

# Model for “BCT”

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## General Condition

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

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## Group and Unit Cell

- Group: SG No. 139  $D_{4h}^{17}$   $I4/mmm$  [ tetragonal ]
- Associated point group: PG No. 139  $D_{4h}$   $4/mmm$  [ tetragonal ]
- Unit cell:
  - $a = 1.00000$ ,  $b = 1.00000$ ,  $c = 2.32000$ ,  $\alpha = 90.0$ ,  $\beta = 90.0$ ,  $\gamma = 90.0$
- Lattice vectors (conventional cell):
  - $\mathbf{a}_1 = [ 1.00000, 0.00000, 0.00000 ]$
  - $\mathbf{a}_2 = [ 0.00000, 1.00000, 0.00000 ]$
  - $\mathbf{a}_3 = [ 0.00000, 0.00000, 2.32000 ]$

- Plus sets:  
 $+ [0, 0, 0], \quad + [\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$

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## Symmetry Operation

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Table 1: Symmetry operation

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

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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	$G, M$	-	-	$-\frac{x^2}{2} - \frac{y^2}{2} + z^2$

*continued ...*

Table 2

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

continued ...

Table 2

#	symbol	irrep.	rank	X	multiplicity	component	symmetry
26	$\mathbb{Q}_{2,1}(E_g)$	$E_g$	2	$Q, T$	-	1	$\sqrt{3}yz$
27	$\mathbb{Q}_{2,2}(E_g)$					2	$\sqrt{3}xz$
28	$\mathbb{G}_{3,1}(E_g, 1)$	$E_g$	3	$G, M$	1	1	$\frac{x(2x^2-3y^2-3z^2)}{2}$
29	$\mathbb{G}_{3,2}(E_g, 1)$					2	$\frac{y(3x^2-2y^2+3z^2)}{2}$
30	$\mathbb{G}_{3,1}(E_g, 2)$	$E_g$	3	$G, M$	2	1	$\frac{\sqrt{15}x(y-z)(y+z)}{2}$
31	$\mathbb{G}_{3,2}(E_g, 2)$					2	$-\frac{\sqrt{15}y(x-z)(x+z)}{2}$
32	$\mathbb{Q}_{4,1}(E_g, 1)$	$E_g$	4	$Q, T$	1	1	$\frac{\sqrt{35}yz(y-z)(y+z)}{2}$
33	$\mathbb{Q}_{4,2}(E_g, 1)$					2	$\frac{\sqrt{35}xz(x-z)(x+z)}{2}$
34	$\mathbb{Q}_{1,1}(E_u)$	$E_u$	1	$Q, T$	-	1	$x$
35	$\mathbb{Q}_{1,2}(E_u)$					2	$y$
36	$\mathbb{G}_{2,1}(E_u)$	$E_u$	2	$G, M$	-	1	$\sqrt{3}yz$
37	$\mathbb{G}_{2,2}(E_u)$					2	$-\sqrt{3}xz$
38	$\mathbb{Q}_{3,1}(E_u, 1)$	$E_u$	3	$Q, T$	1	1	$\frac{x(2x^2-3y^2-3z^2)}{2}$
39	$\mathbb{Q}_{3,2}(E_u, 1)$					2	$-\frac{y(3x^2-2y^2+3z^2)}{2}$
40	$\mathbb{Q}_{3,1}(E_u, 2)$	$E_u$	3	$Q, T$	2	1	$\frac{\sqrt{15}x(y-z)(y+z)}{2}$
41	$\mathbb{Q}_{3,2}(E_u, 2)$					2	$\frac{\sqrt{15}y(x-z)(x+z)}{2}$
42	$\mathbb{G}_{4,1}(E_u, 1)$	$E_u$	4	$G, M$	1	1	$\frac{\sqrt{35}yz(y-z)(y+z)}{2}$
43	$\mathbb{G}_{4,2}(E_u, 1)$					2	$-\frac{\sqrt{35}xz(x-z)(x+z)}{2}$

Table 3: dimension = 6

#	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)$								

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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267 (all 267) SAMBs

- 'A' site-cluster : **A**
  - \* bra:  $\langle s, \uparrow|, \langle s, \downarrow|$
  - \* ket:  $|s, \uparrow\rangle, |s, \downarrow\rangle$
  - \* wyckoff: **2a**

z1

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

• 'A' site-cluster : A

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

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

\* wyckoff: 2a

$$\boxed{\text{z113}} \quad \mathbb{G}_2^{(1,-1;c)}(A_{1u}) = \mathbb{G}_2^{(1,-1;a)}(A_{1u})\mathbb{Q}_0^{(s)}(A_{1g})$$

$$\boxed{\text{z136}} \quad \mathbb{Q}_1^{(1,0;c)}(A_{2u}) = \mathbb{Q}_1^{(1,0;a)}(A_{2u})\mathbb{Q}_0^{(s)}(A_{1g})$$

$$\boxed{\text{z153}} \quad \mathbb{G}_2^{(1,-1;c)}(B_{1u}) = \mathbb{G}_2^{(1,-1;a)}(B_{1u})\mathbb{Q}_0^{(s)}(A_{1g})$$

$$\boxed{\text{z171}} \quad \mathbb{G}_2^{(1,-1;c)}(B_{2u}) = \mathbb{G}_2^{(1,-1;a)}(B_{2u})\mathbb{Q}_0^{(s)}(A_{1g})$$

$$\boxed{\text{z192}} \quad \mathbb{Q}_{1,1}^{(c)}(E_u) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

$$\boxed{\text{z193}} \quad \mathbb{Q}_{1,2}^{(c)}(E_u) = \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

$$\boxed{\text{z194}} \quad \mathbb{Q}_{1,1}^{(1,0;c)}(E_u) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(1,0;a)}(E_u)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

$$\boxed{\text{z195}} \quad \mathbb{Q}_{1,2}^{(1,0;c)}(E_u) = \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(1,0;a)}(E_u)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

• 'A' site-cluster : A

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

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

\* wyckoff: 2a

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

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

$$\boxed{\text{z33}} \quad \mathbb{Q}_2^{(c)}(B_{1g}) = \mathbb{Q}_2^{(a)}(B_{1g})\mathbb{Q}_0^{(s)}(A_{1g})$$

$$\boxed{\text{z48}} \quad \mathbb{Q}_2^{(c)}(B_{2g}) = \mathbb{Q}_2^{(a)}(B_{2g})\mathbb{Q}_0^{(s)}(A_{1g})$$

$$\boxed{\text{z63}} \quad \mathbb{Q}_{2,1}^{(1,-1;c)}(E_g) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

$$\boxed{\text{z64}} \quad \mathbb{Q}_{2,2}^{(1,-1;c)}(E_g) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

- 'A'-'A' bond-cluster : **A;A\_001\_1**
  - \* bra:  $\langle s, \uparrow |, \langle s, \downarrow |$
  - \* ket:  $|s, \uparrow \rangle, |s, \downarrow \rangle$
  - \* wyckoff: **4b@4c**

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

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

$$\boxed{\text{z114}} \quad \mathbb{Q}_1^{(1,-1;c)}(A_{2u}) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

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

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

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

$$\boxed{\text{z196}} \quad \mathbb{Q}_{1,1}^{(1,-1;c)}(E_u) = -\frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z197}} \quad \mathbb{Q}_{1,2}^{(1,-1;c)}(E_u) = \frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

- 'A'-'A' bond-cluster : **A;A\_001\_1**
  - \* bra:  $\langle s, \uparrow |, \langle s, \downarrow |$
  - \* ket:  $|p_x, \uparrow \rangle, |p_x, \downarrow \rangle, |p_y, \uparrow \rangle, |p_y, \downarrow \rangle$
  - \* wyckoff: **4b@4c**

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

$$\boxed{\text{z6}} \quad \mathbb{Q}_2^{(1,-1;c)}(A_{1g}) = -\frac{\sqrt{2}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

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

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

$$\boxed{\text{z35}} \quad \mathbb{G}_1^{(c)}(A_{2g}) = \frac{\sqrt{2}\mathbb{T}_{1,1}^{(a)}(Eu)\mathbb{T}_{1,2}^{(b)}(Eu)}{2} - \frac{\sqrt{2}\mathbb{T}_{1,2}^{(a)}(Eu)\mathbb{T}_{1,1}^{(b)}(Eu)}{2}$$

$$\boxed{\text{z36}} \quad \mathbb{G}_1^{(1,-1;c)}(A_{2g}) = \frac{\sqrt{2}\mathbb{M}_{2,1}^{(1,-1;a)}(Eu)\mathbb{T}_{1,2}^{(b)}(Eu)}{2} - \frac{\sqrt{2}\mathbb{M}_{2,2}^{(1,-1;a)}(Eu)\mathbb{T}_{1,1}^{(b)}(Eu)}{2}$$

$$\boxed{\text{z49}} \quad \mathbb{Q}_1^{(1,-1;c)}(A_{2u}) = -\mathbb{G}_2^{(1,-1;a)}(B_{2u})\mathbb{Q}_2^{(b)}(B_{1g})$$

