}(B_{3u})\mathbb{Q}_0^{(b)}(A_g)$$

$$\boxed{\text{z326}} \quad \mathbb{G}_2^{(1,-1;c)}(B_{3u}) = \mathbb{G}_2^{(1,-1;a)}(B_{3u})\mathbb{Q}_0^{(b)}(A_g)$$

• '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@1c**

$$\boxed{\text{z32}} \quad \mathbb{Q}_0^{(c)}(A_g) = \mathbb{Q}_0^{(a)}(A_g)\mathbb{Q}_0^{(b)}(A_g)$$

$$\boxed{\text{z33}} \quad \mathbb{Q}_2^{(c)}(A_g, 1) = \mathbb{Q}_2^{(a)}(A_g, 1)\mathbb{Q}_0^{(b)}(A_g)$$

$$\boxed{\text{z34}} \quad \mathbb{Q}_2^{(c)}(A_g, 2) = \mathbb{Q}_2^{(a)}(A_g, 2)\mathbb{Q}_0^{(b)}(A_g)$$

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

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

$$\boxed{\text{z37}} \quad \mathbb{Q}_0^{(1,1;c)}(A_g) = \mathbb{Q}_0^{(1,1;a)}(A_g)\mathbb{Q}_0^{(b)}(A_g)$$

$$\boxed{\text{z72}} \quad \mathbb{Q}_3^{(1,-1;c)}(A_u) = -\mathbb{M}_3^{(1,-1;a)}(B_{1g}, 2)\mathbb{T}_1^{(b)}(B_{1u})$$

$$\boxed{\text{z73}} \quad \mathbb{Q}_3^{(1,0;c)}(A_u) = \mathbb{T}_2^{(1,0;a)}(B_{1g})\mathbb{T}_1^{(b)}(B_{1u})$$

$$\boxed{\text{z74}} \quad \mathbb{G}_0^{(c)}(A_u) = \mathbb{M}_1^{(a)}(B_{1g})\mathbb{T}_1^{(b)}(B_{1u})$$

$$\boxed{\text{z109}} \quad \mathbb{G}_0^{(1,-1;c)}(A_u) = \mathbb{M}_1^{(1,-1;a)}(B_{1g})\mathbb{T}_1^{(b)}(B_{1u})$$

$$\boxed{\text{z110}} \quad \mathbb{G}_2^{(1,-1;c)}(A_u, 1) = \mathbb{M}_3^{(1,-1;a)}(B_{1g}, 1)\mathbb{T}_1^{(b)}(B_{1u})$$

$$\boxed{\text{z111}} \quad \mathbb{G}_0^{(1,1;c)}(A_u) = \mathbb{M}_1^{(1,1;a)}(B_{1g})\mathbb{T}_1^{(b)}(B_{1u})$$

$$\boxed{\text{z142}} \quad \mathbb{Q}_2^{(c)}(B_{1g}) = \mathbb{Q}_2^{(a)}(B_{1g})\mathbb{Q}_0^{(b)}(A_g)$$

$$\boxed{\text{z143}} \quad \mathbb{Q}_2^{(1,-1;c)}(B_{1g}) = \mathbb{Q}_2^{(1,-1;a)}(B_{1g})\mathbb{Q}_0^{(b)}(A_g)$$

$$\boxed{\text{z144}} \quad \mathbb{G}_1^{(1,0;c)}(B_{1g}) = \mathbb{G}_1^{(1,0;a)}(B_{1g})\mathbb{Q}_0^{(b)}(A_g)$$

$$\boxed{\text{z184}} \quad \mathbb{Q}_3^{(1,-1;c)}(B_{1u}, 2) = \mathbb{M}_3^{(1,-1;a)}(A_g)\mathbb{T}_1^{(b)}(B_{1u})$$

$$\boxed{\text{z185}} \quad \mathbb{Q}_1^{(1,0;c)}(B_{1u}) = \mathbb{T}_2^{(1,0;a)}(A_g, 1)\mathbb{T}_1^{(b)}(B_{1u})$$

$$\boxed{\text{z186}} \quad \mathbb{Q}_3^{(1,0;c)}(B_{1u}, 2) = \mathbb{T}_2^{(1,0;a)}(A_g, 2)\mathbb{T}_1^{(b)}(B_{1u})$$

$$\boxed{\text{z187}} \quad \mathbb{Q}_2^{(c)}(B_{2g}) = \mathbb{Q}_2^{(a)}(B_{2g})\mathbb{Q}_0^{(b)}(A_g)$$

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

$$\boxed{\text{z189}} \quad \mathbb{G}_1^{(1,0;c)}(B_{2g}) = \mathbb{G}_1^{(1,0;a)}(B_{2g})\mathbb{Q}_0^{(b)}(A_g)$$

$$\boxed{\text{z236}} \quad \mathbb{Q}_1^{(c)}(B_{2u}) = -\mathbb{M}_1^{(a)}(B_{3g})\mathbb{T}_1^{(b)}(B_{1u})$$

$$\boxed{\text{z237}} \quad \mathbb{Q}_1^{(1,-1;c)}(B_{2u}) = -\mathbb{M}_1^{(1,-1;a)}(B_{3g})\mathbb{T}_1^{(b)}(B_{1u})$$

$$\boxed{\text{z238}} \quad \mathbb{Q}_3^{(1,-1;c)}(B_{2u}, 1) = \frac{\sqrt{6}\mathbb{M}_3^{(1,-1;a)}(B_{3g}, 1)\mathbb{T}_1^{(b)}(B_{1u})}{4} - \frac{\sqrt{10}\mathbb{M}_3^{(1,-1;a)}(B_{3g}, 2)\mathbb{T}_1^{(b)}(B_{1u})}{4}$$

$$\boxed{\text{z282}} \quad \mathbb{Q}_3^{(1,-1;c)}(B_{2u}, 2) = \frac{\sqrt{10}\mathbb{M}_3^{(1,-1;a)}(B_{3g}, 1)\mathbb{T}_1^{(b)}(B_{1u})}{4} + \frac{\sqrt{6}\mathbb{M}_3^{(1,-1;a)}(B_{3g}, 2)\mathbb{T}_1^{(b)}(B_{1u})}{4}$$

$$\boxed{\text{z283}} \quad \mathbb{Q}_1^{(1,0;c)}(B_{2u}) = \mathbb{T}_2^{(1,0;a)}(B_{3g})\mathbb{T}_1^{(b)}(B_{1u})$$

$$\boxed{\text{z284}} \quad \mathbb{Q}_1^{(1,1;c)}(B_{2u}) = -\mathbb{M}_1^{(1,1;a)}(B_{3g})\mathbb{T}_1^{(b)}(B_{1u})$$

$$\boxed{\text{z285}} \quad \mathbb{Q}_2^{(c)}(B_{3g}) = \mathbb{Q}_2^{(a)}(B_{3g})\mathbb{Q}_0^{(b)}(A_g)$$

$$\boxed{\text{z286}} \quad \mathbb{Q}_2^{(1,-1;c)}(B_{3g}) = \mathbb{Q}_2^{(1,-1;a)}(B_{3g})\mathbb{Q}_0^{(b)}(A_g)$$

$$\boxed{\text{z287}} \quad \mathbb{G}_1^{(1,0;c)}(B_{3g}) = \mathbb{G}_1^{(1,0;a)}(B_{3g})\mathbb{Q}_0^{(b)}(A_g)$$

$$\boxed{\text{z327}} \quad \mathbb{Q}_1^{(c)}(B_{3u}) = \mathbb{M}_1^{(a)}(B_{2g})\mathbb{T}_1^{(b)}(B_{1u})$$

$$\boxed{\text{z328}} \quad \mathbb{Q}_1^{(1,-1;c)}(B_{3u}) = \mathbb{M}_1^{(1,-1;a)}(B_{2g})\mathbb{T}_1^{(b)}(B_{1u})$$

$$\boxed{\text{z329}} \quad \mathbb{Q}_3^{(1,-1;c)}(B_{3u}, 1) = -\frac{\sqrt{6}\mathbb{M}_3^{(1,-1;a)}(B_{2g}, 1)\mathbb{T}_1^{(b)}(B_{1u})}{4} - \frac{\sqrt{10}\mathbb{M}_3^{(1,-1;a)}(B_{2g}, 2)\mathbb{T}_1^{(b)}(B_{1u})}{4}$$

$$\boxed{\text{z330}} \quad \mathbb{Q}_3^{(1,-1;c)}(B_{3u}, 2) = \frac{\sqrt{10}\mathbb{M}_3^{(1,-1;a)}(B_{2g}, 1)\mathbb{T}_1^{(b)}(B_{1u})}{4} - \frac{\sqrt{6}\mathbb{M}_3^{(1,-1;a)}(B_{2g}, 2)\mathbb{T}_1^{(b)}(B_{1u})}{4}$$

$$\boxed{\text{z331}} \quad \mathbb{Q}_1^{(1,0;c)}(B_{3u}) = \mathbb{T}_2^{(1,0;a)}(B_{2g})\mathbb{T}_1^{(b)}(B_{1u})$$

$$\boxed{\text{z332}} \quad \mathbb{Q}_1^{(1,1;c)}(B_{3u}) = \mathbb{M}_1^{(1,1;a)}(B_{2g})\mathbb{T}_1^{(b)}(B_{1u})$$

