

# Model for “C3v1”

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## General Condition

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- Basis type: 1gs
- SAMB selection:
  - Type: [Q, G]
  - Rank: [0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11]
  - Irrep.: [A<sub>1</sub>, A<sub>2</sub>, E]
  - Spin (s): [0, 1]
- Atomic selection:
  - Type: [Q, G, M, T]
  - Rank: [0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11]
  - Irrep.: [A<sub>1</sub>, A<sub>2</sub>, E]
  - Spin (s): [0, 1]
- Site-cluster selection:
  - Rank: [0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11]
  - Irrep.: [A<sub>1</sub>, A<sub>2</sub>, E]
- Bond-cluster selection:
  - Type: [Q, G, M, T]
  - Rank: [0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11]
  - Irrep.: [A<sub>1</sub>, A<sub>2</sub>, E]
- 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. 156 C<sub>3v</sub><sup>1</sup> P3m1 [ trigonal ]
- Associated point group: PG No. 156 C<sub>3v</sub> 3m (3m1 setting) [ trigonal ]
- Unit cell:  
 $a = 1.00000, b = 1.00000, c = 1.00000, \alpha = 90.0, \beta = 90.0, \gamma = 120.0$
- Lattice vectors (conventional cell):  
 $\mathbf{a}_1 = [1.00000, 0.00000, 0.00000]$   
 $\mathbf{a}_2 = [-0.50000, 0.86603, 0.00000]$   
 $\mathbf{a}_3 = [0.00000, 0.00000, 1.00000]$

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 — Symmetry Operation —

Table 1: Symmetry operation

#	SO	#	SO	#	SO	#	SO	#	SO
1	{1 0}	2	{3 <sup>+</sup> <sub>001</sub>  0}	3	{3 <sup>-</sup> <sub>001</sub>  0}	4	{m <sub>110</sub>  0}	5	{m <sub>100</sub>  0}
6	{m <sub>010</sub>  0}								

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 — Harmonics —

Table 2: Harmonics

#	symbol	irrep.	rank	X	multiplicity	component	symmetry
1	$\mathbb{Q}_0(A_1)$	$A_1$	0	$Q, T$	-	-	1
2	$\mathbb{Q}_1(A_1)$	$A_1$	1	$Q, T$	-	-	$z$
3	$\mathbb{Q}_2(A_1)$	$A_1$	2	$Q, T$	-	-	$-\frac{x^2}{2} - \frac{y^2}{2} + z^2$
4	$\mathbb{G}_3(A_1)$	$A_1$	3	$G, M$	-	-	$\frac{\sqrt{10}x(x^2 - 3y^2)}{4}$
5	$\mathbb{Q}_3(A_1, 1)$	$A_1$	3	$Q, T$	1	-	$-\frac{z(3x^2 + 3y^2 - 2z^2)}{2}$
6	$\mathbb{Q}_3(A_1, 2)$	$A_1$	3	$Q, T$	2	-	$\frac{\sqrt{10}y(3x^2 - y^2)}{4}$
7	$\mathbb{G}_0(A_2)$	$A_2$	0	$G, M$	-	-	1
8	$\mathbb{G}_1(A_2)$	$A_2$	1	$G, M$	-	-	$z$