$$\boxed{\text{z50}} \quad \mathbb{Q}_1^{(1,0;c)}(A_{2u}) = \mathbb{Q}_1^{(1,0;a)}(A_{2u})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z65}} \quad \mathbb{Q}_2^{(c)}(B_{1g}) = \frac{\sqrt{2}\mathbb{T}_{1,1}^{(a)}(Eu)\mathbb{T}_{1,1}^{(b)}(Eu)}{2} - \frac{\sqrt{2}\mathbb{T}_{1,2}^{(a)}(Eu)\mathbb{T}_{1,2}^{(b)}(Eu)}{2}$$

$$\boxed{\text{z66}} \quad \mathbb{Q}_2^{(1,-1;c)}(B_{1g}) = -\frac{\sqrt{2}\mathbb{M}_{2,1}^{(1,-1;a)}(Eu)\mathbb{T}_{1,1}^{(b)}(Eu)}{2} + \frac{\sqrt{2}\mathbb{M}_{2,2}^{(1,-1;a)}(Eu)\mathbb{T}_{1,2}^{(b)}(Eu)}{2}$$

$$\boxed{\text{z67}} \quad \mathbb{Q}_3^{(1,-1;c)}(B_{1u}) = \mathbb{G}_2^{(1,-1;a)}(A_{1u})\mathbb{Q}_2^{(b)}(B_{1g})$$

$$\boxed{\text{z68}} \quad \mathbb{G}_2^{(1,-1;c)}(B_{1u}) = \mathbb{G}_2^{(1,-1;a)}(B_{1u})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z69}} \quad \mathbb{Q}_2^{(c)}(B_{2g}) = \frac{\sqrt{2}\mathbb{T}_{1,1}^{(a)}(Eu)\mathbb{T}_{1,2}^{(b)}(Eu)}{2} + \frac{\sqrt{2}\mathbb{T}_{1,2}^{(a)}(Eu)\mathbb{T}_{1,1}^{(b)}(Eu)}{2}$$

$$\boxed{\text{z70}} \quad \mathbb{Q}_2^{(1,-1;c)}(B_{2g}) = -\frac{\sqrt{2}\mathbb{M}_{2,1}^{(1,-1;a)}(Eu)\mathbb{T}_{1,2}^{(b)}(Eu)}{2} - \frac{\sqrt{2}\mathbb{M}_{2,2}^{(1,-1;a)}(Eu)\mathbb{T}_{1,1}^{(b)}(Eu)}{2}$$

$$\boxed{\text{z71}} \quad \mathbb{Q}_3^{(1,0;c)}(B_{2u}) = \mathbb{Q}_1^{(1,0;a)}(A_{2u})\mathbb{Q}_2^{(b)}(B_{1g})$$

$$\boxed{\text{z72}} \quad \mathbb{G}_2^{(1,-1;c)}(B_{2u}) = \mathbb{G}_2^{(1,-1;a)}(B_{2u})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z115}} \quad \mathbb{Q}_{2,1}^{(1,-1;c)}(E_g) = \frac{\sqrt{30}\mathbb{M}_2^{(1,-1;a)}(A_{1u})\mathbb{T}_{1,1}^{(b)}(Eu)}{10} + \frac{\sqrt{10}\mathbb{M}_2^{(1,-1;a)}(B_{1u})\mathbb{T}_{1,1}^{(b)}(Eu)}{10} + \frac{\sqrt{10}\mathbb{M}_2^{(1,-1;a)}(B_{2u})\mathbb{T}_{1,2}^{(b)}(Eu)}{10}$$

$$\boxed{\text{z116}} \quad \mathbb{Q}_{2,2}^{(1,-1;c)}(E_g) = -\frac{\sqrt{30}\mathbb{M}_2^{(1,-1;a)}(A_{1u})\mathbb{T}_{1,2}^{(b)}(Eu)}{10} + \frac{\sqrt{10}\mathbb{M}_2^{(1,-1;a)}(B_{1u})\mathbb{T}_{1,2}^{(b)}(Eu)}{10} - \frac{\sqrt{10}\mathbb{M}_2^{(1,-1;a)}(B_{2u})\mathbb{T}_{1,1}^{(b)}(Eu)}{10}$$



$$\boxed{\text{z138}} \quad \mathbb{Q}_{2,1}^{(1,0;c)}(E_g) = \frac{\sqrt{2}\mathbb{T}_1^{(1,0;a)}(A_{2u})\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z139}} \quad \mathbb{Q}_{2,2}^{(1,0;c)}(E_g) = \frac{\sqrt{2}\mathbb{T}_1^{(1,0;a)}(A_{2u})\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z155}} \quad \mathbb{G}_{1,1}^{(1,-1;c)}(E_g) = -\frac{\sqrt{5}\mathbb{M}_2^{(1,-1;a)}(A_{1u})\mathbb{T}_{1,1}^{(b)}(E_u)}{5} + \frac{\sqrt{15}\mathbb{M}_2^{(1,-1;a)}(B_{1u})\mathbb{T}_{1,1}^{(b)}(E_u)}{10} + \frac{\sqrt{15}\mathbb{M}_2^{(1,-1;a)}(B_{2u})\mathbb{T}_{1,2}^{(b)}(E_u)}{10}$$

$$\boxed{\text{z156}} \quad \mathbb{G}_{1,2}^{(1,-1;c)}(E_g) = \frac{\sqrt{5}\mathbb{M}_2^{(1,-1;a)}(A_{1u})\mathbb{T}_{1,2}^{(b)}(E_u)}{5} + \frac{\sqrt{15}\mathbb{M}_2^{(1,-1;a)}(B_{1u})\mathbb{T}_{1,2}^{(b)}(E_u)}{10} - \frac{\sqrt{15}\mathbb{M}_2^{(1,-1;a)}(B_{2u})\mathbb{T}_{1,1}^{(b)}(E_u)}{10}$$

$$\boxed{\text{z173}} \quad \mathbb{G}_{3,1}^{(1,-1;c)}(E_g, 1) = \frac{\mathbb{M}_2^{(1,-1;a)}(B_{1u})\mathbb{T}_{1,1}^{(b)}(E_u)}{2} - \frac{\mathbb{M}_2^{(1,-1;a)}(B_{2u})\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z174}} \quad \mathbb{G}_{3,2}^{(1,-1;c)}(E_g, 1) = \frac{\mathbb{M}_2^{(1,-1;a)}(B_{1u})\mathbb{T}_{1,2}^{(b)}(E_u)}{2} + \frac{\mathbb{M}_2^{(1,-1;a)}(B_{2u})\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z198}} \quad \mathbb{Q}_{1,1}^{(c)}(E_u, a) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z199}} \quad \mathbb{Q}_{1,2}^{(c)}(E_u, a) = \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z200}} \quad \mathbb{Q}_{1,1}^{(c)}(E_u, b) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_2^{(b)}(B_{1g})}{2}$$

$$\boxed{\text{z201}} \quad \mathbb{Q}_{1,2}^{(c)}(E_u, b) = -\frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_2^{(b)}(B_{1g})}{2}$$

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

$$\boxed{\text{z203}} \quad \mathbb{Q}_{1,2}^{(1,0;c)}(E_u, a) = \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(1,0;a)}(E_u)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z204}} \quad \mathbb{Q}_{1,1}^{(1,0;c)}(E_u, b) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(1,0;a)}(E_u)\mathbb{Q}_2^{(b)}(B_{1g})}{2}$$

$$\boxed{\text{z205}} \quad \mathbb{Q}_{1,2}^{(1,0;c)}(E_u, b) = -\frac{\sqrt{2}\mathbb{Q}_{1,2}^{(1,0;a)}(E_u)\mathbb{Q}_2^{(b)}(B_{1g})}{2}$$

• 'A'-'A' bond-cluster : A;A\_001\_1

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

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

\* wyckoff: 4b04c

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

$$\boxed{\text{z8}} \quad \mathbb{Q}_0^{(c)}(A_{1g}, b) = \mathbb{Q}_2^{(a)}(B_{1g})\mathbb{Q}_2^{(b)}(B_{1g})$$

$$\boxed{\text{z9}} \quad \mathbb{Q}_2^{(1,-1;c)}(A_{1g}) = \mathbb{Q}_2^{(1,-1;a)}(A_{1g})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z25}} \quad \mathbb{G}_0^{(1,-1;c)}(A_{1u}) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z37}} \quad \mathbb{G}_2^{(1,-1;c)}(A_{1u}) = -\frac{\sqrt{3}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g, 1)\mathbb{T}_{1,1}^{(b)}(E_u)}{4} - \frac{\sqrt{5}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g, 2)\mathbb{T}_{1,1}^{(b)}(E_u)}{4} + \frac{\sqrt{3}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g, 1)\mathbb{T}_{1,2}^{(b)}(E_u)}{4} + \frac{\sqrt{5}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g, 2)\mathbb{T}_{1,2}^{(b)}(E_u)}{4}$$

$$\boxed{\text{z38}} \quad \mathbb{G}_4^{(1,-1;c)}(A_{1u}, 1) = \frac{\sqrt{5}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g, 1)\mathbb{T}_{1,1}^{(b)}(E_u)}{4} - \frac{\sqrt{3}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g, 2)\mathbb{T}_{1,1}^{(b)}(E_u)}{4} - \frac{\sqrt{5}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g, 1)\mathbb{T}_{1,2}^{(b)}(E_u)}{4} + \frac{\sqrt{3}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g, 2)\mathbb{T}_{1,2}^{(b)}(E_u)}{4}$$

$$\boxed{\text{z39}} \quad \mathbb{Q}_4^{(c)}(A_{2g}) = \mathbb{Q}_2^{(a)}(B_{2g})\mathbb{Q}_2^{(b)}(B_{1g})$$