• 'A'-'A' bond-cluster : **A;A\_004\_1**

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

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

\* wyckoff: **2d01f**

$$\boxed{\text{z38}} \quad \mathbb{Q}_0^{(c)}(A_g) = \mathbb{Q}_0^{(a)}(A_g)\mathbb{Q}_0^{(b)}(A_g)$$

$$\boxed{\text{z75}} \quad \mathbb{G}_0^{(1,-1;c)}(A_u) = \frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(B_{2g})\mathbb{T}_1^{(b)}(B_{2u})}{2} + \frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(B_{3g})\mathbb{T}_1^{(b)}(B_{3u})}{2}$$

$$\boxed{\text{z190}} \quad \mathbb{G}_2^{(1,-1;c)}(A_u, 2) = -\frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(B_{2g})\mathbb{T}_1^{(b)}(B_{2u})}{2} + \frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(B_{3g})\mathbb{T}_1^{(b)}(B_{3u})}{2}$$

$$\boxed{\text{z191}} \quad \mathbb{Q}_2^{(c)}(B_{1g}) = \mathbb{Q}_0^{(a)}(A_g)\mathbb{Q}_2^{(b)}(B_{1g})$$

$$\boxed{\text{z239}} \quad \mathbb{Q}_1^{(1,-1;c)}(B_{1u}) = -\frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(B_{2g})\mathbb{T}_1^{(b)}(B_{3u})}{2} + \frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(B_{3g})\mathbb{T}_1^{(b)}(B_{2u})}{2}$$

$$\boxed{\text{z240}} \quad \mathbb{G}_2^{(1,-1;c)}(B_{1u}) = \frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(B_{2g})\mathbb{T}_1^{(b)}(B_{3u})}{2} + \frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(B_{3g})\mathbb{T}_1^{(b)}(B_{2u})}{2}$$

$$\boxed{\text{z288}} \quad \mathbb{Q}_1^{(1,-1;c)}(B_{2u}) = \mathbb{M}_1^{(1,-1;a)}(B_{1g})\mathbb{T}_1^{(b)}(B_{3u})$$

$$\boxed{\text{z333}} \quad \mathbb{Q}_1^{(1,-1;c)}(B_{3u}) = -\mathbb{M}_1^{(1,-1;a)}(B_{1g})\mathbb{T}_1^{(b)}(B_{2u})$$

• '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: 2d01f

$$\boxed{\text{z39}} \quad \mathbb{Q}_0^{(c)}(A_g) = \frac{\sqrt{2}\mathbb{T}_1^{(a)}(B_{2u})\mathbb{T}_1^{(b)}(B_{2u})}{2} + \frac{\sqrt{2}\mathbb{T}_1^{(a)}(B_{3u})\mathbb{T}_1^{(b)}(B_{3u})}{2}$$

$$\boxed{\text{z40}} \quad \mathbb{Q}_2^{(c)}(A_g, 2) = -\frac{\sqrt{2}\mathbb{T}_1^{(a)}(B_{2u})\mathbb{T}_1^{(b)}(B_{2u})}{2} + \frac{\sqrt{2}\mathbb{T}_1^{(a)}(B_{3u})\mathbb{T}_1^{(b)}(B_{3u})}{2}$$

$$\boxed{\text{z41}} \quad \mathbb{Q}_2^{(1,-1;c)}(A_g, 1) = \frac{\sqrt{2}\mathbb{M}_2^{(1,-1;a)}(B_{2u})\mathbb{T}_1^{(b)}(B_{2u})}{2} - \frac{\sqrt{2}\mathbb{M}_2^{(1,-1;a)}(B_{3u})\mathbb{T}_1^{(b)}(B_{3u})}{2}$$

$$\boxed{\text{z42}} \quad \mathbb{Q}_2^{(1,-1;c)}(A_g, 2) = -\frac{\sqrt{2}\mathbb{M}_2^{(1,-1;a)}(B_{2u})\mathbb{T}_1^{(b)}(B_{2u})}{2} - \frac{\sqrt{2}\mathbb{M}_2^{(1,-1;a)}(B_{3u})\mathbb{T}_1^{(b)}(B_{3u})}{2}$$

$$\boxed{\text{z43}} \quad \mathbb{Q}_0^{(1,0;c)}(A_g) = \frac{\sqrt{2}\mathbb{T}_1^{(1,0;a)}(B_{2u})\mathbb{T}_1^{(b)}(B_{2u})}{2} + \frac{\sqrt{2}\mathbb{T}_1^{(1,0;a)}(B_{3u})\mathbb{T}_1^{(b)}(B_{3u})}{2}$$

$$\boxed{\text{z44}} \quad \mathbb{Q}_2^{(1,0;c)}(A_g, 2) = -\frac{\sqrt{2}\mathbb{T}_1^{(1,0;a)}(B_{2u})\mathbb{T}_1^{(b)}(B_{2u})}{2} + \frac{\sqrt{2}\mathbb{T}_1^{(1,0;a)}(B_{3u})\mathbb{T}_1^{(b)}(B_{3u})}{2}$$

$$\boxed{\text{z76}} \quad \mathbb{Q}_3^{(c)}(A_u) = \mathbb{Q}_1^{(a)}(B_{1u})\mathbb{Q}_2^{(b)}(B_{1g})$$

$$\boxed{\text{z77}} \quad \mathbb{Q}_3^{(1,0;c)}(A_u) = \mathbb{Q}_1^{(1,0;a)}(B_{1u})\mathbb{Q}_2^{(b)}(B_{1g})$$

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

$$\boxed{\text{z79}} \quad \mathbb{G}_2^{(1,-1;c)}(A_u, 1) = \mathbb{G}_2^{(1,-1;a)}(A_u, 1)\mathbb{Q}_0^{(b)}(A_g)$$

$$\boxed{\text{z80}} \quad \mathbb{G}_2^{(1,-1;c)}(A_u, 2) = \mathbb{G}_2^{(1,-1;a)}(A_u, 2)\mathbb{Q}_0^{(b)}(A_g)$$

$$\boxed{\text{z81}} \quad \mathbb{G}_0^{(1,1;c)}(A_u) = \mathbb{G}_0^{(1,1;a)}(A_u)\mathbb{Q}_0^{(b)}(A_g)$$

$$\boxed{\text{z112}} \quad \mathbb{Q}_2^{(c)}(B_{1g}) = \frac{\sqrt{2}\mathbb{T}_1^{(a)}(B_{2u})\mathbb{T}_1^{(b)}(B_{3u})}{2} + \frac{\sqrt{2}\mathbb{T}_1^{(a)}(B_{3u})\mathbb{T}_1^{(b)}(B_{2u})}{2}$$

$$\boxed{\text{z113}} \quad \mathbb{Q}_2^{(1,-1;c)}(B_{1g}) = \frac{\sqrt{2}\mathbb{M}_2^{(1,-1;a)}(B_{2u})\mathbb{T}_1^{(b)}(B_{3u})}{2} - \frac{\sqrt{2}\mathbb{M}_2^{(1,-1;a)}(B_{3u})\mathbb{T}_1^{(b)}(B_{2u})}{2}$$

$$\boxed{\text{z114}} \quad \mathbb{Q}_2^{(1,0;c)}(B_{1g}) = \frac{\sqrt{2}\mathbb{T}_1^{(1,0;a)}(B_{2u})\mathbb{T}_1^{(b)}(B_{3u})}{2} + \frac{\sqrt{2}\mathbb{T}_1^{(1,0;a)}(B_{3u})\mathbb{T}_1^{(b)}(B_{2u})}{2}$$

$$\boxed{\text{z115}} \quad \mathbb{G}_1^{(c)}(B_{1g}) = -\frac{\sqrt{2}\mathbb{T}_1^{(a)}(B_{2u})\mathbb{T}_1^{(b)}(B_{3u})}{2} + \frac{\sqrt{2}\mathbb{T}_1^{(a)}(B_{3u})\mathbb{T}_1^{(b)}(B_{2u})}{2}$$

$$\boxed{\text{z116}} \quad \mathbb{G}_1^{(1,-1;c)}(B_{1g}) = \frac{\sqrt{2}\mathbb{M}_2^{(1,-1;a)}(B_{2u})\mathbb{T}_1^{(b)}(B_{3u})}{2} + \frac{\sqrt{2}\mathbb{M}_2^{(1,-1;a)}(B_{3u})\mathbb{T}_1^{(b)}(B_{2u})}{2}$$

$$\boxed{\text{z117}} \quad \mathbb{G}_1^{(1,0;c)}(B_{1g}) = -\frac{\sqrt{2}\mathbb{T}_1^{(1,0;a)}(B_{2u})\mathbb{T}_1^{(b)}(B_{3u})}{2} + \frac{\sqrt{2}\mathbb{T}_1^{(1,0;a)}(B_{3u})\mathbb{T}_1^{(b)}(B_{2u})}{2}$$

$$\boxed{\text{z145}} \quad \mathbb{Q}_1^{(c)}(B_{1u}) = \mathbb{Q}_1^{(a)}(B_{1u})\mathbb{Q}_0^{(b)}(A_g)$$