*continued ...*

Table 2

#	symbol	irrep.	rank	X	multiplicity	component	symmetry
9	$\mathbb{G}_2(A_2)$	$A_2$	2	$G, M$	-	-	$-\frac{x^2}{2} - \frac{y^2}{2} + z^2$
10	$\mathbb{G}_3(A_2, 2)$	$A_2$	3	$G, M$	2	-	$\frac{\sqrt{10}y(3x^2-y^2)}{4}$
11	$\mathbb{Q}_3(A_2)$	$A_2$	3	$Q, T$	-	-	$\frac{\sqrt{10}x(x^2-3y^2)}{4}$
12	$\mathbb{G}_{1,1}(E)$	$E$	1	$G, M$	-	1	$-y$
13	$\mathbb{G}_{1,2}(E)$					2	$x$
14	$\mathbb{Q}_{1,1}(E)$	$E$	1	$Q, T$	-	1	$x$
15	$\mathbb{Q}_{1,2}(E)$					2	$y$
16	$\mathbb{G}_{2,1}(E, 2)$	$E$	2	$G, M$	2	1	$\frac{\sqrt{3}(x-y)(x+y)}{2}$
17	$\mathbb{G}_{2,2}(E, 2)$					2	$-\sqrt{3}xy$
18	$\mathbb{Q}_{2,1}(E, 1)$	$E$	2	$Q, T$	1	1	$\sqrt{3}xz$
19	$\mathbb{Q}_{2,2}(E, 1)$					2	$\sqrt{3}yz$
20	$\mathbb{Q}_{2,1}(E, 2)$	$E$	2	$Q, T$	2	1	$\sqrt{3}xy$
21	$\mathbb{Q}_{2,2}(E, 2)$					2	$\frac{\sqrt{3}(x-y)(x+y)}{2}$
22	$\mathbb{G}_{3,1}(E, 1)$	$E$	3	$G, M$	1	1	$\frac{\sqrt{6}y(x^2+y^2-4z^2)}{4}$
23	$\mathbb{G}_{3,2}(E, 1)$					2	$-\frac{\sqrt{6}x(x^2+y^2-4z^2)}{4}$
24	$\mathbb{G}_{3,1}(E, 2)$	$E$	3	$G, M$	2	1	$-\frac{\sqrt{15}z(x-y)(x+y)}{2}$
25	$\mathbb{G}_{3,2}(E, 2)$					2	$\sqrt{15}xyz$
26	$\mathbb{Q}_{3,1}(E, 1)$	$E$	3	$Q, T$	1	1	$-\frac{\sqrt{6}x(x^2+y^2-4z^2)}{4}$
27	$\mathbb{Q}_{3,2}(E, 1)$					2	$-\frac{\sqrt{6}y(x^2+y^2-4z^2)}{4}$
28	$\mathbb{Q}_{3,1}(E, 2)$	$E$	3	$Q, T$	2	1	$\sqrt{15}xyz$
29	$\mathbb{Q}_{3,2}(E, 2)$					2	$\frac{\sqrt{15}z(x-y)(x+y)}{2}$

continued ...

Table 2

#	symbol	irrep.	rank	X	multiplicity	component	symmetry
30	$\mathbb{G}_{4,1}(E, 2)$	$E$	4	$G, M$	2	1	$\frac{\sqrt{35}(x^2 - 2xy - y^2)(x^2 + 2xy - y^2)}{8}$
31	$\mathbb{G}_{4,2}(E, 2)$					2	$\frac{\sqrt{35}xy(x-y)(x+y)}{2}$

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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	$ p_x, \uparrow\rangle @A(1)$	1	$ p_x, \downarrow\rangle @A(1)$	2	$ p_y, \uparrow\rangle @A(1)$	3	$ p_y, \downarrow\rangle @A(1)$	4	$ p_x, \uparrow\rangle @B(1)$
5	$ p_x, \downarrow\rangle @B(1)$	6	$ p_y, \uparrow\rangle @B(1)$	7	$ p_y, \downarrow\rangle @B(1)$				

Table 4: Atomic basis (orbital part only)

orbital	definition
$ p_x\rangle$	$x$
$ p_y\rangle$	$y$

*continued ...*

Table 4

orbital	definition
$ p_z\rangle$	$z$

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— SAMB —

60 (all 60) SAMBs

- '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: 1b

$$\boxed{\text{z1}} \quad \mathbb{Q}_0^{(c)}(A_1) = \mathbb{Q}_0^{(a)}(A_1)\mathbb{Q}_0^{(s)}(A_1)$$

$$\boxed{\text{z2}} \quad \mathbb{Q}_2^{(1,-1;c)}(A_1) = \mathbb{Q}_2^{(1,-1;a)}(A_1)\mathbb{Q}_0^{(s)}(A_1)$$

$$\boxed{\text{z21}} \quad \mathbb{Q}_{2,1}^{(c)}(E, 2) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E, 2)\mathbb{Q}_0^{(s)}(A_1)}{2}$$

$$\boxed{\text{z22}} \quad \mathbb{Q}_{2,2}^{(c)}(E, 2) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E, 2)\mathbb{Q}_0^{(s)}(A_1)}{2}$$

$$\boxed{\text{z23}} \quad \mathbb{Q}_{2,1}^{(1,-1;c)}(E, 1) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(1,-1;a)}(E, 1)\mathbb{Q}_0^{(s)}(A_1)}{2}$$

$$\boxed{\text{z24}} \quad \mathbb{Q}_{2,2}^{(1,-1;c)}(E, 1) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(1,-1;a)}(E, 1)\mathbb{Q}_0^{(s)}(A_1)}{2}$$