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

$$\boxed{\text{z73}} \quad \mathbb{Q}_3^{(1,-1;c)}(A_{2u}) = -\frac{\sqrt{3}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g, 1)\mathbb{T}_{1,2}^{(b)}(E_u)}{4} - \frac{\sqrt{5}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g, 2)\mathbb{T}_{1,2}^{(b)}(E_u)}{4} - \frac{\sqrt{3}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g, 1)\mathbb{T}_{1,1}^{(b)}(E_u)}{4} - \frac{\sqrt{5}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g, 2)\mathbb{T}_{1,1}^{(b)}(E_u)}{4}$$

$$\boxed{\text{z74}} \quad \mathbb{G}_4^{(1,-1;c)}(A_{2u}) = \frac{\sqrt{5}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g, 1)\mathbb{T}_{1,2}^{(b)}(E_u)}{4} - \frac{\sqrt{3}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g, 2)\mathbb{T}_{1,2}^{(b)}(E_u)}{4} + \frac{\sqrt{5}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g, 1)\mathbb{T}_{1,1}^{(b)}(E_u)}{4} - \frac{\sqrt{3}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g, 2)\mathbb{T}_{1,1}^{(b)}(E_u)}{4}$$

$$\boxed{\text{z75}} \quad \mathbb{Q}_2^{(c)}(B_{1g}, a) = \mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_2^{(b)}(B_{1g})$$

$$\boxed{\text{z76}} \quad \mathbb{Q}_2^{(c)}(B_{1g}, b) = \mathbb{Q}_2^{(a)}(B_{1g})\mathbb{Q}_0^{(b)}(A_{1g})$$

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

$$\boxed{\text{z118}} \quad \mathbb{Q}_3^{(1,-1;c)}(B_{1u}) = -\frac{\sqrt{2}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g, 2)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g, 2)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z119}} \quad \mathbb{G}_2^{(1,-1;c)}(B_{1u}, a) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z140}} \quad \mathbb{G}_2^{(1,-1;c)}(B_{1u}, b) = \frac{\sqrt{2}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g, 1)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g, 1)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z141}} \quad \mathbb{Q}_2^{(c)}(B_{2g}) = \mathbb{Q}_2^{(a)}(B_{2g})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z142}} \quad \mathbb{Q}_3^{(1,-1;c)}(B_{2u}) = \frac{\sqrt{30}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g, 1)\mathbb{T}_{1,2}^{(b)}(E_u)}{8} + \frac{\sqrt{2}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g, 2)\mathbb{T}_{1,2}^{(b)}(E_u)}{8} - \frac{\sqrt{30}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g, 1)\mathbb{T}_{1,1}^{(b)}(E_u)}{8} - \frac{\sqrt{2}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g, 2)\mathbb{T}_{1,1}^{(b)}(E_u)}{8}$$

$$\boxed{\text{z157}} \quad \mathbb{G}_2^{(1,-1;c)}(B_{2u}, a) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z158}} \quad \mathbb{G}_2^{(1,-1;c)}(B_{2u}, b) = -\frac{\sqrt{2}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g, 1)\mathbb{T}_{1,2}^{(b)}(E_u)}{8} + \frac{\sqrt{30}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g, 2)\mathbb{T}_{1,2}^{(b)}(E_u)}{8} + \frac{\sqrt{2}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g, 1)\mathbb{T}_{1,1}^{(b)}(E_u)}{8} - \frac{\sqrt{30}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g, 2)\mathbb{T}_{1,1}^{(b)}(E_u)}{8}$$

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

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

$$\boxed{\text{z176}} \quad \mathbb{Q}_{2,1}^{(1,-1;c)}(E_g, b) = -\frac{\sqrt{2}\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_2^{(b)}(B_{1g})}{2}$$

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

$$\boxed{\text{z206}} \quad \mathbb{Q}_{1,1}^{(c)}(E_u) = -\frac{\sqrt{2}\mathbb{M}_1^{(a)}(A_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z207}} \quad \mathbb{Q}_{1,2}^{(c)}(E_u) = \frac{\sqrt{2}\mathbb{M}_1^{(a)}(A_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z208}} \quad \mathbb{Q}_{1,1}^{(1,-1;c)}(E_u) = -\frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z209}} \quad \mathbb{Q}_{1,2}^{(1,-1;c)}(E_u) = \frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z210}} \quad \mathbb{Q}_{3,1}^{(1,-1;c)}(E_u, 1) = -\frac{\sqrt{2}\mathbb{M}_3^{(1,-1;a)}(B_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z211}} \quad \mathbb{Q}_{3,2}^{(1,-1;c)}(E_u, 1) = -\frac{\sqrt{2}\mathbb{M}_3^{(1,-1;a)}(B_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z212}} \quad \mathbb{Q}_{3,1}^{(1,-1;c)}(E_u, 2) = \frac{\sqrt{2}\mathbb{M}_3^{(1,-1;a)}(B_{1g})\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z213}} \quad \mathbb{Q}_{3,2}^{(1,-1;c)}(E_u, 2) = -\frac{\sqrt{2}\mathbb{M}_3^{(1,-1;a)}(B_{1g})\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

• 'A'-'A' bond-cluster : A;A\_002\_1

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

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

\* wyckoff: **8a08f**

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

$$\boxed{\text{z52}} \quad \mathbb{G}_0^{(1,-1;c)}(A_{1u}) = \frac{\sqrt{3}\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{3} - \frac{\sqrt{3}\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{3} + \frac{\sqrt{3}\mathbb{M}_1^{(1,-1;a)}(A_{2g})\mathbb{T}_1^{(b)}(A_{2u})}{3}$$

$$\boxed{\text{z77}} \quad \mathbb{G}_2^{(1,-1;c)}(A_{1u}) = -\frac{\sqrt{6}\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{6} + \frac{\sqrt{6}\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{6} + \frac{\sqrt{6}\mathbb{M}_1^{(1,-1;a)}(A_{2g})\mathbb{T}_1^{(b)}(A_{2u})}{3}$$

$$\boxed{\text{z78}} \quad \mathbb{Q}_1^{(1,-1;c)}(A_{2u}) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

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

$$\boxed{\text{z121}} \quad \mathbb{Q}_2^{(c)}(B_{2g}) = \mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_2^{(b)}(B_{2g})$$

$$\boxed{\text{z143}} \quad \mathbb{Q}_3^{(1,-1;c)}(B_{2u}) = \mathbb{M}_1^{(1,-1;a)}(A_{2g})\mathbb{M}_2^{(b)}(B_{1u})$$

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

$$\boxed{\text{z178}} \quad \mathbb{Q}_{2,1}^{(c)}(E_g) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z179}} \quad \mathbb{Q}_{2,2}^{(c)}(E_g) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$$

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

$$\boxed{\text{z215}} \quad \mathbb{Q}_{1,2}^{(1,-1;c)}(E_u, a) = -\frac{\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_1^{(b)}(A_{2u})}{2} + \frac{\mathbb{M}_1^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z216}} \quad \mathbb{Q}_{1,1}^{(1,-1;c)}(E_u, b) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{M}_2^{(b)}(B_{1u})}{2}$$

$$\boxed{\text{z217}} \quad \mathbb{Q}_{1,2}^{(1,-1;c)}(E_u, b) = \frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{M}_2^{(b)}(B_{1u})}{2}$$

$$\boxed{\text{z218}} \quad \mathbb{G}_{2,1}^{(1,-1;c)}(E_u) = -\frac{\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_1^{(b)}(A_{2u})}{2} + \frac{\mathbb{M}_1^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z219}} \quad \mathbb{G}_{2,2}^{(1,-1;c)}(E_u) = -\frac{\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_1^{(b)}(A_{2u})}{2} - \frac{\mathbb{M}_1^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