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

$$\boxed{\text{z147}} \quad \mathbb{Q}_3^{(1,-1;c)}(B_{1u}, 2) = -\mathbb{G}_2^{(1,-1;a)}(A_u, 1)\mathbb{Q}_2^{(b)}(B_{1g})$$

$$\boxed{\text{z148}} \quad \mathbb{Q}_1^{(1,0;c)}(B_{1u}) = \mathbb{Q}_1^{(1,0;a)}(B_{1u})\mathbb{Q}_0^{(b)}(A_g)$$

$$\boxed{\text{z149}} \quad \mathbb{G}_2^{(1,-1;c)}(B_{1u}) = \mathbb{G}_2^{(1,-1;a)}(B_{1u})\mathbb{Q}_0^{(b)}(A_g)$$

$$\boxed{\text{z150}} \quad \mathbb{G}_2^{(1,1;c)}(B_{1u}) = \mathbb{G}_0^{(1,1;a)}(A_u)\mathbb{Q}_2^{(b)}(B_{1g})$$

$$\boxed{\text{z192}} \quad \mathbb{Q}_2^{(c)}(B_{2g}) = \mathbb{T}_1^{(a)}(B_{1u})\mathbb{T}_1^{(b)}(B_{3u})$$

$$\boxed{\text{z193}} \quad \mathbb{Q}_2^{(1,-1;c)}(B_{2g}) = -\frac{\sqrt{15}\mathbb{M}_2^{(1,-1;a)}(A_u, 1)\mathbb{T}_1^{(b)}(B_{2u})}{5} + \frac{\sqrt{5}\mathbb{M}_2^{(1,-1;a)}(A_u, 2)\mathbb{T}_1^{(b)}(B_{2u})}{5} - \frac{\sqrt{5}\mathbb{M}_2^{(1,-1;a)}(B_{1u})\mathbb{T}_1^{(b)}(B_{3u})}{5}$$

$$\boxed{\text{z194}} \quad \mathbb{Q}_2^{(1,0;c)}(B_{2g}) = \mathbb{T}_1^{(1,0;a)}(B_{1u})\mathbb{T}_1^{(b)}(B_{3u})$$

$$\boxed{\text{z195}} \quad \mathbb{G}_1^{(1,-1;c)}(B_{2g}) = -\frac{\sqrt{10}\mathbb{M}_2^{(1,-1;a)}(A_u, 1)\mathbb{T}_1^{(b)}(B_{2u})}{5} - \frac{\sqrt{30}\mathbb{M}_2^{(1,-1;a)}(A_u, 2)\mathbb{T}_1^{(b)}(B_{2u})}{10} + \frac{\sqrt{30}\mathbb{M}_2^{(1,-1;a)}(B_{1u})\mathbb{T}_1^{(b)}(B_{3u})}{10}$$

$$\boxed{\text{z196}} \quad \mathbb{G}_3^{(1,-1;c)}(B_{2g}, 1) = -\frac{\sqrt{2}\mathbb{M}_2^{(1,-1;a)}(A_u, 2)\mathbb{T}_1^{(b)}(B_{2u})}{2} - \frac{\sqrt{2}\mathbb{M}_2^{(1,-1;a)}(B_{1u})\mathbb{T}_1^{(b)}(B_{3u})}{2}$$

$$\boxed{\text{z197}} \quad \mathbb{G}_1^{(1,1;c)}(B_{2g}) = \mathbb{M}_0^{(1,1;a)}(A_u)\mathbb{T}_1^{(b)}(B_{2u})$$

$$\boxed{\text{z241}} \quad \mathbb{Q}_1^{(c)}(B_{2u}, a) = \mathbb{Q}_1^{(a)}(B_{2u})\mathbb{Q}_0^{(b)}(A_g)$$

$$\boxed{\text{z242}} \quad \mathbb{Q}_1^{(c)}(B_{2u}, b) = \mathbb{Q}_1^{(a)}(B_{3u})\mathbb{Q}_2^{(b)}(B_{1g})$$

$$\boxed{\text{z243}} \quad \mathbb{Q}_1^{(1,-1;c)}(B_{2u}) = \mathbb{G}_2^{(1,-1;a)}(B_{3u})\mathbb{Q}_2^{(b)}(B_{1g})$$

$$\boxed{\text{z244}} \quad \mathbb{Q}_1^{(1,0;c)}(B_{2u}, a) = \mathbb{Q}_1^{(1,0;a)}(B_{2u})\mathbb{Q}_0^{(b)}(A_g)$$

$$\boxed{\text{z245}} \quad \mathbb{Q}_1^{(1,0;c)}(B_{2u}, b) = \mathbb{Q}_1^{(1,0;a)}(B_{3u})\mathbb{Q}_2^{(b)}(B_{1g})$$

$$\boxed{\text{z246}} \quad \mathbb{G}_2^{(1,-1;c)}(B_{2u}) = \mathbb{G}_2^{(1,-1;a)}(B_{2u})\mathbb{Q}_0^{(b)}(A_g)$$

$$\boxed{\text{z289}} \quad \mathbb{Q}_2^{(c)}(B_{3g}) = \mathbb{T}_1^{(a)}(B_{1u})\mathbb{T}_1^{(b)}(B_{2u})$$

$$\boxed{\text{z290}} \quad \mathbb{Q}_2^{(1,-1;c)}(B_{3g}) = \frac{\sqrt{15}\mathbb{M}_2^{(1,-1;a)}(A_u, 1)\mathbb{T}_1^{(b)}(B_{3u})}{5} + \frac{\sqrt{5}\mathbb{M}_2^{(1,-1;a)}(A_u, 2)\mathbb{T}_1^{(b)}(B_{3u})}{5} + \frac{\sqrt{5}\mathbb{M}_2^{(1,-1;a)}(B_{1u})\mathbb{T}_1^{(b)}(B_{2u})}{5}$$

$$\boxed{\text{z291}} \quad \mathbb{Q}_2^{(1,0;c)}(B_{3g}) = \mathbb{T}_1^{(1,0;a)}(B_{1u})\mathbb{T}_1^{(b)}(B_{2u})$$

$$\boxed{\text{z292}} \quad \mathbb{G}_1^{(1,-1;c)}(B_{3g}) = -\frac{\sqrt{10}\mathbb{M}_2^{(1,-1;a)}(A_u, 1)\mathbb{T}_1^{(b)}(B_{3u})}{5} + \frac{\sqrt{30}\mathbb{M}_2^{(1,-1;a)}(A_u, 2)\mathbb{T}_1^{(b)}(B_{3u})}{10} + \frac{\sqrt{30}\mathbb{M}_2^{(1,-1;a)}(B_{1u})\mathbb{T}_1^{(b)}(B_{2u})}{10}$$

$$\boxed{\text{z293}} \quad \mathbb{G}_3^{(1,-1;c)}(B_{3g}, 1) = \frac{\sqrt{2}\mathbb{M}_2^{(1,-1;a)}(A_u, 2)\mathbb{T}_1^{(b)}(B_{3u})}{2} - \frac{\sqrt{2}\mathbb{M}_2^{(1,-1;a)}(B_{1u})\mathbb{T}_1^{(b)}(B_{2u})}{2}$$

$$\boxed{\text{z294}} \quad \mathbb{G}_1^{(1,1;c)}(B_{3g}) = \mathbb{M}_0^{(1,1;a)}(A_u)\mathbb{T}_1^{(b)}(B_{3u})$$

$$\boxed{\text{z334}} \quad \mathbb{Q}_1^{(c)}(B_{3u}, a) = \mathbb{Q}_1^{(a)}(B_{3u})\mathbb{Q}_0^{(b)}(A_g)$$

$$\boxed{\text{z335}} \quad \mathbb{Q}_1^{(c)}(B_{3u}, b) = \mathbb{Q}_1^{(a)}(B_{2u})\mathbb{Q}_2^{(b)}(B_{1g})$$

$$\boxed{\text{z336}} \quad \mathbb{Q}_1^{(1,-1;c)}(B_{3u}) = -\mathbb{G}_2^{(1,-1;a)}(B_{2u})\mathbb{Q}_2^{(b)}(B_{1g})$$

$$\boxed{\text{z337}} \quad \mathbb{Q}_1^{(1,0;c)}(B_{3u}, a) = \mathbb{Q}_1^{(1,0;a)}(B_{3u})\mathbb{Q}_0^{(b)}(A_g)$$

$$\boxed{\text{z338}} \quad \mathbb{Q}_1^{(1,0;c)}(B_{3u}, b) = \mathbb{Q}_1^{(1,0;a)}(B_{2u})\mathbb{Q}_2^{(b)}(B_{1g})$$

$$\boxed{\text{z339}} \quad \mathbb{G}_2^{(1,-1;c)}(B_{3u}) = \mathbb{G}_2^{(1,-1;a)}(B_{3u})\mathbb{Q}_0^{(b)}(A_g)$$

• '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: 2d@1f

$$\boxed{\text{z45}} \quad \mathbb{Q}_0^{(c)}(A_g, a) = \mathbb{Q}_0^{(a)}(A_g)\mathbb{Q}_0^{(b)}(A_g)$$

$$\boxed{\text{z46}} \quad \mathbb{Q}_0^{(c)}(A_g, b) = \mathbb{Q}_2^{(a)}(B_{1g})\mathbb{Q}_2^{(b)}(B_{1g})$$

$$\boxed{\text{z47}} \quad \mathbb{Q}_2^{(c)}(A_g, 1) = \mathbb{Q}_2^{(a)}(A_g, 1)\mathbb{Q}_0^{(b)}(A_g)$$

$$\boxed{\text{z48}} \quad \mathbb{Q}_2^{(c)}(A_g, 2) = \mathbb{Q}_2^{(a)}(A_g, 2)\mathbb{Q}_0^{(b)}(A_g)$$

$$\boxed{\text{z49}} \quad \mathbb{Q}_0^{(1,-1;c)}(A_g) = \mathbb{Q}_2^{(1,-1;a)}(B_{1g})\mathbb{Q}_2^{(b)}(B_{1g})$$

$$\boxed{\text{z50}} \quad \mathbb{Q}_2^{(1,-1;c)}(A_g, 1) = \mathbb{Q}_2^{(1,-1;a)}(A_g, 1)\mathbb{Q}_0^{(b)}(A_g)$$

$$\boxed{\text{z51}} \quad \mathbb{Q}_2^{(1,-1;c)}(A_g, 2) = \mathbb{Q}_2^{(1,-1;a)}(A_g, 2)\mathbb{Q}_0^{(b)}(A_g)$$

$$\boxed{\text{z52}} \quad \mathbb{Q}_2^{(1,0;c)}(A_g, 2) = -\mathbb{G}_1^{(1,0;a)}(B_{1g})\mathbb{Q}_2^{(b)}(B_{1g})$$

$$\boxed{\text{z53}} \quad \mathbb{Q}_0^{(1,1;c)}(A_g) = \mathbb{Q}_0^{(1,1;a)}(A_g)\mathbb{Q}_0^{(b)}(A_g)$$