- 'B' site-cluster : B
  - \* 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: 1c

$$\boxed{z3} \quad \mathbb{Q}_0^{(c)}(A_1) = \mathbb{Q}_0^{(a)}(A_1)\mathbb{Q}_0^{(s)}(A_1)$$

$$\boxed{z4} \quad \mathbb{Q}_2^{(1,-1;c)}(A_1) = \mathbb{Q}_2^{(1,-1;a)}(A_1)\mathbb{Q}_0^{(s)}(A_1)$$

$$\boxed{z25} \quad \mathbb{Q}_{2,1}^{(c)}(E, 2) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E, 2)\mathbb{Q}_0^{(s)}(A_1)}{2}$$

$$\boxed{z26} \quad \mathbb{Q}_{2,2}^{(c)}(E, 2) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E, 2)\mathbb{Q}_0^{(s)}(A_1)}{2}$$

$$\boxed{z27} \quad \mathbb{Q}_{2,1}^{(1,-1;c)}(E, 1) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(1,-1;a)}(E, 1)\mathbb{Q}_0^{(s)}(A_1)}{2}$$

$$\boxed{z28} \quad \mathbb{Q}_{2,2}^{(1,-1;c)}(E, 1) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(1,-1;a)}(E, 1)\mathbb{Q}_0^{(s)}(A_1)}{2}$$

• 'A'-'B' bond-cluster : B;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: 3a@3d

$$\boxed{z5} \quad \mathbb{Q}_0^{(c)}(A_1) = \mathbb{Q}_0^{(a)}(A_1)\mathbb{Q}_0^{(b)}(A_1)$$

$$\boxed{z6} \quad \mathbb{Q}_3^{(c)}(A_1, 2) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E, 2)\mathbb{Q}_{1,1}^{(b)}(E)}{2} + \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E, 2)\mathbb{Q}_{1,2}^{(b)}(E)}{2}$$

$$\boxed{z7} \quad \mathbb{Q}_1^{(1,-1;c)}(A_1, a) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(1,-1;a)}(E, 1)\mathbb{Q}_{1,1}^{(b)}(E)}{2} + \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(1,-1;a)}(E, 1)\mathbb{Q}_{1,2}^{(b)}(E)}{2}$$

$$\boxed{z8} \quad \mathbb{Q}_1^{(1,-1;c)}(A_1, b) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E)\mathbb{T}_{1,1}^{(b)}(E)}{2} + \frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E)\mathbb{T}_{1,2}^{(b)}(E)}{2}$$

$$\boxed{z9} \quad \mathbb{Q}_2^{(1,-1;c)}(A_1) = \mathbb{Q}_2^{(1,-1;a)}(A_1)\mathbb{Q}_0^{(b)}(A_1)$$

$$\boxed{z10} \quad \mathbb{Q}_3^{(1,-1;c)}(A_1, 1) = \frac{\sqrt{2}\mathbb{M}_{3,1}^{(1,-1;a)}(E, 1)\mathbb{T}_{1,1}^{(b)}(E)}{2} + \frac{\sqrt{2}\mathbb{M}_{3,2}^{(1,-1;a)}(E, 1)\mathbb{T}_{1,2}^{(b)}(E)}{2}$$

$$\boxed{\text{z11}} \quad \mathbb{Q}_3^{(1,-1;c)}(A_1, 2) = -\frac{\sqrt{2}\mathbb{M}_{3,1}^{(1,-1;a)}(E, 2)\mathbb{T}_{1,1}^{(b)}(E)}{2} - \frac{\sqrt{2}\mathbb{M}_{3,2}^{(1,-1;a)}(E, 2)\mathbb{T}_{1,2}^{(b)}(E)}{2}$$

$$\boxed{\text{z12}} \quad \mathbb{G}_3^{(1,-1;c)}(A_1) = \mathbb{M}_3^{(1,-1;a)}(A_1)\mathbb{T}_0^{(b)}(A_1)$$

$$\boxed{\text{z13}} \quad \mathbb{Q}_3^{(c)}(A_2) = -\frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E, 2)\mathbb{Q}_{1,2}^{(b)}(E)}{2} + \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E, 2)\mathbb{Q}_{1,1}^{(b)}(E)}{2}$$