• 'A'-'A' bond-cluster : A;A\_002\_1

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

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

\* wyckoff: 8a08f

$$\boxed{\text{z11}} \quad \mathbb{Q}_0^{(c)}(A_{1g}) = \frac{\sqrt{2}\mathbb{T}_{1,1}^{(a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{T}_{1,2}^{(a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z12}} \quad \mathbb{Q}_0^{(1,-1;c)}(A_{1g}) = \mathbb{M}_2^{(1,-1;a)}(B_{1u})\mathbb{M}_2^{(b)}(B_{1u})$$

$$\boxed{\text{z13}} \quad \mathbb{Q}_2^{(1,-1;c)}(A_{1g}) = -\frac{\sqrt{2}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z14}} \quad \mathbb{Q}_0^{(1,0;c)}(A_{1g}) = \mathbb{T}_1^{(1,0;a)}(A_{2u})\mathbb{T}_1^{(b)}(A_{2u})$$

$$\boxed{\text{z26}} \quad \mathbb{G}_2^{(c)}(A_{1u}) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} - \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z27}} \quad \mathbb{G}_0^{(1,-1;c)}(A_{1u}) = \mathbb{G}_2^{(1,-1;a)}(B_{2u})\mathbb{Q}_2^{(b)}(B_{2g})$$

$$\boxed{\text{z28}} \quad \mathbb{G}_2^{(1,-1;c)}(A_{1u}) = \mathbb{G}_2^{(1,-1;a)}(A_{1u})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z29}} \quad \mathbb{G}_2^{(1,0;c)}(A_{1u}) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(1,0;a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} - \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(1,0;a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z40}} \quad \mathbb{Q}_4^{(1,-1;c)}(A_{2g}) = \mathbb{M}_2^{(1,-1;a)}(B_{2u})\mathbb{M}_2^{(b)}(B_{1u})$$

$$\boxed{\text{z41}} \quad \mathbb{G}_1^{(c)}(A_{2g}) = \frac{\sqrt{2}\mathbb{T}_{1,1}^{(a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{T}_{1,2}^{(a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z42}} \quad \mathbb{G}_1^{(1,-1;c)}(A_{2g}) = \frac{\sqrt{30}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{10} - \frac{\sqrt{30}\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{10} + \frac{\sqrt{10}\mathbb{M}_2^{(1,-1;a)}(A_{1u})\mathbb{T}_1^{(b)}(A_{2u})}{5}$$

$$\boxed{\text{z43}} \quad \mathbb{G}_3^{(1,-1;c)}(A_{2g}) = -\frac{\sqrt{5}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{5} + \frac{\sqrt{5}\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{5} + \frac{\sqrt{15}\mathbb{M}_2^{(1,-1;a)}(A_{1u})\mathbb{T}_1^{(b)}(A_{2u})}{5}$$

$$\boxed{\text{z53}} \quad \mathbb{Q}_1^{(c)}(A_{2u}) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2} + \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z54}} \quad \mathbb{Q}_1^{(1,-1;c)}(A_{2u}) = \mathbb{G}_2^{(1,-1;a)}(B_{1u})\mathbb{Q}_2^{(b)}(B_{2g})$$

$$\boxed{\text{z55}} \quad \mathbb{Q}_1^{(1,0;c)}(A_{2u}, a) = \mathbb{Q}_1^{(1,0;a)}(A_{2u})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z56}} \quad \mathbb{Q}_1^{(1,0;c)}(A_{2u}, b) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(1,0;a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2} + \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(1,0;a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z79}} \quad \mathbb{Q}_2^{(c)}(B_{1g}) = \frac{\sqrt{2}\mathbb{T}_{1,1}^{(a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{T}_{1,2}^{(a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z80}} \quad \mathbb{Q}_2^{(1,-1;c)}(B_{1g}, a) = -\frac{\sqrt{6}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{6} + \frac{\sqrt{6}\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{6} + \frac{\sqrt{6}\mathbb{M}_2^{(1,-1;a)}(B_{2u})\mathbb{T}_1^{(b)}(A_{2u})}{3}$$

$$\boxed{\text{z81}} \quad \mathbb{Q}_2^{(1,-1;c)}(B_{1g}, b) = -\mathbb{M}_2^{(1,-1;a)}(A_{1u})\mathbb{M}_2^{(b)}(B_{1u})$$

$$\boxed{\text{z82}} \quad \mathbb{G}_3^{(1,-1;c)}(B_{1g}) = \frac{\sqrt{3}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{3} - \frac{\sqrt{3}\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{3} + \frac{\sqrt{3}\mathbb{M}_2^{(1,-1;a)}(B_{2u})\mathbb{T}_1^{(b)}(A_{2u})}{3}$$

$$\boxed{\text{z83}} \quad \mathbb{Q}_3^{(c)}(B_{1u}) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} + \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z84}} \quad \mathbb{Q}_3^{(1,0;c)}(B_{1u}) = \frac{\sqrt{3}\mathbb{Q}_{1,1}^{(1,0;a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{3} + \frac{\sqrt{3}\mathbb{Q}_{1,2}^{(1,0;a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{3} + \frac{\sqrt{3}\mathbb{Q}_1^{(1,0;a)}(A_{2u})\mathbb{Q}_2^{(b)}(B_{2g})}{3}$$

$$\boxed{\text{z85}} \quad \mathbb{G}_2^{(1,-1;c)}(B_{1u}) = \mathbb{G}_2^{(1,-1;a)}(B_{1u})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z86}} \quad \mathbb{G}_2^{(1,0;c)}(B_{1u}) = \frac{\sqrt{6}\mathbb{Q}_{1,1}^{(1,0;a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{6} + \frac{\sqrt{6}\mathbb{Q}_{1,2}^{(1,0;a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{6} - \frac{\sqrt{6}\mathbb{Q}_1^{(1,0;a)}(A_{2u})\mathbb{Q}_2^{(b)}(B_{2g})}{3}$$

$$\boxed{\text{z87}} \quad \mathbb{Q}_2^{(c)}(B_{2g}) = \frac{\sqrt{2}\mathbb{T}_{1,1}^{(a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{T}_{1,2}^{(a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z88}} \quad \mathbb{Q}_2^{(1,-1;c)}(B_{2g}) = -\frac{\sqrt{6}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{6} - \frac{\sqrt{6}\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{6} - \frac{\sqrt{6}\mathbb{M}_2^{(1,-1;a)}(B_{1u})\mathbb{T}_1^{(b)}(A_{2u})}{3}$$

$$\boxed{\text{z89}} \quad \mathbb{Q}_2^{(1,0;c)}(B_{2g}) = \mathbb{T}_1^{(1,0;a)}(A_{2u})\mathbb{M}_2^{(b)}(B_{1u})$$

$$\boxed{\text{z90}} \quad \mathbb{G}_3^{(1,-1;c)}(B_{2g}) = -\frac{\sqrt{3}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{3} - \frac{\sqrt{3}\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{3} + \frac{\sqrt{3}\mathbb{M}_2^{(1,-1;a)}(B_{1u})\mathbb{T}_1^{(b)}(A_{2u})}{3}$$

$$\boxed{\text{z91}} \quad \mathbb{Q}_3^{(c)}(B_{2u}) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2} - \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z92}} \quad \mathbb{Q}_3^{(1,-1;c)}(B_{2u}) = -\mathbb{G}_2^{(1,-1;a)}(A_{1u})\mathbb{Q}_2^{(b)}(B_{2g})$$

$$\boxed{\text{z93}} \quad \mathbb{Q}_3^{(1,0;c)}(B_{2u}) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(1,0;a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2} - \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(1,0;a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z94}} \quad \mathbb{G}_2^{(1,-1;c)}(B_{2u}) = \mathbb{G}_2^{(1,-1;a)}(B_{2u})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z122}} \quad \mathbb{Q}_{2,1}^{(c)}(E_g, a) = \frac{\sqrt{2}\mathbb{T}_{1,2}^{(a)}(E_u)\mathbb{T}_1^{(b)}(A_{2u})}{2}$$

$$\boxed{\text{z123}} \quad \mathbb{Q}_{2,2}^{(c)}(E_g, a) = \frac{\sqrt{2}\mathbb{T}_{1,1}^{(a)}(E_u)\mathbb{T}_1^{(b)}(A_{2u})}{2}$$

$$\boxed{\text{z124}} \quad \mathbb{Q}_{2,1}^{(c)}(E_g, b) = -\frac{\sqrt{2}\mathbb{T}_{1,1}^{(a)}(E_u)\mathbb{M}_2^{(b)}(B_{1u})}{2}$$

$$\boxed{\text{z125}} \quad \mathbb{Q}_{2,2}^{(c)}(E_g, b) = -\frac{\sqrt{2}\mathbb{T}_{1,2}^{(a)}(E_u)\mathbb{M}_2^{(b)}(B_{1u})}{2}$$

$$\begin{aligned}
\text{z144} \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} \\
\text{z145} \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} \\
\text{z146} \quad \mathbb{Q}_{2,1}^{(1,-1;c)}(E_g, b) &= -\frac{\sqrt{2}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{M}_2^{(b)}(B_{1u})}{2} \\
\text{z147} \quad \mathbb{Q}_{2,2}^{(1,-1;c)}(E_g, b) &= -\frac{\sqrt{2}\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{M}_2^{(b)}(B_{1u})}{2} \\
\text{z161} \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} \\
\text{z162} \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} \\
\text{z163} \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} \\
\text{z164} \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} \\
\text{z180} \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} \\
\text{z181} \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} \\
\text{z182} \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} \\
\text{z183} \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} \\
\text{z220} \quad \mathbb{Q}_{1,1}^{(c)}(E_u, a) &= \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_0^{(b)}(A_{1g})}{2} \\
\text{z221} \quad \mathbb{Q}_{1,2}^{(c)}(E_u, a) &= \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_0^{(b)}(A_{1g})}{2}
\end{aligned}$$