$$\boxed{\text{z82}} \quad \mathbb{Q}_3^{(1,-1;c)}(A_u) = -\frac{\sqrt{2}\mathbb{M}_3^{(1,-1;a)}(B_{2g}, 2)\mathbb{T}_1^{(b)}(B_{2u})}{2} - \frac{\sqrt{2}\mathbb{M}_3^{(1,-1;a)}(B_{3g}, 2)\mathbb{T}_1^{(b)}(B_{3u})}{2}$$

$$\boxed{\text{z83}} \quad \mathbb{Q}_3^{(1,0;c)}(A_u) = \frac{\sqrt{2}\mathbb{T}_2^{(1,0;a)}(B_{2g})\mathbb{T}_1^{(b)}(B_{2u})}{2} + \frac{\sqrt{2}\mathbb{T}_2^{(1,0;a)}(B_{3g})\mathbb{T}_1^{(b)}(B_{3u})}{2}$$

$$\boxed{\text{z84}} \quad \mathbb{G}_0^{(c)}(A_u) = \frac{\sqrt{2}\mathbb{M}_1^{(a)}(B_{2g})\mathbb{T}_1^{(b)}(B_{2u})}{2} + \frac{\sqrt{2}\mathbb{M}_1^{(a)}(B_{3g})\mathbb{T}_1^{(b)}(B_{3u})}{2}$$

$$\boxed{\text{z85}} \quad \mathbb{G}_2^{(c)}(A_u, 2) = -\frac{\sqrt{2}\mathbb{M}_1^{(a)}(B_{2g})\mathbb{T}_1^{(b)}(B_{2u})}{2} + \frac{\sqrt{2}\mathbb{M}_1^{(a)}(B_{3g})\mathbb{T}_1^{(b)}(B_{3u})}{2}$$

$$\boxed{\text{z86}} \quad \mathbb{G}_0^{(1,-1;c)}(A_u) = \frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(B_{2g})\mathbb{T}_1^{(b)}(B_{2u})}{2} + \frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(B_{3g})\mathbb{T}_1^{(b)}(B_{3u})}{2}$$

$$\boxed{\text{z87}} \quad \mathbb{G}_2^{(1,-1;c)}(A_u, 1) = -\frac{\sqrt{3}\mathbb{M}_3^{(1,-1;a)}(B_{2g}, 1)\mathbb{T}_1^{(b)}(B_{2u})}{4} + \frac{\sqrt{5}\mathbb{M}_3^{(1,-1;a)}(B_{2g}, 2)\mathbb{T}_1^{(b)}(B_{2u})}{4} - \frac{\sqrt{3}\mathbb{M}_3^{(1,-1;a)}(B_{3g}, 1)\mathbb{T}_1^{(b)}(B_{3u})}{4} - \frac{\sqrt{5}\mathbb{M}_3^{(1,-1;a)}(B_{3g}, 2)\mathbb{T}_1^{(b)}(B_{3u})}{4}$$

$$\boxed{\text{z88}} \quad \mathbb{G}_2^{(1,-1;c)}(A_u, 2a) = -\frac{\sqrt{2}\mathbb{M}_3^{(1,-1;a)}(B_{2g}, 1)\mathbb{T}_1^{(b)}(B_{2u})}{2} + \frac{\sqrt{2}\mathbb{M}_3^{(1,-1;a)}(B_{3g}, 1)\mathbb{T}_1^{(b)}(B_{3u})}{2}$$

$$\boxed{\text{z89}} \quad \mathbb{G}_2^{(1,-1;c)}(A_u, 2b) = -\frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(B_{2g})\mathbb{T}_1^{(b)}(B_{2u})}{2} + \frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(B_{3g})\mathbb{T}_1^{(b)}(B_{3u})}{2}$$

$$\boxed{\text{z90}} \quad \mathbb{G}_4^{(1,-1;c)}(A_u, 1) = \frac{\sqrt{5}\mathbb{M}_3^{(1,-1;a)}(B_{2g}, 1)\mathbb{T}_1^{(b)}(B_{2u})}{4} + \frac{\sqrt{3}\mathbb{M}_3^{(1,-1;a)}(B_{2g}, 2)\mathbb{T}_1^{(b)}(B_{2u})}{4} + \frac{\sqrt{5}\mathbb{M}_3^{(1,-1;a)}(B_{3g}, 1)\mathbb{T}_1^{(b)}(B_{3u})}{4} - \frac{\sqrt{3}\mathbb{M}_3^{(1,-1;a)}(B_{3g}, 2)\mathbb{T}_1^{(b)}(B_{3u})}{4}$$

$$\boxed{\text{z118}} \quad \mathbb{G}_2^{(1,0;c)}(A_u, 1) = \frac{\sqrt{2}\mathbb{T}_2^{(1,0;a)}(B_{2g})\mathbb{T}_1^{(b)}(B_{2u})}{2} - \frac{\sqrt{2}\mathbb{T}_2^{(1,0;a)}(B_{3g})\mathbb{T}_1^{(b)}(B_{3u})}{2}$$

$$\boxed{\text{z119}} \quad \mathbb{G}_0^{(1,1;c)}(A_u) = \frac{\sqrt{2}\mathbb{M}_1^{(1,1;a)}(B_{2g})\mathbb{T}_1^{(b)}(B_{2u})}{2} + \frac{\sqrt{2}\mathbb{M}_1^{(1,1;a)}(B_{3g})\mathbb{T}_1^{(b)}(B_{3u})}{2}$$

$$\boxed{\text{z120}} \quad \mathbb{G}_2^{(1,1;c)}(A_u, 2) = -\frac{\sqrt{2}\mathbb{M}_1^{(1,1;a)}(B_{2g})\mathbb{T}_1^{(b)}(B_{2u})}{2} + \frac{\sqrt{2}\mathbb{M}_1^{(1,1;a)}(B_{3g})\mathbb{T}_1^{(b)}(B_{3u})}{2}$$

$$\boxed{\text{z121}} \quad \mathbb{Q}_2^{(c)}(B_{1g}, a) = \mathbb{Q}_0^{(a)}(A_g)\mathbb{Q}_2^{(b)}(B_{1g})$$

$$\boxed{\text{z122}} \quad \mathbb{Q}_2^{(c)}(B_{1g}, b) = \mathbb{Q}_2^{(a)}(B_{1g})\mathbb{Q}_0^{(b)}(A_g)$$

$$\boxed{\text{z123}} \quad \mathbb{Q}_2^{(c)}(B_{1g}, c) = -\mathbb{Q}_2^{(a)}(A_g, 1)\mathbb{Q}_2^{(b)}(B_{1g})$$

$$\boxed{\text{z151}} \quad \mathbb{Q}_4^{(c)}(B_{1g}, 1) = \mathbb{Q}_2^{(a)}(A_g, 2)\mathbb{Q}_2^{(b)}(B_{1g})$$

$$\boxed{\text{z152}} \quad \mathbb{Q}_2^{(1,-1;c)}(B_{1g}, a) = \mathbb{Q}_2^{(1,-1;a)}(B_{1g})\mathbb{Q}_0^{(b)}(A_g)$$

$$\boxed{\text{z153}} \quad \mathbb{Q}_2^{(1,-1;c)}(B_{1g}, b) = -\mathbb{Q}_2^{(1,-1;a)}(A_g, 1)\mathbb{Q}_2^{(b)}(B_{1g})$$

$$\boxed{\text{z154}} \quad \mathbb{Q}_4^{(1,-1;c)}(B_{1g}, 1) = \mathbb{Q}_2^{(1,-1;a)}(A_g, 2)\mathbb{Q}_2^{(b)}(B_{1g})$$

$$\boxed{\text{z155}} \quad \mathbb{Q}_2^{(1,1;c)}(B_{1g}) = \mathbb{Q}_0^{(1,1;a)}(A_g)\mathbb{Q}_2^{(b)}(B_{1g})$$

$$\boxed{\text{z156}} \quad \mathbb{G}_1^{(1,0;c)}(B_{1g}) = \mathbb{G}_1^{(1,0;a)}(B_{1g})\mathbb{Q}_0^{(b)}(A_g)$$

$$\boxed{\text{z198}} \quad \mathbb{Q}_1^{(c)}(B_{1u}) = -\frac{\sqrt{2}\mathbb{M}_1^{(a)}(B_{2g})\mathbb{T}_1^{(b)}(B_{3u})}{2} + \frac{\sqrt{2}\mathbb{M}_1^{(a)}(B_{3g})\mathbb{T}_1^{(b)}(B_{2u})}{2}$$

$$\boxed{\text{z199}} \quad \mathbb{Q}_1^{(1,-1;c)}(B_{1u}) = -\frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(B_{2g})\mathbb{T}_1^{(b)}(B_{3u})}{2} + \frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(B_{3g})\mathbb{T}_1^{(b)}(B_{2u})}{2}$$

$$\boxed{\text{z200}} \quad \mathbb{Q}_3^{(1,-1;c)}(B_{1u}, 1) = \frac{\sqrt{3}\mathbb{M}_3^{(1,-1;a)}(B_{2g}, 1)\mathbb{T}_1^{(b)}(B_{3u})}{4} - \frac{\sqrt{5}\mathbb{M}_3^{(1,-1;a)}(B_{2g}, 2)\mathbb{T}_1^{(b)}(B_{3u})}{4} - \frac{\sqrt{3}\mathbb{M}_3^{(1,-1;a)}(B_{3g}, 1)\mathbb{T}_1^{(b)}(B_{2u})}{4} - \frac{\sqrt{5}\mathbb{M}_3^{(1,-1;a)}(B_{3g}, 2)\mathbb{T}_1^{(b)}(B_{2u})}{4}$$