$$\boxed{\text{z14}} \quad \mathbb{Q}_3^{(1,-1;c)}(A_2) = \frac{\sqrt{2}\mathbb{M}_{3,1}^{(1,-1;a)}(E, 2)\mathbb{T}_{1,2}^{(b)}(E)}{2} - \frac{\sqrt{2}\mathbb{M}_{3,2}^{(1,-1;a)}(E, 2)\mathbb{T}_{1,1}^{(b)}(E)}{2}$$

$$\boxed{\text{z15}} \quad \mathbb{G}_1^{(c)}(A_2) = \mathbb{M}_1^{(a)}(A_2)\mathbb{T}_0^{(b)}(A_1)$$

$$\boxed{\text{z16}} \quad \mathbb{G}_0^{(1,-1;c)}(A_2) = -\frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E)\mathbb{T}_{1,2}^{(b)}(E)}{2} + \frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E)\mathbb{T}_{1,1}^{(b)}(E)}{2}$$

$$\boxed{\text{z17}} \quad \mathbb{G}_1^{(1,-1;c)}(A_2) = \mathbb{M}_1^{(1,-1;a)}(A_2)\mathbb{T}_0^{(b)}(A_1)$$

$$\boxed{\text{z18}} \quad \mathbb{G}_2^{(1,-1;c)}(A_2, a) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(1,-1;a)}(E, 1)\mathbb{Q}_{1,2}^{(b)}(E)}{2} - \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(1,-1;a)}(E, 1)\mathbb{Q}_{1,1}^{(b)}(E)}{2}$$

$$\boxed{\text{z19}} \quad \mathbb{G}_2^{(1,-1;c)}(A_2, b) = -\frac{\sqrt{2}\mathbb{M}_{3,1}^{(1,-1;a)}(E, 1)\mathbb{T}_{1,2}^{(b)}(E)}{2} + \frac{\sqrt{2}\mathbb{M}_{3,2}^{(1,-1;a)}(E, 1)\mathbb{T}_{1,1}^{(b)}(E)}{2}$$

$$\boxed{\text{z20}} \quad \mathbb{G}_3^{(1,-1;c)}(A_2, 2) = \mathbb{M}_3^{(1,-1;a)}(A_2, 2)\mathbb{T}_0^{(b)}(A_1)$$

$$\boxed{\text{z29}} \quad \mathbb{Q}_{1,1}^{(c)}(E, a) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_1)\mathbb{Q}_{1,1}^{(b)}(E)}{2}$$

$$\boxed{\text{z30}} \quad \mathbb{Q}_{1,2}^{(c)}(E, a) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_1)\mathbb{Q}_{1,2}^{(b)}(E)}{2}$$

$$\boxed{\text{z31}} \quad \mathbb{Q}_{1,1}^{(c)}(E, b) = \frac{\mathbb{Q}_{2,1}^{(a)}(E, 2)\mathbb{Q}_{1,2}^{(b)}(E)}{2} + \frac{\mathbb{Q}_{2,2}^{(a)}(E, 2)\mathbb{Q}_{1,1}^{(b)}(E)}{2}$$

$$\boxed{\text{z32}} \quad \mathbb{Q}_{1,2}^{(c)}(E, b) = \frac{\mathbb{Q}_{2,1}^{(a)}(E, 2)\mathbb{Q}_{1,1}^{(b)}(E)}{2} - \frac{\mathbb{Q}_{2,2}^{(a)}(E, 2)\mathbb{Q}_{1,2}^{(b)}(E)}{2}$$

$$\boxed{\text{z33}} \quad \mathbb{Q}_{1,1}^{(c)}(E, c) = -\frac{\sqrt{2}\mathbb{M}_1^{(a)}(A_2)\mathbb{T}_{1,2}^{(b)}(E)}{2}$$

$$\boxed{\text{z34}} \quad \mathbb{Q}_{1,2}^{(c)}(E, c) = \frac{\sqrt{2}\mathbb{M}_1^{(a)}(A_2)\mathbb{T}_{1,1}^{(b)}(E)}{2}$$

$$\boxed{\text{z35}} \quad \mathbb{Q}_{2,1}^{(c)}(E, 2) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E, 2)\mathbb{Q}_0^{(b)}(A_1)}{2}$$