$$\begin{aligned}
\boxed{\text{z222}} \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{z223}} \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{z224}} \quad \mathbb{Q}_{1,1}^{(1,-1;c)}(E_u) &= -\frac{\sqrt{30}\mathbb{G}_2^{(1,-1;a)}(A_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{10} - \frac{\sqrt{10}\mathbb{G}_2^{(1,-1;a)}(B_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{10} + \frac{\sqrt{10}\mathbb{G}_2^{(1,-1;a)}(B_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{10} \\
\boxed{\text{z225}} \quad \mathbb{Q}_{1,2}^{(1,-1;c)}(E_u) &= \frac{\sqrt{30}\mathbb{G}_2^{(1,-1;a)}(A_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{10} - \frac{\sqrt{10}\mathbb{G}_2^{(1,-1;a)}(B_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{10} - \frac{\sqrt{10}\mathbb{G}_2^{(1,-1;a)}(B_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{10} \\
\boxed{\text{z226}} \quad \mathbb{Q}_{3,1}^{(1,-1;c)}(E_u, 1) &= \frac{\sqrt{30}\mathbb{G}_2^{(1,-1;a)}(A_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{20} + \frac{\sqrt{10}\mathbb{G}_2^{(1,-1;a)}(B_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{20} + \frac{\sqrt{10}\mathbb{G}_2^{(1,-1;a)}(B_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{5} \\
\boxed{\text{z227}} \quad \mathbb{Q}_{3,2}^{(1,-1;c)}(E_u, 1) &= -\frac{\sqrt{30}\mathbb{G}_2^{(1,-1;a)}(A_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{20} + \frac{\sqrt{10}\mathbb{G}_2^{(1,-1;a)}(B_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{20} - \frac{\sqrt{10}\mathbb{G}_2^{(1,-1;a)}(B_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{5} \\
\boxed{\text{z228}} \quad \mathbb{Q}_{3,1}^{(1,-1;c)}(E_u, 2) &= \frac{\sqrt{2}\mathbb{G}_2^{(1,-1;a)}(A_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{4} - \frac{\sqrt{6}\mathbb{G}_2^{(1,-1;a)}(B_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{4} \\
\boxed{\text{z229}} \quad \mathbb{Q}_{3,2}^{(1,-1;c)}(E_u, 2) &= -\frac{\sqrt{2}\mathbb{G}_2^{(1,-1;a)}(A_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{4} - \frac{\sqrt{6}\mathbb{G}_2^{(1,-1;a)}(B_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{4} \\
\boxed{\text{z230}} \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{z231}} \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{z232}} \quad \mathbb{Q}_{1,1}^{(1,0;c)}(E_u, b) &= \frac{\mathbb{Q}_{1,2}^{(1,0;a)}(E_u)\mathbb{Q}_2^{(b)}(B_{2g})}{2} + \frac{\mathbb{Q}_1^{(1,0;a)}(A_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2} \\
\boxed{\text{z233}} \quad \mathbb{Q}_{1,2}^{(1,0;c)}(E_u, b) &= \frac{\mathbb{Q}_{1,1}^{(1,0;a)}(E_u)\mathbb{Q}_2^{(b)}(B_{2g})}{2} + \frac{\mathbb{Q}_1^{(1,0;a)}(A_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} \\
\boxed{\text{z234}} \quad \mathbb{Q}_{3,1}^{(1,0;c)}(E_u, 2) &= \frac{\mathbb{Q}_{1,2}^{(1,0;a)}(E_u)\mathbb{Q}_2^{(b)}(B_{2g})}{2} - \frac{\mathbb{Q}_1^{(1,0;a)}(A_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2} \\
\boxed{\text{z235}} \quad \mathbb{Q}_{3,2}^{(1,0;c)}(E_u, 2) &= \frac{\mathbb{Q}_{1,1}^{(1,0;a)}(E_u)\mathbb{Q}_2^{(b)}(B_{2g})}{2} - \frac{\mathbb{Q}_1^{(1,0;a)}(A_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}
\end{aligned}$$

• 'A'-A' bond-cluster : A;A\_002\_1

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

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

\* wyckoff: 8a08f

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

$$\boxed{\text{z16}} \quad \mathbb{Q}_0^{(c)}(A_{1g}, b) = \mathbb{Q}_2^{(a)}(B_{2g})\mathbb{Q}_2^{(b)}(B_{2g})$$

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

$$\boxed{\text{z18}} \quad \mathbb{Q}_2^{(1,-1;c)}(A_{1g}) = \mathbb{Q}_2^{(1,-1;a)}(A_{1g})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z30}} \quad \mathbb{Q}_5^{(1,-1;c)}(A_{1u}) = \mathbb{M}_3^{(1,-1;a)}(B_{1g})\mathbb{M}_2^{(b)}(B_{1u})$$

$$\boxed{\text{z31}} \quad \mathbb{G}_0^{(c)}(A_{1u}) = \mathbb{M}_1^{(a)}(A_{2g})\mathbb{T}_1^{(b)}(A_{2u})$$

$$\boxed{\text{z44}} \quad \mathbb{G}_0^{(1,-1;c)}(A_{1u}) = \frac{\sqrt{3}\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{3} - \frac{\sqrt{3}\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{3} + \frac{\sqrt{3}\mathbb{M}_1^{(1,-1;a)}(A_{2g})\mathbb{T}_1^{(b)}(A_{2u})}{3}$$

$$\boxed{\text{z45}} \quad \mathbb{G}_2^{(1,-1;c)}(A_{1u}, a) = -\frac{\sqrt{6}\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{6} + \frac{\sqrt{6}\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{6} + \frac{\sqrt{6}\mathbb{M}_1^{(1,-1;a)}(A_{2g})\mathbb{T}_1^{(b)}(A_{2u})}{3}$$

$$\boxed{\text{z57}} \quad \mathbb{G}_2^{(1,-1;c)}(A_{1u}, b) = -\frac{\sqrt{3}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g, 1)\mathbb{T}_{1,1}^{(b)}(E_u)}{4} - \frac{\sqrt{5}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g, 2)\mathbb{T}_{1,1}^{(b)}(E_u)}{4} + \frac{\sqrt{3}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g, 1)\mathbb{T}_{1,2}^{(b)}(E_u)}{4} + \frac{\sqrt{5}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g, 2)\mathbb{T}_{1,2}^{(b)}(E_u)}{4}$$

$$\boxed{\text{z58}} \quad \mathbb{G}_4^{(1,-1;c)}(A_{1u}, 1) = \frac{\sqrt{5}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g, 1)\mathbb{T}_{1,1}^{(b)}(E_u)}{4} - \frac{\sqrt{3}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g, 2)\mathbb{T}_{1,1}^{(b)}(E_u)}{4} - \frac{\sqrt{5}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g, 1)\mathbb{T}_{1,2}^{(b)}(E_u)}{4} + \frac{\sqrt{3}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g, 2)\mathbb{T}_{1,2}^{(b)}(E_u)}{4}$$

$$\boxed{\text{z59}} \quad \mathbb{Q}_4^{(c)}(A_{2g}) = \mathbb{Q}_2^{(a)}(B_{1g})\mathbb{Q}_2^{(b)}(B_{2g})$$

$$\boxed{\text{z60}} \quad \mathbb{G}_1^{(1,-1;c)}(A_{2g}) = -\frac{\sqrt{2}\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2} + \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z95}} \quad \mathbb{Q}_1^{(1,-1;c)}(A_{2u}, a) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z96}} \quad \mathbb{Q}_1^{(1,-1;c)}(A_{2u}, b) = \mathbb{M}_3^{(1,-1;a)}(B_{2g})\mathbb{M}_2^{(b)}(B_{1u})$$

$$\begin{aligned}
\boxed{\text{z97}} \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{z98}} \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{z99}} \quad \mathbb{Q}_2^{(c)}(B_{1g}) &= \mathbb{Q}_2^{(a)}(B_{1g})\mathbb{Q}_0^{(b)}(A_{1g}) \\
\boxed{\text{z100}} \quad \mathbb{Q}_2^{(1,-1;c)}(B_{1g}) &= -\frac{\sqrt{2}\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} + \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2} \\
\boxed{\text{z101}} \quad \mathbb{Q}_3^{(1,-1;c)}(B_{1u}) &= -\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{z102}} \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{z103}} \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} \\
&\quad - \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{z104}} \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{z105}} \quad \mathbb{Q}_2^{(c)}(B_{2g}, a) &= \mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_2^{(b)}(B_{2g}) \\
\boxed{\text{z106}} \quad \mathbb{Q}_2^{(c)}(B_{2g}, b) &= \mathbb{Q}_2^{(a)}(B_{2g})\mathbb{Q}_0^{(b)}(A_{1g}) \\
\boxed{\text{z126}} \quad \mathbb{Q}_2^{(1,-1;c)}(B_{2g}) &= \frac{\sqrt{30}\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(E_g)}{10} + \frac{\sqrt{30}\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(E_g)}{10} - \frac{\sqrt{10}\mathbb{Q}_2^{(1,-1;a)}(A_{1g})\mathbb{Q}_2^{(b)}(B_{2g})}{5} \\
\boxed{\text{z127}} \quad \mathbb{Q}_4^{(1,-1;c)}(B_{2g}) &= \frac{\sqrt{5}\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(E_g)}{5} + \frac{\sqrt{5}\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(E_g)}{5} + \frac{\sqrt{15}\mathbb{Q}_2^{(1,-1;a)}(A_{1g})\mathbb{Q}_2^{(b)}(B_{2g})}{5} \\
\boxed{\text{z128}} \quad \mathbb{Q}_3^{(c)}(B_{2u}) &= \mathbb{M}_1^{(a)}(A_{2g})\mathbb{M}_2^{(b)}(B_{1u}) \\
\boxed{\text{z129}} \quad \mathbb{Q}_3^{(1,-1;c)}(B_{2u}, a) &= \mathbb{M}_1^{(1,-1;a)}(A_{2g})\mathbb{M}_2^{(b)}(B_{1u})
\end{aligned}$$