$$\boxed{\text{z201}} \quad \mathbb{Q}_3^{(1,-1;c)}(B_{1u}, 2) = \frac{\sqrt{30}\mathbb{M}_3^{(1,-1;a)}(B_{2g}, 1)\mathbb{T}_1^{(b)}(B_{3u})}{8} - \frac{\sqrt{2}\mathbb{M}_3^{(1,-1;a)}(B_{2g}, 2)\mathbb{T}_1^{(b)}(B_{3u})}{8} + \frac{\sqrt{30}\mathbb{M}_3^{(1,-1;a)}(B_{3g}, 1)\mathbb{T}_1^{(b)}(B_{2u})}{8} + \frac{\sqrt{2}\mathbb{M}_3^{(1,-1;a)}(B_{3g}, 2)\mathbb{T}_1^{(b)}(B_{2u})}{8}$$

$$\boxed{\text{z202}} \quad \mathbb{Q}_1^{(1,0;c)}(B_{1u}) = \frac{\sqrt{2}\mathbb{T}_2^{(1,0;a)}(B_{2g})\mathbb{T}_1^{(b)}(B_{3u})}{2} + \frac{\sqrt{2}\mathbb{T}_2^{(1,0;a)}(B_{3g})\mathbb{T}_1^{(b)}(B_{2u})}{2}$$

$$\boxed{\text{z203}} \quad \mathbb{Q}_3^{(1,0;c)}(B_{1u}, 2) = \frac{\sqrt{2}\mathbb{T}_2^{(1,0;a)}(B_{2g})\mathbb{T}_1^{(b)}(B_{3u})}{2} - \frac{\sqrt{2}\mathbb{T}_2^{(1,0;a)}(B_{3g})\mathbb{T}_1^{(b)}(B_{2u})}{2}$$

$$\boxed{\text{z204}} \quad \mathbb{Q}_1^{(1,1;c)}(B_{1u}) = -\frac{\sqrt{2}\mathbb{M}_1^{(1,1;a)}(B_{2g})\mathbb{T}_1^{(b)}(B_{3u})}{2} + \frac{\sqrt{2}\mathbb{M}_1^{(1,1;a)}(B_{3g})\mathbb{T}_1^{(b)}(B_{2u})}{2}$$

$$\boxed{\text{z205}} \quad \mathbb{G}_2^{(c)}(B_{1u}) = \frac{\sqrt{2}\mathbb{M}_1^{(a)}(B_{2g})\mathbb{T}_1^{(b)}(B_{3u})}{2} + \frac{\sqrt{2}\mathbb{M}_1^{(a)}(B_{3g})\mathbb{T}_1^{(b)}(B_{2u})}{2}$$

$$\boxed{\text{z206}} \quad \mathbb{G}_2^{(1,-1;c)}(B_{1u}, a) = -\frac{\sqrt{2}\mathbb{M}_3^{(1,-1;a)}(B_{2g}, 1)\mathbb{T}_1^{(b)}(B_{3u})}{8} - \frac{\sqrt{30}\mathbb{M}_3^{(1,-1;a)}(B_{2g}, 2)\mathbb{T}_1^{(b)}(B_{3u})}{8} - \frac{\sqrt{2}\mathbb{M}_3^{(1,-1;a)}(B_{3g}, 1)\mathbb{T}_1^{(b)}(B_{2u})}{8} + \frac{\sqrt{30}\mathbb{M}_3^{(1,-1;a)}(B_{3g}, 2)\mathbb{T}_1^{(b)}(B_{2u})}{8}$$

$$\boxed{\text{z207}} \quad \mathbb{G}_2^{(1,-1;c)}(B_{1u}, b) = \frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(B_{2g})\mathbb{T}_1^{(b)}(B_{3u})}{2} + \frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(B_{3g})\mathbb{T}_1^{(b)}(B_{2u})}{2}$$

$$\boxed{\text{z208}} \quad \mathbb{G}_4^{(1,-1;c)}(B_{1u}, 1) = -\frac{\sqrt{5}\mathbb{M}_3^{(1,-1;a)}(B_{2g}, 1)\mathbb{T}_1^{(b)}(B_{3u})}{4} - \frac{\sqrt{3}\mathbb{M}_3^{(1,-1;a)}(B_{2g}, 2)\mathbb{T}_1^{(b)}(B_{3u})}{4} + \frac{\sqrt{5}\mathbb{M}_3^{(1,-1;a)}(B_{3g}, 1)\mathbb{T}_1^{(b)}(B_{2u})}{4} - \frac{\sqrt{3}\mathbb{M}_3^{(1,-1;a)}(B_{3g}, 2)\mathbb{T}_1^{(b)}(B_{2u})}{4}$$

$$\boxed{\text{z209}} \quad \mathbb{G}_2^{(1,1;c)}(B_{1u}) = \frac{\sqrt{2}\mathbb{M}_1^{(1,1;a)}(B_{2g})\mathbb{T}_1^{(b)}(B_{3u})}{2} + \frac{\sqrt{2}\mathbb{M}_1^{(1,1;a)}(B_{3g})\mathbb{T}_1^{(b)}(B_{2u})}{2}$$

$$\boxed{\text{z247}} \quad \mathbb{Q}_2^{(c)}(B_{2g}, a) = \mathbb{Q}_2^{(a)}(B_{2g})\mathbb{Q}_0^{(b)}(A_g)$$

$$\boxed{\text{z248}} \quad \mathbb{Q}_2^{(c)}(B_{2g}, b) = \mathbb{Q}_2^{(a)}(B_{3g})\mathbb{Q}_2^{(b)}(B_{1g})$$

$$\boxed{\text{z249}} \quad \mathbb{Q}_2^{(1,-1;c)}(B_{2g}, a) = \mathbb{Q}_2^{(1,-1;a)}(B_{2g})\mathbb{Q}_0^{(b)}(A_g)$$

$$\boxed{\text{z250}} \quad \mathbb{Q}_2^{(1,-1;c)}(B_{2g}, b) = \mathbb{Q}_2^{(1,-1;a)}(B_{3g})\mathbb{Q}_2^{(b)}(B_{1g})$$

$$\boxed{\text{z251}} \quad \mathbb{Q}_2^{(1,0;c)}(B_{2g}) = \mathbb{G}_1^{(1,0;a)}(B_{3g})\mathbb{Q}_2^{(b)}(B_{1g})$$

$$\boxed{\text{z252}} \quad \mathbb{G}_1^{(1,0;c)}(B_{2g}) = \mathbb{G}_1^{(1,0;a)}(B_{2g})\mathbb{Q}_0^{(b)}(A_g)$$

$$\boxed{\text{z253}} \quad \mathbb{Q}_1^{(c)}(B_{2u}) = \mathbb{M}_1^{(a)}(B_{1g})\mathbb{T}_1^{(b)}(B_{3u})$$

$$\boxed{\text{z254}} \quad \mathbb{Q}_1^{(1,-1;c)}(B_{2u}) = \mathbb{M}_1^{(1,-1;a)}(B_{1g})\mathbb{T}_1^{(b)}(B_{3u})$$

$$\boxed{\text{z255}} \quad \mathbb{Q}_3^{(1,-1;c)}(B_{2u}, 1) = -\frac{\sqrt{6}\mathbb{M}_3^{(1,-1;a)}(B_{1g}, 1)\mathbb{T}_1^{(b)}(B_{3u})}{4} - \frac{\sqrt{10}\mathbb{M}_3^{(1,-1;a)}(B_{1g}, 2)\mathbb{T}_1^{(b)}(B_{3u})}{4}$$

$$\boxed{\text{z256}} \quad \mathbb{Q}_3^{(1,-1;c)}(B_{2u}, 2) = \frac{2\sqrt{22}\mathbb{M}_3^{(1,-1;a)}(A_g)\mathbb{T}_1^{(b)}(B_{2u})}{11} + \frac{\sqrt{330}\mathbb{M}_3^{(1,-1;a)}(B_{1g}, 1)\mathbb{T}_1^{(b)}(B_{3u})}{44} - \frac{3\sqrt{22}\mathbb{M}_3^{(1,-1;a)}(B_{1g}, 2)\mathbb{T}_1^{(b)}(B_{3u})}{44}$$

$$\boxed{\text{z257}} \quad \mathbb{Q}_1^{(1,0;c)}(B_{2u}) = -\frac{\sqrt{7}\mathbb{T}_2^{(1,0;a)}(A_g, 1)\mathbb{T}_1^{(b)}(B_{2u})}{7} - \frac{\sqrt{21}\mathbb{T}_2^{(1,0;a)}(A_g, 2)\mathbb{T}_1^{(b)}(B_{2u})}{7} + \frac{\sqrt{21}\mathbb{T}_2^{(1,0;a)}(B_{1g})\mathbb{T}_1^{(b)}(B_{3u})}{7}$$

$$\boxed{\text{z258}} \quad \mathbb{Q}_3^{(1,0;c)}(B_{2u}, 1) = -\frac{\sqrt{21}\mathbb{T}_2^{(1,0;a)}(A_g, 1)\mathbb{T}_1^{(b)}(B_{2u})}{14} - \frac{3\sqrt{7}\mathbb{T}_2^{(1,0;a)}(A_g, 2)\mathbb{T}_1^{(b)}(B_{2u})}{14} - \frac{2\sqrt{7}\mathbb{T}_2^{(1,0;a)}(B_{1g})\mathbb{T}_1^{(b)}(B_{3u})}{7}$$

$$\boxed{\text{z295}} \quad \mathbb{Q}_3^{(1,0;c)}(B_{2u}, 2) = \frac{\sqrt{3}\mathbb{T}_2^{(1,0;a)}(A_g, 1)\mathbb{T}_1^{(b)}(B_{2u})}{2} - \frac{\mathbb{T}_2^{(1,0;a)}(A_g, 2)\mathbb{T}_1^{(b)}(B_{2u})}{2}$$