$$\boxed{\text{z36}} \quad \mathbb{Q}_{2,2}^{(c)}(E, 2) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E, 2)\mathbb{Q}_0^{(b)}(A_1)}{2}$$

$$\boxed{\text{z37}} \quad \mathbb{Q}_{1,1}^{(1,-1;c)}(E, a) = -\frac{\sqrt{2}\mathbb{Q}_2^{(1,-1;a)}(A_1)\mathbb{Q}_{1,1}^{(b)}(E)}{2}$$

$$\boxed{\text{z38}} \quad \mathbb{Q}_{1,2}^{(1,-1;c)}(E, a) = -\frac{\sqrt{2}\mathbb{Q}_2^{(1,-1;a)}(A_1)\mathbb{Q}_{1,2}^{(b)}(E)}{2}$$

$$\boxed{\text{z39}} \quad \mathbb{Q}_{1,1}^{(1,-1;c)}(E, b) = -\frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(A_2)\mathbb{T}_{1,2}^{(b)}(E)}{2}$$

$$\boxed{\text{z40}} \quad \mathbb{Q}_{1,2}^{(1,-1;c)}(E, b) = \frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(A_2)\mathbb{T}_{1,1}^{(b)}(E)}{2}$$

$$\boxed{\text{z41}} \quad \mathbb{Q}_{2,1}^{(1,-1;c)}(E, 1) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(1,-1;a)}(E, 1)\mathbb{Q}_0^{(b)}(A_1)}{2}$$

$$\boxed{\text{z42}} \quad \mathbb{Q}_{2,2}^{(1,-1;c)}(E, 1) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(1,-1;a)}(E, 1)\mathbb{Q}_0^{(b)}(A_1)}{2}$$

$$\boxed{\text{z43}} \quad \mathbb{Q}_{3,1}^{(1,-1;c)}(E, 1) = -\frac{\mathbb{M}_{3,1}^{(1,-1;a)}(E, 2)\mathbb{T}_{1,2}^{(b)}(E)}{2} - \frac{\mathbb{M}_{3,2}^{(1,-1;a)}(E, 2)\mathbb{T}_{1,1}^{(b)}(E)}{2}$$

$$\boxed{\text{z44}} \quad \mathbb{Q}_{3,2}^{(1,-1;c)}(E, 1) = -\frac{\mathbb{M}_{3,1}^{(1,-1;a)}(E, 2)\mathbb{T}_{1,1}^{(b)}(E)}{2} + \frac{\mathbb{M}_{3,2}^{(1,-1;a)}(E, 2)\mathbb{T}_{1,2}^{(b)}(E)}{2}$$

$$\boxed{\text{z45}} \quad \mathbb{Q}_{3,1}^{(1,-1;c)}(E, 2a) = \frac{\mathbb{Q}_{2,1}^{(1,-1;a)}(E, 1)\mathbb{Q}_{1,2}^{(b)}(E)}{2} + \frac{\mathbb{Q}_{2,2}^{(1,-1;a)}(E, 1)\mathbb{Q}_{1,1}^{(b)}(E)}{2}$$

$$\boxed{\text{z46}} \quad \mathbb{Q}_{3,2}^{(1,-1;c)}(E, 2a) = \frac{\mathbb{Q}_{2,1}^{(1,-1;a)}(E, 1)\mathbb{Q}_{1,1}^{(b)}(E)}{2} - \frac{\mathbb{Q}_{2,2}^{(1,-1;a)}(E, 1)\mathbb{Q}_{1,2}^{(b)}(E)}{2}$$

$$\boxed{\text{z47}} \quad \mathbb{Q}_{3,1}^{(1,-1;c)}(E, 2b) = \frac{\sqrt{10}\mathbb{M}_{3,1}^{(1,-1;a)}(E, 1)\mathbb{T}_{1,2}^{(b)}(E)}{8} + \frac{\sqrt{10}\mathbb{M}_{3,2}^{(1,-1;a)}(E, 1)\mathbb{T}_{1,1}^{(b)}(E)}{8} + \frac{\sqrt{6}\mathbb{M}_3^{(1,-1;a)}(A_1)\mathbb{T}_{1,1}^{(b)}(E)}{8} + \frac{\sqrt{6}\mathbb{M}_3^{(1,-1;a)}(A_2, 2)\mathbb{T}_{1,2}^{(b)}(E)}{8}$$