$$\begin{aligned}
\text{z130} \quad \mathbb{Q}_3^{(1,-1;c)}(B_{2u}, b) &= \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} \\
\text{z131} \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} \\
\text{z148} \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} \\
&\quad - \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} \\
\text{z149} \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} \\
\text{z150} \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} \\
\text{z151} \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} \\
\text{z165} \quad \mathbb{Q}_{2,1}^{(c)}(E_g, b) &= -\frac{\mathbb{Q}_2^{(a)}(B_{1g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} + \frac{\mathbb{Q}_2^{(a)}(B_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2} \\
\text{z166} \quad \mathbb{Q}_{2,2}^{(c)}(E_g, b) &= \frac{\mathbb{Q}_2^{(a)}(B_{1g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2} + \frac{\mathbb{Q}_2^{(a)}(B_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} \\
\text{z167} \quad \mathbb{Q}_{4,1}^{(c)}(E_g, 1) &= -\frac{\mathbb{Q}_2^{(a)}(B_{1g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} - \frac{\mathbb{Q}_2^{(a)}(B_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2} \\
\text{z168} \quad \mathbb{Q}_{4,2}^{(c)}(E_g, 1) &= \frac{\mathbb{Q}_2^{(a)}(B_{1g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2} - \frac{\mathbb{Q}_2^{(a)}(B_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} \\
\text{z184} \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} \\
\text{z185} \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} \\
\text{z186} \quad \mathbb{Q}_{2,1}^{(1,-1;c)}(E_g, b) &= \frac{\sqrt{6}\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_2^{(b)}(B_{2g})}{4} + \frac{\sqrt{2}\mathbb{Q}_2^{(1,-1;a)}(A_{1g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{4}
\end{aligned}$$

$$\boxed{\text{z187}} \quad \mathbb{Q}_{2,2}^{(1,-1;c)}(E_g, b) = \frac{\sqrt{6}\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_2^{(b)}(B_{2g})}{4} + \frac{\sqrt{2}\mathbb{Q}_2^{(1,-1;a)}(A_{1g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{4}$$

$$\boxed{\text{z188}} \quad \mathbb{Q}_{4,1}^{(1,-1;c)}(E_g, 1) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_2^{(b)}(B_{2g})}{4} - \frac{\sqrt{6}\mathbb{Q}_2^{(1,-1;a)}(A_{1g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{4}$$

$$\boxed{\text{z189}} \quad \mathbb{Q}_{4,2}^{(1,-1;c)}(E_g, 1) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_2^{(b)}(B_{2g})}{4} - \frac{\sqrt{6}\mathbb{Q}_2^{(1,-1;a)}(A_{1g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{4}$$

$$\boxed{\text{z236}} \quad \mathbb{Q}_{1,1}^{(c)}(E_u) = -\frac{\sqrt{2}\mathbb{M}_1^{(a)}(A_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z237}} \quad \mathbb{Q}_{1,2}^{(c)}(E_u) = \frac{\sqrt{2}\mathbb{M}_1^{(a)}(A_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z238}} \quad \mathbb{Q}_{1,1}^{(1,-1;c)}(E_u, a) = -\frac{\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_1^{(b)}(A_{2u})}{2} - \frac{\mathbb{M}_1^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

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

$$\boxed{\text{z240}} \quad \mathbb{Q}_{1,1}^{(1,-1;c)}(E_u, b) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{M}_2^{(b)}(B_{1u})}{2}$$

$$\boxed{\text{z241}} \quad \mathbb{Q}_{1,2}^{(1,-1;c)}(E_u, b) = \frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{M}_2^{(b)}(B_{1u})}{2}$$

$$\boxed{\text{z242}} \quad \mathbb{Q}_{1,1}^{(1,-1;c)}(E_u, c) = \frac{3\sqrt{3}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g, 1)\mathbb{M}_2^{(b)}(B_{1u})}{8} - \frac{\sqrt{5}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g, 2)\mathbb{M}_2^{(b)}(B_{1u})}{8}$$

$$\boxed{\text{z243}} \quad \mathbb{Q}_{1,2}^{(1,-1;c)}(E_u, c) = \frac{3\sqrt{3}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g, 1)\mathbb{M}_2^{(b)}(B_{1u})}{8} - \frac{\sqrt{5}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g, 2)\mathbb{M}_2^{(b)}(B_{1u})}{8}$$

$$\boxed{\text{z244}} \quad \mathbb{Q}_{3,1}^{(1,-1;c)}(E_u, 1a) = \frac{\sqrt{78}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g, 1)\mathbb{T}_1^{(b)}(A_{2u})}{26} - \frac{\sqrt{130}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g, 2)\mathbb{T}_1^{(b)}(A_{2u})}{26} - \frac{\sqrt{130}\mathbb{M}_3^{(1,-1;a)}(B_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{26}$$

$$\boxed{\text{z245}} \quad \mathbb{Q}_{3,2}^{(1,-1;c)}(E_u, 1a) = \frac{\sqrt{78}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g, 1)\mathbb{T}_1^{(b)}(A_{2u})}{26} - \frac{\sqrt{130}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g, 2)\mathbb{T}_1^{(b)}(A_{2u})}{26} - \frac{\sqrt{130}\mathbb{M}_3^{(1,-1;a)}(B_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{26}$$

$$\boxed{\text{z246}} \quad \mathbb{Q}_{3,1}^{(1,-1;c)}(E_u, 1b) = \frac{\sqrt{5}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g, 1)\mathbb{M}_2^{(b)}(B_{1u})}{8} + \frac{3\sqrt{3}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g, 2)\mathbb{M}_2^{(b)}(B_{1u})}{8}$$

$$\begin{aligned}
\text{z247} \quad \mathbb{Q}_{3,2}^{(1,-1;c)}(E_u, 1b) &= \frac{\sqrt{5}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g, 1)\mathbb{M}_2^{(b)}(B_{1u})}{8} + \frac{3\sqrt{3}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g, 2)\mathbb{M}_2^{(b)}(B_{1u})}{8} \\
\text{z248} \quad \mathbb{Q}_{3,1}^{(1,-1;c)}(E_u, 2) &= -\frac{5\sqrt{65}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g, 1)\mathbb{T}_1^{(b)}(A_{2u})}{104} - \frac{\sqrt{39}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g, 2)\mathbb{T}_1^{(b)}(A_{2u})}{312} + \frac{\sqrt{39}\mathbb{M}_3^{(1,-1;a)}(B_{1g})\mathbb{T}_{1,1}^{(b)}(E_u)}{12} - \frac{7\sqrt{39}\mathbb{M}_3^{(1,-1;a)}(B_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{156} \\
\text{z249} \quad \mathbb{Q}_{3,2}^{(1,-1;c)}(E_u, 2) &= -\frac{5\sqrt{65}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g, 1)\mathbb{T}_1^{(b)}(A_{2u})}{104} - \frac{\sqrt{39}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g, 2)\mathbb{T}_1^{(b)}(A_{2u})}{312} - \frac{\sqrt{39}\mathbb{M}_3^{(1,-1;a)}(B_{1g})\mathbb{T}_{1,2}^{(b)}(E_u)}{12} - \frac{7\sqrt{39}\mathbb{M}_3^{(1,-1;a)}(B_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{156} \\
\text{z250} \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} \\
\text{z251} \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} \\
\text{z252} \quad \mathbb{G}_{2,1}^{(1,-1;c)}(E_u, b) &= \frac{\sqrt{10}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g, 1)\mathbb{T}_1^{(b)}(A_{2u})}{8} + \frac{5\sqrt{6}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g, 2)\mathbb{T}_1^{(b)}(A_{2u})}{24} + \frac{\sqrt{6}\mathbb{M}_3^{(1,-1;a)}(B_{1g})\mathbb{T}_{1,1}^{(b)}(E_u)}{12} - \frac{\sqrt{6}\mathbb{M}_3^{(1,-1;a)}(B_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{12} \\
\text{z253} \quad \mathbb{G}_{2,2}^{(1,-1;c)}(E_u, b) &= \frac{\sqrt{10}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g, 1)\mathbb{T}_1^{(b)}(A_{2u})}{8} + \frac{5\sqrt{6}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g, 2)\mathbb{T}_1^{(b)}(A_{2u})}{24} - \frac{\sqrt{6}\mathbb{M}_3^{(1,-1;a)}(B_{1g})\mathbb{T}_{1,2}^{(b)}(E_u)}{12} - \frac{\sqrt{6}\mathbb{M}_3^{(1,-1;a)}(B_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{12} \\
\text{z254} \quad \mathbb{G}_{4,1}^{(1,-1;c)}(E_u, 1) &= -\frac{\sqrt{5}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g, 1)\mathbb{T}_1^{(b)}(A_{2u})}{8} + \frac{\sqrt{3}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g, 2)\mathbb{T}_1^{(b)}(A_{2u})}{8} - \frac{\sqrt{3}\mathbb{M}_3^{(1,-1;a)}(B_{1g})\mathbb{T}_{1,1}^{(b)}(E_u)}{4} - \frac{\sqrt{3}\mathbb{M}_3^{(1,-1;a)}(B_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{4} \\
\text{z255} \quad \mathbb{G}_{4,2}^{(1,-1;c)}(E_u, 1) &= -\frac{\sqrt{5}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g, 1)\mathbb{T}_1^{(b)}(A_{2u})}{8} + \frac{\sqrt{3}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g, 2)\mathbb{T}_1^{(b)}(A_{2u})}{8} + \frac{\sqrt{3}\mathbb{M}_3^{(1,-1;a)}(B_{1g})\mathbb{T}_{1,2}^{(b)}(E_u)}{4} - \frac{\sqrt{3}\mathbb{M}_3^{(1,-1;a)}(B_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{4}
\end{aligned}$$