$$\boxed{\text{z296}} \quad \mathbb{Q}_1^{(1,1;c)}(B_{2u}) = \mathbb{M}_1^{(1,1;a)}(B_{1g})\mathbb{T}_1^{(b)}(B_{3u})$$

$$\boxed{\text{z297}} \quad \mathbb{G}_2^{(1,-1;c)}(B_{2u}) = \frac{\sqrt{33}\mathbb{M}_3^{(1,-1;a)}(A_g)\mathbb{T}_1^{(b)}(B_{2u})}{11} - \frac{\sqrt{55}\mathbb{M}_3^{(1,-1;a)}(B_{1g}, 1)\mathbb{T}_1^{(b)}(B_{3u})}{11} + \frac{\sqrt{33}\mathbb{M}_3^{(1,-1;a)}(B_{1g}, 2)\mathbb{T}_1^{(b)}(B_{3u})}{11}$$

$$\boxed{\text{z298}} \quad \mathbb{Q}_2^{(c)}(B_{3g}, a) = \mathbb{Q}_2^{(a)}(B_{3g})\mathbb{Q}_0^{(b)}(A_g)$$

$$\boxed{\text{z299}} \quad \mathbb{Q}_2^{(c)}(B_{3g}, b) = \mathbb{Q}_2^{(a)}(B_{2g})\mathbb{Q}_2^{(b)}(B_{1g})$$

$$\boxed{\text{z300}} \quad \mathbb{Q}_2^{(1,-1;c)}(B_{3g}, a) = \mathbb{Q}_2^{(1,-1;a)}(B_{3g})\mathbb{Q}_0^{(b)}(A_g)$$

$$\boxed{\text{z301}} \quad \mathbb{Q}_2^{(1,-1;c)}(B_{3g}, b) = \mathbb{Q}_2^{(1,-1;a)}(B_{2g})\mathbb{Q}_2^{(b)}(B_{1g})$$

$$\boxed{\text{z302}} \quad \mathbb{Q}_2^{(1,0;c)}(B_{3g}) = -\mathbb{G}_1^{(1,0;a)}(B_{2g})\mathbb{Q}_2^{(b)}(B_{1g})$$

$$\boxed{\text{z303}} \quad \mathbb{G}_1^{(1,0;c)}(B_{3g}) = \mathbb{G}_1^{(1,0;a)}(B_{3g})\mathbb{Q}_0^{(b)}(A_g)$$

$$\boxed{\text{z340}} \quad \mathbb{Q}_1^{(c)}(B_{3u}) = -\mathbb{M}_1^{(a)}(B_{1g})\mathbb{T}_1^{(b)}(B_{2u})$$

$$\boxed{\text{z341}} \quad \mathbb{Q}_1^{(1,-1;c)}(B_{3u}) = -\mathbb{M}_1^{(1,-1;a)}(B_{1g})\mathbb{T}_1^{(b)}(B_{2u})$$

$$\boxed{\text{z342}} \quad \mathbb{Q}_3^{(1,-1;c)}(B_{3u}, 1) = \frac{\sqrt{6}\mathbb{M}_3^{(1,-1;a)}(B_{1g}, 1)\mathbb{T}_1^{(b)}(B_{2u})}{4} - \frac{\sqrt{10}\mathbb{M}_3^{(1,-1;a)}(B_{1g}, 2)\mathbb{T}_1^{(b)}(B_{2u})}{4}$$

$$\boxed{\text{z343}} \quad \mathbb{Q}_3^{(1,-1;c)}(B_{3u}, 2) = \frac{2\sqrt{22}\mathbb{M}_3^{(1,-1;a)}(A_g)\mathbb{T}_1^{(b)}(B_{3u})}{11} + \frac{\sqrt{330}\mathbb{M}_3^{(1,-1;a)}(B_{1g}, 1)\mathbb{T}_1^{(b)}(B_{2u})}{44} + \frac{3\sqrt{22}\mathbb{M}_3^{(1,-1;a)}(B_{1g}, 2)\mathbb{T}_1^{(b)}(B_{2u})}{44}$$

$$\boxed{\text{z344}} \quad \mathbb{Q}_1^{(1,0;c)}(B_{3u}) = -\frac{\sqrt{7}\mathbb{T}_2^{(1,0;a)}(A_g, 1)\mathbb{T}_1^{(b)}(B_{3u})}{7} + \frac{\sqrt{21}\mathbb{T}_2^{(1,0;a)}(A_g, 2)\mathbb{T}_1^{(b)}(B_{3u})}{7} + \frac{\sqrt{21}\mathbb{T}_2^{(1,0;a)}(B_{1g})\mathbb{T}_1^{(b)}(B_{2u})}{7}$$

$$\boxed{\text{z345}} \quad \mathbb{Q}_3^{(1,0;c)}(B_{3u}, 1) = -\frac{\sqrt{21}\mathbb{T}_2^{(1,0;a)}(A_g, 1)\mathbb{T}_1^{(b)}(B_{3u})}{14} + \frac{3\sqrt{7}\mathbb{T}_2^{(1,0;a)}(A_g, 2)\mathbb{T}_1^{(b)}(B_{3u})}{14} - \frac{2\sqrt{7}\mathbb{T}_2^{(1,0;a)}(B_{1g})\mathbb{T}_1^{(b)}(B_{2u})}{7}$$

$$\boxed{\text{z346}} \quad \mathbb{Q}_3^{(1,0;c)}(B_{3u}, 2) = -\frac{\sqrt{3}\mathbb{T}_2^{(1,0;a)}(A_g, 1)\mathbb{T}_1^{(b)}(B_{3u})}{2} - \frac{\mathbb{T}_2^{(1,0;a)}(A_g, 2)\mathbb{T}_1^{(b)}(B_{3u})}{2}$$

$$\boxed{\text{z347}} \quad \mathbb{Q}_1^{(1,1;c)}(B_{3u}) = -\mathbb{M}_1^{(1,1;a)}(B_{1g})\mathbb{T}_1^{(b)}(B_{2u})$$

$$\boxed{\text{z348}} \quad \mathbb{G}_2^{(1,-1;c)}(B_{3u}) = \frac{\sqrt{33}\mathbb{M}_3^{(1,-1;a)}(A_g)\mathbb{T}_1^{(b)}(B_{3u})}{11} - \frac{\sqrt{55}\mathbb{M}_3^{(1,-1;a)}(B_{1g}, 1)\mathbb{T}_1^{(b)}(B_{2u})}{11} - \frac{\sqrt{33}\mathbb{M}_3^{(1,-1;a)}(B_{1g}, 2)\mathbb{T}_1^{(b)}(B_{2u})}{11}$$

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## — Atomic SAMB —

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

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

$$\boxed{\text{x2}} \quad \mathbb{M}_1^{(1,-1;a)}(B_{1g}) = \begin{bmatrix} \frac{\sqrt{2}}{2} & 0 \\ 0 & -\frac{\sqrt{2}}{2} \end{bmatrix}$$

$$\boxed{x3} \quad \mathbb{M}_1^{(1,-1;a)}(B_{2g}) = \begin{bmatrix} 0 & -\frac{\sqrt{2}i}{2} \\ \frac{\sqrt{2}i}{2} & 0 \end{bmatrix}$$

$$\boxed{x4} \quad \mathbb{M}_1^{(1,-1;a)}(B_{3g}) = \begin{bmatrix} 0 & \frac{\sqrt{2}}{2} \\ \frac{\sqrt{2}}{2} & 0 \end{bmatrix}$$

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

$$\boxed{x5} \quad \mathbb{Q}_1^{(a)}(B_{1u}) = \begin{bmatrix} 0 & 0 & 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{2} \end{bmatrix}$$

$$\boxed{x6} \quad \mathbb{Q}_1^{(a)}(B_{2u}) = \begin{bmatrix} 0 & 0 & \frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2} & 0 & 0 \end{bmatrix}$$

$$\boxed{x7} \quad \mathbb{Q}_1^{(a)}(B_{3u}) = \begin{bmatrix} \frac{1}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{x8} \quad \mathbb{Q}_1^{(1,0;a)}(B_{1u}) = \begin{bmatrix} 0 & -\frac{\sqrt{2}}{4} & 0 & \frac{\sqrt{2}i}{4} & 0 & 0 \\ \frac{\sqrt{2}}{4} & 0 & \frac{\sqrt{2}i}{4} & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{x9} \quad \mathbb{Q}_1^{(1,0;a)}(B_{2u}) = \begin{bmatrix} \frac{\sqrt{2}i}{4} & 0 & 0 & 0 & 0 & -\frac{\sqrt{2}i}{4} \\ 0 & -\frac{\sqrt{2}i}{4} & 0 & 0 & -\frac{\sqrt{2}i}{4} & 0 \end{bmatrix}$$

$$\boxed{x10} \quad \mathbb{Q}_1^{(1,0;a)}(B_{3u}) = \begin{bmatrix} 0 & 0 & -\frac{\sqrt{2}i}{4} & 0 & 0 & \frac{\sqrt{2}}{4} \\ 0 & 0 & 0 & \frac{\sqrt{2}i}{4} & -\frac{\sqrt{2}}{4} & 0 \end{bmatrix}$$

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

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

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

$$\boxed{x14} \quad \mathbb{G}_2^{(1,-1;a)}(B_{2u}) = \begin{bmatrix} \frac{\sqrt{2}i}{4} & 0 & 0 & 0 & \frac{\sqrt{2}i}{4} \\ 0 & -\frac{\sqrt{2}i}{4} & 0 & 0 & \frac{\sqrt{2}i}{4} & 0 \end{bmatrix}$$

$$\boxed{x15} \quad \mathbb{G}_2^{(1,-1;a)}(B_{3u}) = \begin{bmatrix} 0 & 0 & \frac{\sqrt{2}i}{4} & 0 & 0 & \frac{\sqrt{2}}{4} \\ 0 & 0 & 0 & -\frac{\sqrt{2}i}{4} & -\frac{\sqrt{2}}{4} & 0 \end{bmatrix}$$