$$\boxed{\text{z48}} \quad \mathbb{Q}_{3,2}^{(1,-1;c)}(E, 2b) = \frac{\sqrt{10}\mathbb{M}_{3,1}^{(1,-1;a)}(E, 1)\mathbb{T}_{1,1}^{(b)}(E)}{8} - \frac{\sqrt{10}\mathbb{M}_{3,2}^{(1,-1;a)}(E, 1)\mathbb{T}_{1,2}^{(b)}(E)}{8} + \frac{\sqrt{6}\mathbb{M}_3^{(1,-1;a)}(A_1)\mathbb{T}_{1,2}^{(b)}(E)}{8} - \frac{\sqrt{6}\mathbb{M}_3^{(1,-1;a)}(A_2, 2)\mathbb{T}_{1,1}^{(b)}(E)}{8}$$

$$\boxed{\text{z49}} \quad \mathbb{G}_{1,1}^{(1,-1;c)}(E) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E)\mathbb{T}_0^{(b)}(A_1)}{2}$$

$$\boxed{\text{z50}} \quad \mathbb{G}_{1,2}^{(1,-1;c)}(E) = \frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E)\mathbb{T}_0^{(b)}(A_1)}{2}$$

$$\boxed{\text{z51}} \quad \mathbb{G}_{2,1}^{(1,-1;c)}(E, 2a) = -\frac{\sqrt{6}\mathbb{M}_{3,1}^{(1,-1;a)}(E, 1)\mathbb{T}_{1,2}^{(b)}(E)}{8} - \frac{\sqrt{6}\mathbb{M}_{3,2}^{(1,-1;a)}(E, 1)\mathbb{T}_{1,1}^{(b)}(E)}{8} + \frac{\sqrt{10}\mathbb{M}_3^{(1,-1;a)}(A_1)\mathbb{T}_{1,1}^{(b)}(E)}{8} + \frac{\sqrt{10}\mathbb{M}_3^{(1,-1;a)}(A_2, 2)\mathbb{T}_{1,2}^{(b)}(E)}{8}$$

$$\boxed{\text{z52}} \quad \mathbb{G}_{2,2}^{(1,-1;c)}(E, 2a) = -\frac{\sqrt{6}\mathbb{M}_{3,1}^{(1,-1;a)}(E, 1)\mathbb{T}_{1,1}^{(b)}(E)}{8} + \frac{\sqrt{6}\mathbb{M}_{3,2}^{(1,-1;a)}(E, 1)\mathbb{T}_{1,2}^{(b)}(E)}{8} + \frac{\sqrt{10}\mathbb{M}_3^{(1,-1;a)}(A_1)\mathbb{T}_{1,2}^{(b)}(E)}{8} - \frac{\sqrt{10}\mathbb{M}_3^{(1,-1;a)}(A_2, 2)\mathbb{T}_{1,1}^{(b)}(E)}{8}$$

$$\boxed{\text{z53}} \quad \mathbb{G}_{2,1}^{(1,-1;c)}(E, 2b) = \frac{\mathbb{M}_{1,1}^{(1,-1;a)}(E)\mathbb{T}_{1,2}^{(b)}(E)}{2} + \frac{\mathbb{M}_{1,2}^{(1,-1;a)}(E)\mathbb{T}_{1,1}^{(b)}(E)}{2}$$

$$\boxed{\text{z54}} \quad \mathbb{G}_{2,2}^{(1,-1;c)}(E, 2b) = \frac{\mathbb{M}_{1,1}^{(1,-1;a)}(E)\mathbb{T}_{1,1}^{(b)}(E)}{2} - \frac{\mathbb{M}_{1,2}^{(1,-1;a)}(E)\mathbb{T}_{1,2}^{(b)}(E)}{2}$$

$$\boxed{\text{z55}} \quad \mathbb{G}_{3,1}^{(1,-1;c)}(E, 1) = \frac{\sqrt{2}\mathbb{M}_{3,1}^{(1,-1;a)}(E, 1)\mathbb{T}_0^{(b)}(A_1)}{2}$$

$$\boxed{\text{z56}} \quad \mathbb{G}_{3,2}^{(1,-1;c)}(E, 1) = \frac{\sqrt{2}\mathbb{M}_{3,2}^{(1,-1;a)}(E, 1)\mathbb{T}_0^{(b)}(A_1)}{2}$$