• 'A'-'A' bond-cluster : A;A\_007\_1

- \* bra:  $\langle s, \uparrow |, \langle s, \downarrow |$
- \* ket:  $|s, \uparrow\rangle, |s, \downarrow\rangle$
- \* wyckoff: 2a02b

$$\begin{aligned}
\text{z19} \quad \mathbb{Q}_0^{(c)}(A_{1g}) &= \mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_0^{(b)}(A_{1g}) \\
\text{z132} \quad \mathbb{G}_0^{(1,-1;c)}(A_{1u}) &= \mathbb{M}_1^{(1,-1;a)}(A_{2g})\mathbb{T}_1^{(b)}(A_{2u}) \\
\text{z256} \quad \mathbb{Q}_{1,1}^{(1,-1;c)}(E_u) &= -\frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_1^{(b)}(A_{2u})}{2}
\end{aligned}$$

$$\boxed{\text{z257}} \quad \mathbb{Q}_{1,2}^{(1,-1;c)}(E_u) = -\frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_1^{(b)}(A_{2u})}{2}$$

- 'A'-'A' bond-cluster : **A;A\_007\_1**
  - \* bra:  $\langle s, \uparrow |, \langle s, \downarrow |$
  - \* ket:  $|p_x, \uparrow\rangle, |p_x, \downarrow\rangle, |p_y, \uparrow\rangle, |p_y, \downarrow\rangle$
  - \* wyckoff: **2a@2b**

$$\boxed{\text{z20}} \quad \mathbb{Q}_0^{(1,0;c)}(A_{1g}) = \mathbb{T}_1^{(1,0;a)}(A_{2u})\mathbb{T}_1^{(b)}(A_{2u})$$

$$\boxed{\text{z32}} \quad \mathbb{G}_2^{(1,-1;c)}(A_{1u}) = \mathbb{G}_2^{(1,-1;a)}(A_{1u})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z46}} \quad \mathbb{G}_1^{(1,-1;c)}(A_{2g}) = \mathbb{M}_2^{(1,-1;a)}(A_{1u})\mathbb{T}_1^{(b)}(A_{2u})$$

$$\boxed{\text{z61}} \quad \mathbb{Q}_1^{(1,0;c)}(A_{2u}) = \mathbb{Q}_1^{(1,0;a)}(A_{2u})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z107}} \quad \mathbb{Q}_2^{(1,-1;c)}(B_{1g}) = \mathbb{M}_2^{(1,-1;a)}(B_{2u})\mathbb{T}_1^{(b)}(A_{2u})$$

$$\boxed{\text{z108}} \quad \mathbb{G}_2^{(1,-1;c)}(B_{1u}) = \mathbb{G}_2^{(1,-1;a)}(B_{1u})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z109}} \quad \mathbb{Q}_2^{(1,-1;c)}(B_{2g}) = -\mathbb{M}_2^{(1,-1;a)}(B_{1u})\mathbb{T}_1^{(b)}(A_{2u})$$

$$\boxed{\text{z110}} \quad \mathbb{G}_2^{(1,-1;c)}(B_{2u}) = \mathbb{G}_2^{(1,-1;a)}(B_{2u})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z133}} \quad \mathbb{Q}_{2,1}^{(c)}(E_g) = \frac{\sqrt{2}\mathbb{T}_{1,2}^{(a)}(E_u)\mathbb{T}_1^{(b)}(A_{2u})}{2}$$

$$\boxed{\text{z152}} \quad \mathbb{Q}_{2,2}^{(c)}(E_g) = \frac{\sqrt{2}\mathbb{T}_{1,1}^{(a)}(E_u)\mathbb{T}_1^{(b)}(A_{2u})}{2}$$

$$\boxed{\text{z169}} \quad \mathbb{Q}_{2,1}^{(1,-1;c)}(E_g) = \frac{\sqrt{2}\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{T}_1^{(b)}(A_{2u})}{2}$$

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

$$\boxed{\text{z258}} \quad \mathbb{Q}_{1,1}^{(c)}(E_u) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z259}} \quad \mathbb{Q}_{1,2}^{(c)}(E_u) = \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z260}} \quad \mathbb{Q}_{1,1}^{(1,0;c)}(E_u) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(1,0;a)}(E_u)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z261}} \quad \mathbb{Q}_{1,2}^{(1,0;c)}(E_u) = \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(1,0;a)}(E_u)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

• 'A'-'A' bond-cluster : A;A\_007\_1

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

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

\* wyckoff: 2a@2b

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

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

$$\boxed{\text{z47}} \quad \mathbb{G}_0^{(c)}(A_{1u}) = \mathbb{M}_1^{(a)}(A_{2g})\mathbb{T}_1^{(b)}(A_{2u})$$

$$\boxed{\text{z62}} \quad \mathbb{G}_0^{(1,-1;c)}(A_{1u}) = \mathbb{M}_1^{(1,-1;a)}(A_{2g})\mathbb{T}_1^{(b)}(A_{2u})$$

$$\boxed{\text{z111}} \quad \mathbb{Q}_2^{(c)}(B_{1g}) = \mathbb{Q}_2^{(a)}(B_{1g})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z112}} \quad \mathbb{Q}_3^{(1,-1;c)}(B_{1u}) = -\mathbb{M}_3^{(1,-1;a)}(B_{2g})\mathbb{T}_1^{(b)}(A_{2u})$$

$$\boxed{\text{z134}} \quad \mathbb{Q}_2^{(c)}(B_{2g}) = \mathbb{Q}_2^{(a)}(B_{2g})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z135}} \quad \mathbb{Q}_3^{(1,-1;c)}(B_{2u}) = \mathbb{M}_3^{(1,-1;a)}(B_{1g})\mathbb{T}_1^{(b)}(A_{2u})$$

$$\boxed{\text{z170}} \quad \mathbb{Q}_{2,1}^{(1,-1;c)}(E_g) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z191}} \quad \mathbb{Q}_{2,2}^{(1,-1;c)}(E_g) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z262}} \quad \mathbb{Q}_{1,1}^{(1,-1;c)}(E_u) = -\frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_1^{(b)}(A_{2u})}{2}$$



$$\boxed{\text{z263}} \quad \mathbb{Q}_{1,2}^{(1,-1;c)}(E_u) = -\frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_1^{(b)}(A_{2u})}{2}$$

$$\boxed{\text{z264}} \quad \mathbb{Q}_{3,1}^{(1,-1;c)}(E_u, 1) = \frac{\sqrt{3}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g, 1)\mathbb{T}_1^{(b)}(A_{2u})}{4} - \frac{\sqrt{5}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g, 2)\mathbb{T}_1^{(b)}(A_{2u})}{4}$$

$$\boxed{\text{z265}} \quad \mathbb{Q}_{3,2}^{(1,-1;c)}(E_u, 1) = \frac{\sqrt{3}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g, 1)\mathbb{T}_1^{(b)}(A_{2u})}{4} - \frac{\sqrt{5}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g, 2)\mathbb{T}_1^{(b)}(A_{2u})}{4}$$

$$\boxed{\text{z266}} \quad \mathbb{Q}_{3,1}^{(1,-1;c)}(E_u, 2) = -\frac{\sqrt{5}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g, 1)\mathbb{T}_1^{(b)}(A_{2u})}{4} - \frac{\sqrt{3}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g, 2)\mathbb{T}_1^{(b)}(A_{2u})}{4}$$

$$\boxed{\text{z267}} \quad \mathbb{Q}_{3,2}^{(1,-1;c)}(E_u, 2) = -\frac{\sqrt{5}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g, 1)\mathbb{T}_1^{(b)}(A_{2u})}{4} - \frac{\sqrt{3}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g, 2)\mathbb{T}_1^{(b)}(A_{2u})}{4}$$

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#### Atomic SAMB

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

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

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

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

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

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

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

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

$$\boxed{\text{x7}} \quad \mathbb{Q}_1^{(1,0;a)}(A_{2u}) = \begin{bmatrix} 0 & -\frac{\sqrt{2}}{4} & 0 & \frac{\sqrt{2}i}{4} \\ \frac{\sqrt{2}}{4} & 0 & \frac{\sqrt{2}i}{4} & 0 \end{bmatrix}$$

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

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

$$\boxed{\text{x10}} \quad \mathbb{G}_2^{(1,-1;a)}(A_{1u}) = \begin{bmatrix} 0 & -\frac{\sqrt{2}i}{4} & 0 & -\frac{\sqrt{2}}{4} \\ -\frac{\sqrt{2}i}{4} & 0 & \frac{\sqrt{2}}{4} & 0 \end{bmatrix}$$

$$\boxed{\text{x11}} \quad \mathbb{G}_2^{(1,-1;a)}(B_{1u}) = \begin{bmatrix} 0 & \frac{\sqrt{2}i}{4} & 0 & -\frac{\sqrt{2}}{4} \\ \frac{\sqrt{2}i}{4} & 0 & \frac{\sqrt{2}}{4} & 0 \end{bmatrix}$$