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

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

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

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

$$\boxed{x20} \quad \mathbb{M}_2^{(1,-1;a)}(B_{2u}) = \begin{bmatrix} \frac{\sqrt{2}}{4} & 0 & 0 & 0 & 0 & \frac{\sqrt{2}}{4} \\ 0 & -\frac{\sqrt{2}}{4} & 0 & 0 & \frac{\sqrt{2}}{4} & 0 \end{bmatrix}$$

$$\boxed{x21} \quad \mathbb{M}_2^{(1,-1;a)}(B_{3u}) = \begin{bmatrix} 0 & 0 & \frac{\sqrt{2}}{4} & 0 & 0 & -\frac{\sqrt{2}i}{4} \\ 0 & 0 & 0 & -\frac{\sqrt{2}}{4} & \frac{\sqrt{2}i}{4} & 0 \end{bmatrix}$$

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

$$\boxed{x23} \quad \mathbb{T}_1^{(a)}(B_{1u}) = \begin{bmatrix} 0 & 0 & 0 & 0 & \frac{i}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{i}{2} \end{bmatrix}$$

$$\boxed{x24} \quad \mathbb{T}_1^{(a)}(B_{2u}) = \begin{bmatrix} 0 & 0 & \frac{i}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{i}{2} & 0 & 0 \end{bmatrix}$$

$$\boxed{x25} \quad \mathbb{T}_1^{(a)}(B_{3u}) = \begin{bmatrix} \frac{i}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{i}{2} & 0 & 0 & 0 & 0 \end{bmatrix}$$

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

$$\boxed{x27} \quad \mathbb{T}_1^{(1,0;a)}(B_{2u}) = \begin{bmatrix} \frac{\sqrt{2}}{4} & 0 & 0 & 0 & 0 & -\frac{\sqrt{2}}{4} \\ 0 & -\frac{\sqrt{2}}{4} & 0 & 0 & -\frac{\sqrt{2}}{4} & 0 \end{bmatrix}$$

$$\boxed{x28} \quad \mathbb{T}_1^{(1,0;a)}(B_{3u}) = \begin{bmatrix} 0 & 0 & -\frac{\sqrt{2}}{4} & 0 & 0 & -\frac{\sqrt{2}i}{4} \\ 0 & 0 & 0 & \frac{\sqrt{2}}{4} & \frac{\sqrt{2}i}{4} & 0 \end{bmatrix}$$

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

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

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

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

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

$$\boxed{x33} \quad \mathbb{Q}_2^{(a)}(B_{2g}) = \begin{bmatrix} 0 & 0 & 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{2} \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{1}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{x34} \quad \mathbb{Q}_2^{(a)}(B_{3g}) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{2} \\ 0 & 0 & \frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2} & 0 & 0 \end{bmatrix}$$

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

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

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

$$\boxed{x38} \quad \mathbb{Q}_2^{(1,-1;a)}(B_{2g}) = \begin{bmatrix} 0 & 0 & 0 & -\frac{\sqrt{2}i}{4} & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{2}i}{4} & 0 & 0 & 0 \\ 0 & \frac{\sqrt{2}i}{4} & 0 & 0 & -\frac{\sqrt{2}i}{4} & 0 \\ \frac{\sqrt{2}i}{4} & 0 & 0 & 0 & 0 & \frac{\sqrt{2}i}{4} \\ 0 & 0 & \frac{\sqrt{2}i}{4} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{2}i}{4} & 0 & 0 \end{bmatrix}$$

$$\boxed{x39} \quad \mathbb{Q}_2^{(1,-1;a)}(B_{3g}) = \begin{bmatrix} 0 & 0 & 0 & -\frac{\sqrt{2}}{4} & \frac{\sqrt{2}i}{4} & 0 \\ 0 & 0 & \frac{\sqrt{2}}{4} & 0 & 0 & -\frac{\sqrt{2}i}{4} \\ 0 & \frac{\sqrt{2}}{4} & 0 & 0 & 0 & 0 \\ -\frac{\sqrt{2}}{4} & 0 & 0 & 0 & 0 & 0 \\ -\frac{\sqrt{2}i}{4} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{2}i}{4} & 0 & 0 & 0 & 0 \end{bmatrix}$$

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

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

$$\boxed{x42} \quad \mathbb{G}_1^{(1,0;a)}(B_{2g}) = \begin{bmatrix} 0 & 0 & 0 & \frac{\sqrt{2}i}{4} & 0 & 0 \\ 0 & 0 & \frac{\sqrt{2}i}{4} & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{2}i}{4} & 0 & 0 & -\frac{\sqrt{2}i}{4} & 0 \\ -\frac{\sqrt{2}i}{4} & 0 & 0 & 0 & 0 & \frac{\sqrt{2}i}{4} \\ 0 & 0 & \frac{\sqrt{2}i}{4} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{2}i}{4} & 0 & 0 \end{bmatrix}$$

$$\boxed{x43} \quad \mathbb{G}_1^{(1,0;a)}(B_{3g}) = \begin{bmatrix} 0 & 0 & 0 & -\frac{\sqrt{2}}{4} & -\frac{\sqrt{2}i}{4} & 0 \\ 0 & 0 & \frac{\sqrt{2}}{4} & 0 & 0 & \frac{\sqrt{2}i}{4} \\ 0 & \frac{\sqrt{2}}{4} & 0 & 0 & 0 & 0 \\ -\frac{\sqrt{2}}{4} & 0 & 0 & 0 & 0 & 0 \\ \frac{\sqrt{2}i}{4} & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{2}i}{4} & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x44}} \quad \mathbb{M}_1^{(a)}(B_{1g}) = \begin{bmatrix} 0 & 0 & -\frac{i}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{i}{2} & 0 & 0 \\ \frac{i}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{i}{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x45}} \quad \mathbb{M}_1^{(a)}(B_{2g}) = \begin{bmatrix} 0 & 0 & 0 & 0 & \frac{i}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{i}{2} \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ -\frac{i}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{i}{2} & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x46}} \quad \mathbb{M}_1^{(a)}(B_{3g}) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{i}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{i}{2} \\ 0 & 0 & \frac{i}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{i}{2} & 0 & 0 \end{bmatrix}$$

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

$$\boxed{\text{x48}} \quad \mathbb{M}_1^{(1,-1;a)}(B_{1g}) = \begin{bmatrix} \frac{\sqrt{6}}{6} & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{6}}{6} & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{6}}{6} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{6}}{6} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{6}}{6} & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{6}}{6} \end{bmatrix}$$

$$\boxed{\text{x49}} \quad \mathbb{M}_3^{(1,-1;a)}(B_{1g}, 1) = \begin{bmatrix} -\frac{\sqrt{5}}{10} & 0 & 0 & 0 & 0 & -\frac{\sqrt{5}}{10} \\ 0 & \frac{\sqrt{5}}{10} & 0 & 0 & -\frac{\sqrt{5}}{10} & 0 \\ 0 & 0 & -\frac{\sqrt{5}}{10} & 0 & 0 & \frac{\sqrt{5}i}{10} \\ 0 & 0 & 0 & \frac{\sqrt{5}}{10} & -\frac{\sqrt{5}i}{10} & 0 \\ 0 & -\frac{\sqrt{5}}{10} & 0 & \frac{\sqrt{5}i}{10} & \frac{\sqrt{5}}{5} & 0 \\ -\frac{\sqrt{5}}{10} & 0 & -\frac{\sqrt{5}i}{10} & 0 & 0 & -\frac{\sqrt{5}}{5} \end{bmatrix}$$

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

$$\boxed{x51} \quad \mathbb{M}_1^{(1,-1;a)}(B_{2g}) = \begin{bmatrix} 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 \\ \frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 \\ 0 & 0 & \frac{\sqrt{6}i}{6} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{6}i}{6} \\ 0 & 0 & 0 & 0 & \frac{\sqrt{6}i}{6} & 0 \end{bmatrix}$$

$$\boxed{x52} \quad \mathbb{M}_3^{(1,-1;a)}(B_{2g}, 1) = \begin{bmatrix} 0 & \frac{\sqrt{5}i}{10} & 0 & -\frac{\sqrt{5}}{10} & 0 & 0 \\ -\frac{\sqrt{5}i}{10} & 0 & -\frac{\sqrt{5}}{10} & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{5}}{10} & 0 & -\frac{\sqrt{5}i}{5} & -\frac{\sqrt{5}}{10} & 0 \\ -\frac{\sqrt{5}}{10} & 0 & \frac{\sqrt{5}i}{5} & 0 & 0 & \frac{\sqrt{5}}{10} \\ 0 & 0 & -\frac{\sqrt{5}}{10} & 0 & 0 & \frac{\sqrt{5}i}{10} \\ 0 & 0 & 0 & \frac{\sqrt{5}}{10} & -\frac{\sqrt{5}i}{10} & 0 \end{bmatrix}$$

$$\boxed{x53} \quad \mathbb{M}_3^{(1,-1;a)}(B_{2g}, 2) = \begin{bmatrix} 0 & \frac{\sqrt{3}i}{6} & 0 & -\frac{\sqrt{3}}{6} & 0 & 0 \\ -\frac{\sqrt{3}i}{6} & 0 & -\frac{\sqrt{3}}{6} & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{3}}{6} & 0 & 0 & \frac{\sqrt{3}}{6} & 0 \\ -\frac{\sqrt{3}}{6} & 0 & 0 & 0 & 0 & -\frac{\sqrt{3}}{6} \\ 0 & 0 & \frac{\sqrt{3}}{6} & 0 & 0 & -\frac{\sqrt{3}i}{6} \\ 0 & 0 & 0 & -\frac{\sqrt{3}}{6} & \frac{\sqrt{3}i}{6} & 0 \end{bmatrix}$$