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

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

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

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

$$\boxed{\text{x16}} \quad \mathbb{M}_{2,1}^{(1,-1;a)}(E_u) = \begin{bmatrix} 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & -\frac{1}{2} \end{bmatrix}$$

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

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

$$\boxed{\text{x19}} \quad \mathbb{T}_{1,2}^{(a)}(E_u) = \begin{bmatrix} 0 & 0 & \frac{i}{2} & 0 \\ 0 & 0 & 0 & \frac{i}{2} \end{bmatrix}$$

$$\boxed{\text{x20}} \quad \mathbb{T}_1^{(1,0;a)}(A_{2u}) = \begin{bmatrix} 0 & \frac{\sqrt{2}i}{4} & 0 & \frac{\sqrt{2}}{4} \\ -\frac{\sqrt{2}i}{4} & 0 & \frac{\sqrt{2}}{4} & 0 \end{bmatrix}$$

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

$$\boxed{\text{x21}} \quad \mathbb{Q}_0^{(a)}(A_{1g}) = \begin{bmatrix} \frac{1}{2} & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 \\ 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & \frac{1}{2} \end{bmatrix}$$

$$\boxed{\text{x22}} \quad \mathbb{Q}_2^{(a)}(B_{1g}) = \begin{bmatrix} \frac{1}{2} & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 \\ 0 & 0 & -\frac{1}{2} & 0 \\ 0 & 0 & 0 & -\frac{1}{2} \end{bmatrix}$$

$$\boxed{\text{x23}} \quad \mathbb{Q}_2^{(a)}(B_{2g}) = \begin{bmatrix} 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & \frac{1}{2} \\ \frac{1}{2} & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x24}} \quad \mathbb{Q}_2^{(1,-1;a)}(A_{1g}) = \begin{bmatrix} 0 & 0 & -\frac{i}{2} & 0 \\ 0 & 0 & 0 & \frac{i}{2} \\ \frac{i}{2} & 0 & 0 & 0 \\ 0 & -\frac{i}{2} & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x25}} \quad \mathbb{Q}_{2,1}^{(1,-1;a)}(E_g) = \begin{bmatrix} 0 & 0 & 0 & -\frac{1}{2} \\ 0 & 0 & \frac{1}{2} & 0 \\ 0 & \frac{1}{2} & 0 & 0 \\ -\frac{1}{2} & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x26}} \quad \mathbb{Q}_{2,2}^{(1,-1;a)}(E_g) = \begin{bmatrix} 0 & 0 & 0 & -\frac{i}{2} \\ 0 & 0 & -\frac{i}{2} & 0 \\ 0 & \frac{i}{2} & 0 & 0 \\ \frac{i}{2} & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x27}} \quad \mathbb{M}_1^{(a)}(A_{2g}) = \begin{bmatrix} 0 & 0 & -\frac{i}{2} & 0 \\ 0 & 0 & 0 & -\frac{i}{2} \\ \frac{i}{2} & 0 & 0 & 0 \\ 0 & \frac{i}{2} & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x28}} \quad \mathbb{M}_1^{(1,-1;a)}(A_{2g}) = \begin{bmatrix} \frac{1}{2} & 0 & 0 & 0 \\ 0 & -\frac{1}{2} & 0 & 0 \\ 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & -\frac{1}{2} \end{bmatrix}$$

$$\boxed{\text{x29}} \quad \mathbb{M}_3^{(1,-1;a)}(B_{1g}) = \begin{bmatrix} 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & -\frac{1}{2} \\ \frac{1}{2} & 0 & 0 & 0 \\ 0 & -\frac{1}{2} & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x30}} \quad \mathbb{M}_3^{(1,-1;a)}(B_{2g}) = \begin{bmatrix} \frac{1}{2} & 0 & 0 & 0 \\ 0 & -\frac{1}{2} & 0 & 0 \\ 0 & 0 & -\frac{1}{2} & 0 \\ 0 & 0 & 0 & \frac{1}{2} \end{bmatrix}$$

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

$$\boxed{\text{x32}} \quad \mathbb{M}_{1,2}^{(1,-1;a)}(E_g) = \begin{bmatrix} 0 & \frac{i}{2} & 0 & 0 \\ -\frac{i}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{i}{2} \\ 0 & 0 & -\frac{i}{2} & 0 \end{bmatrix}$$

$$\boxed{\text{x33}} \quad \mathbb{M}_{3,1}^{(1,-1;a)}(E_g, 1) = \begin{bmatrix} 0 & \frac{3\sqrt{13}}{26} & 0 & \frac{\sqrt{13}i}{13} \\ \frac{3\sqrt{13}}{26} & 0 & -\frac{\sqrt{13}i}{13} & 0 \\ 0 & \frac{\sqrt{13}i}{13} & 0 & -\frac{3\sqrt{13}}{26} \\ -\frac{\sqrt{13}i}{13} & 0 & -\frac{3\sqrt{13}}{26} & 0 \end{bmatrix}$$

$$\boxed{\text{x34}} \quad \mathbb{M}_{3,2}^{(1,-1;a)}(E_g, 1) = \begin{bmatrix} 0 & -\frac{3\sqrt{13}i}{26} & 0 & \frac{\sqrt{13}}{13} \\ \frac{3\sqrt{13}i}{26} & 0 & \frac{\sqrt{13}}{13} & 0 \\ 0 & \frac{\sqrt{13}}{13} & 0 & \frac{3\sqrt{13}i}{26} \\ \frac{\sqrt{13}}{13} & 0 & -\frac{3\sqrt{13}i}{26} & 0 \end{bmatrix}$$

$$\boxed{\text{x35}} \quad \mathbb{M}_{3,1}^{(1,-1;a)}(E_g, 2) = \begin{bmatrix} 0 & \frac{\sqrt{13}}{13} & 0 & -\frac{3\sqrt{13}i}{26} \\ \frac{\sqrt{13}}{13} & 0 & \frac{3\sqrt{13}i}{26} & 0 \\ 0 & -\frac{3\sqrt{13}i}{26} & 0 & -\frac{\sqrt{13}}{13} \\ \frac{3\sqrt{13}i}{26} & 0 & -\frac{\sqrt{13}}{13} & 0 \end{bmatrix}$$

$$\boxed{\text{x36}} \quad \mathbb{M}_{3,2}^{(1,-1;a)}(E_g, 2) = \begin{bmatrix} 0 & -\frac{\sqrt{13}i}{13} & 0 & -\frac{3\sqrt{13}}{26} \\ \frac{\sqrt{13}i}{13} & 0 & -\frac{3\sqrt{13}}{26} & 0 \\ 0 & -\frac{3\sqrt{13}}{26} & 0 & \frac{\sqrt{13}i}{13} \\ -\frac{3\sqrt{13}}{26} & 0 & -\frac{\sqrt{13}i}{13} & 0 \end{bmatrix}$$

## Cluster SAMB

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- Site cluster

\*\* Wyckoff: 2a

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

- Bond cluster

\*\* Wyckoff: 2a@2b

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

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

\*\* Wyckoff: 4b@4c

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

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

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

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

\*\* Wyckoff: 8a@8f

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

$$\boxed{\text{y9}} \quad \mathbb{T}_1^{(s)}(A_{2u}) = \left[ \frac{i}{2}, \frac{i}{2}, \frac{i}{2}, \frac{i}{2} \right]$$

$$\boxed{\text{y10}} \quad \mathbb{M}_2^{(s)}(B_{1u}) = \left[ \frac{i}{2}, \frac{i}{2}, -\frac{i}{2}, -\frac{i}{2} \right]$$

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

$$\boxed{\text{y12}} \quad \mathbb{Q}_{2,1}^{(s)}(E_g) = \left[ \frac{1}{2}, -\frac{1}{2}, \frac{1}{2}, -\frac{1}{2} \right]$$

$$\boxed{\text{y13}} \quad \mathbb{Q}_{2,2}^{(s)}(E_g) = \left[ \frac{1}{2}, -\frac{1}{2}, -\frac{1}{2}, \frac{1}{2} \right]$$

$$\boxed{\text{y14}} \quad \mathbb{T}_{1,1}^{(s)}(E_u) = \left[ \frac{i}{2}, -\frac{i}{2}, -\frac{i}{2}, \frac{i}{2} \right]$$

$$\boxed{\text{y15}} \quad \mathbb{T}_{1,2}^{(s)}(E_u) = \left[ \frac{i}{2}, -\frac{i}{2}, \frac{i}{2}, -\frac{i}{2} \right]$$

— Site and Bond —

Table 5: Orbital of each site

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

Table 6: Neighbor and bra-ket of each bond

#	head	tail	neighbor	head (bra)	tail (ket)
1	A	A	[1,2,7]	[s,p]	[s,p]

#### Site in Unit Cell

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

Table 7: 'A' (#1) site cluster (2a), 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]

#### 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 (4b@4c), 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)	[-1,0,-1]
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)	[0,1,1]

Table 9: 2-th 'A'-'A' [1] (#2) bond cluster (8a@8f), ND,  $|\mathbf{v}|=1.35853$  (cartesian)

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