$$\boxed{x54} \quad \mathbb{M}_1^{(1,-1;a)}(B_{3g}) = \begin{bmatrix} 0 & \frac{\sqrt{6}}{6} & 0 & 0 & 0 & 0 \\ \frac{\sqrt{6}}{6} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{6}}{6} & 0 & 0 \\ 0 & 0 & \frac{\sqrt{6}}{6} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{6}}{6} \\ 0 & 0 & 0 & 0 & \frac{\sqrt{6}}{6} & 0 \end{bmatrix}$$

$$\boxed{x55} \quad \mathbb{M}_3^{(1,-1;a)}(B_{3g}, 1) = \begin{bmatrix} 0 & \frac{\sqrt{5}}{5} & 0 & \frac{\sqrt{5}i}{10} & -\frac{\sqrt{5}}{10} & 0 \\ \frac{\sqrt{5}}{5} & 0 & -\frac{\sqrt{5}i}{10} & 0 & 0 & \frac{\sqrt{5}}{10} \\ 0 & \frac{\sqrt{5}i}{10} & 0 & -\frac{\sqrt{5}}{10} & 0 & 0 \\ -\frac{\sqrt{5}i}{10} & 0 & -\frac{\sqrt{5}}{10} & 0 & 0 & 0 \\ -\frac{\sqrt{5}}{10} & 0 & 0 & 0 & 0 & -\frac{\sqrt{5}}{10} \\ 0 & \frac{\sqrt{5}}{10} & 0 & 0 & -\frac{\sqrt{5}}{10} & 0 \end{bmatrix}$$

$$\boxed{x56} \quad \mathbb{M}_3^{(1,-1;a)}(B_{3g}, 2) = \begin{bmatrix} 0 & 0 & 0 & -\frac{\sqrt{3}i}{6} & -\frac{\sqrt{3}}{6} & 0 \\ 0 & 0 & \frac{\sqrt{3}i}{6} & 0 & 0 & \frac{\sqrt{3}}{6} \\ 0 & -\frac{\sqrt{3}i}{6} & 0 & \frac{\sqrt{3}}{6} & 0 & 0 \\ \frac{\sqrt{3}i}{6} & 0 & \frac{\sqrt{3}}{6} & 0 & 0 & 0 \\ -\frac{\sqrt{3}}{6} & 0 & 0 & 0 & 0 & -\frac{\sqrt{3}}{6} \\ 0 & \frac{\sqrt{3}}{6} & 0 & 0 & -\frac{\sqrt{3}}{6} & 0 \end{bmatrix}$$

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

$$\boxed{x58} \quad \mathbb{M}_1^{(1,1;a)}(B_{2g}) = \begin{bmatrix} 0 & \frac{\sqrt{30}i}{30} & 0 & \frac{\sqrt{30}}{20} & 0 & 0 \\ -\frac{\sqrt{30}i}{30} & 0 & \frac{\sqrt{30}}{20} & 0 & 0 & 0 \\ 0 & \frac{\sqrt{30}}{20} & 0 & -\frac{\sqrt{30}i}{15} & \frac{\sqrt{30}}{20} & 0 \\ \frac{\sqrt{30}}{20} & 0 & \frac{\sqrt{30}i}{15} & 0 & 0 & -\frac{\sqrt{30}}{20} \\ 0 & 0 & \frac{\sqrt{30}}{20} & 0 & 0 & \frac{\sqrt{30}i}{30} \\ 0 & 0 & 0 & -\frac{\sqrt{30}}{20} & -\frac{\sqrt{30}i}{30} & 0 \end{bmatrix}$$

$$\boxed{x59} \quad \mathbb{M}_1^{(1,1;a)}(B_{3g}) = \begin{bmatrix} 0 & \frac{\sqrt{30}}{15} & 0 & -\frac{\sqrt{30}i}{20} & \frac{\sqrt{30}}{20} & 0 \\ \frac{\sqrt{30}}{15} & 0 & \frac{\sqrt{30}i}{20} & 0 & 0 & -\frac{\sqrt{30}}{20} \\ 0 & -\frac{\sqrt{30}i}{20} & 0 & -\frac{\sqrt{30}}{30} & 0 & 0 \\ \frac{\sqrt{30}i}{20} & 0 & -\frac{\sqrt{30}}{30} & 0 & 0 & 0 \\ \frac{\sqrt{30}}{20} & 0 & 0 & 0 & 0 & -\frac{\sqrt{30}}{30} \\ 0 & -\frac{\sqrt{30}}{20} & 0 & 0 & -\frac{\sqrt{30}}{30} & 0 \end{bmatrix}$$

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

$$\boxed{x61} \quad \mathbb{T}_2^{(1,0;a)}(A_g, 2) = \begin{bmatrix} 0 & 0 & -\frac{\sqrt{6}}{6} & 0 & 0 & -\frac{\sqrt{6}i}{12} \\ 0 & 0 & 0 & \frac{\sqrt{6}}{6} & \frac{\sqrt{6}i}{12} & 0 \\ -\frac{\sqrt{6}}{6} & 0 & 0 & 0 & 0 & \frac{\sqrt{6}}{12} \\ 0 & \frac{\sqrt{6}}{6} & 0 & 0 & \frac{\sqrt{6}}{12} & 0 \\ 0 & -\frac{\sqrt{6}i}{12} & 0 & \frac{\sqrt{6}}{12} & 0 & 0 \\ \frac{\sqrt{6}i}{12} & 0 & \frac{\sqrt{6}}{12} & 0 & 0 & 0 \end{bmatrix}$$

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

$$\boxed{x63} \quad \mathbb{T}_2^{(1,0;a)}(B_{2g}) = \begin{bmatrix} 0 & \frac{\sqrt{6}i}{6} & 0 & \frac{\sqrt{6}}{12} & 0 & 0 \\ -\frac{\sqrt{6}i}{6} & 0 & \frac{\sqrt{6}}{12} & 0 & 0 & 0 \\ 0 & \frac{\sqrt{6}}{12} & 0 & 0 & -\frac{\sqrt{6}}{12} & 0 \\ \frac{\sqrt{6}}{12} & 0 & 0 & 0 & 0 & \frac{\sqrt{6}}{12} \\ 0 & 0 & -\frac{\sqrt{6}}{12} & 0 & 0 & -\frac{\sqrt{6}i}{6} \\ 0 & 0 & 0 & \frac{\sqrt{6}}{12} & \frac{\sqrt{6}i}{6} & 0 \end{bmatrix}$$

$$\boxed{x64} \quad \mathbb{T}_2^{(1,0;a)}(B_{3g}) = \begin{bmatrix} 0 & 0 & 0 & \frac{\sqrt{6}i}{12} & \frac{\sqrt{6}}{12} & 0 \\ 0 & 0 & -\frac{\sqrt{6}i}{12} & 0 & 0 & -\frac{\sqrt{6}}{12} \\ 0 & \frac{\sqrt{6}i}{12} & 0 & \frac{\sqrt{6}}{6} & 0 & 0 \\ -\frac{\sqrt{6}i}{12} & 0 & \frac{\sqrt{6}}{6} & 0 & 0 & 0 \\ \frac{\sqrt{6}}{12} & 0 & 0 & 0 & 0 & -\frac{\sqrt{6}}{6} \\ 0 & -\frac{\sqrt{6}}{12} & 0 & 0 & -\frac{\sqrt{6}}{6} & 0 \end{bmatrix}$$

- Site cluster

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

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

- Bond cluster

\*\* Wyckoff: **1a@1c**

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

$$\boxed{y3} \quad \mathbb{T}_1^{(s)}(B_{1u}) = [i]$$

\*\* Wyckoff: **1b@1e**

$$\boxed{y4} \quad \mathbb{Q}_0^{(s)}(A_g) = [1]$$

$$\boxed{y5} \quad \mathbb{T}_1^{(s)}(B_{2u}) = [i]$$

\*\* Wyckoff: **1c@1b**

$$\boxed{y6} \quad \mathbb{Q}_0^{(s)}(A_g) = [1]$$

$$\boxed{y7} \quad \mathbb{T}_1^{(s)}(B_{3u}) = [i]$$

\*\* Wyckoff: **2d@1f**

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

$$\boxed{y9} \quad \mathbb{Q}_2^{(s)}(B_{1g}) = \left[ \frac{\sqrt{2}}{2}, -\frac{\sqrt{2}}{2} \right]$$

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

$$\boxed{y11} \quad \mathbb{T}_1^{(s)}(B_{3u}) = \left[ \frac{\sqrt{2}i}{2}, -\frac{\sqrt{2}i}{2} \right]$$

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— Site and Bond —

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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 —

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

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

SL	position ( $s$ )	mapping
1	[ 0.00000, 0.00000, 0.00000]	[1,2,3,4,5,6,7,8]

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### Bond in Unit Cell

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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 (1c@1b), ND,  $|\mathbf{v}|=1.0$  (cartesian)

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

Table 9: 2-th 'A'-'A' [1] (#2) bond cluster (1b@1e), ND,  $|\mathbf{v}|=1.2$  (cartesian)

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

Table 10: 3-th 'A'-'A' [1] (#3) bond cluster (**1a@1c**), 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]	(1,1)	(1,1)	[0,0,1]

Table 11: 4-th 'A'-'A' [1] (#4) bond cluster (**2d@1f**), ND,  $|\mathbf{v}|=1.56205$  (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,-5,6]	(1,1)	(1,1)	[1,1,0]
2	[ 1.00000, -1.00000, 0.00000]	[ 0.50000, 0.50000, 0.00000]	[3,-4,-7,8]	(1,1)	(1,1)	[-1,1,0]