$$\boxed{\text{z57}} \quad \mathbb{G}_{3,1}^{(1,-1;c)}(E, 2) = \frac{\sqrt{2}\mathbb{M}_{3,1}^{(1,-1;a)}(E, 2)\mathbb{T}_0^{(b)}(A_1)}{2}$$

$$\boxed{\text{z58}} \quad \mathbb{G}_{3,2}^{(1,-1;c)}(E, 2) = \frac{\sqrt{2}\mathbb{M}_{3,2}^{(1,-1;a)}(E, 2)\mathbb{T}_0^{(b)}(A_1)}{2}$$

$$\boxed{\text{z59}} \quad \mathbb{G}_{4,1}^{(1,-1;c)}(E, 2) = \frac{\mathbb{M}_3^{(1,-1;a)}(A_1)\mathbb{T}_{1,1}^{(b)}(E)}{2} - \frac{\mathbb{M}_3^{(1,-1;a)}(A_2, 2)\mathbb{T}_{1,2}^{(b)}(E)}{2}$$

$$\boxed{\text{z60}} \quad \mathbb{G}_{4,2}^{(1,-1;c)}(E, 2) = \frac{\mathbb{M}_3^{(1,-1;a)}(A_1)\mathbb{T}_{1,2}^{(b)}(E)}{2} + \frac{\mathbb{M}_3^{(1,-1;a)}(A_2, 2)\mathbb{T}_{1,1}^{(b)}(E)}{2}$$

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

$$\boxed{x1} \quad \mathbb{Q}_0^{(a)}(A_1) = \begin{bmatrix} \frac{1}{2} & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 \\ 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & \frac{1}{2} \end{bmatrix}$$

$$\boxed{x2} \quad \mathbb{Q}_{2,1}^{(a)}(E, 2) = \begin{bmatrix} 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & \frac{1}{2} \\ \frac{1}{2} & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 \end{bmatrix}$$

$$\boxed{x3} \quad \mathbb{Q}_{2,2}^{(a)}(E, 2) = \begin{bmatrix} \frac{1}{2} & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 \\ 0 & 0 & -\frac{1}{2} & 0 \\ 0 & 0 & 0 & -\frac{1}{2} \end{bmatrix}$$

$$\boxed{x4} \quad \mathbb{Q}_2^{(1, -1; a)}(A_1) = \begin{bmatrix} 0 & 0 & -\frac{i}{2} & 0 \\ 0 & 0 & 0 & \frac{i}{2} \\ \frac{i}{2} & 0 & 0 & 0 \\ 0 & -\frac{i}{2} & 0 & 0 \end{bmatrix}$$

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

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

$$\boxed{x7} \quad \mathbb{M}_1^{(a)}(A_2) = \begin{bmatrix} 0 & 0 & -\frac{i}{2} & 0 \\ 0 & 0 & 0 & -\frac{i}{2} \\ \frac{i}{2} & 0 & 0 & 0 \\ 0 & \frac{i}{2} & 0 & 0 \end{bmatrix}$$

$$\boxed{x8} \quad \mathbb{M}_3^{(1,-1;a)}(A_1) = \begin{bmatrix} 0 & \frac{\sqrt{2}}{4} & 0 & \frac{\sqrt{2}i}{4} \\ \frac{\sqrt{2}}{4} & 0 & -\frac{\sqrt{2}i}{4} & 0 \\ 0 & \frac{\sqrt{2}i}{4} & 0 & -\frac{\sqrt{2}}{4} \\ -\frac{\sqrt{2}i}{4} & 0 & -\frac{\sqrt{2}}{4} & 0 \end{bmatrix}$$

$$\boxed{x9} \quad \mathbb{M}_1^{(1,-1;a)}(A_2) = \begin{bmatrix} \frac{1}{2} & 0 & 0 & 0 \\ 0 & -\frac{1}{2} & 0 & 0 \\ 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & -\frac{1}{2} \end{bmatrix}$$

$$\boxed{x10} \quad \mathbb{M}_3^{(1,-1;a)}(A_2, 2) = \begin{bmatrix} 0 & -\frac{\sqrt{2}i}{4} & 0 & \frac{\sqrt{2}}{4} \\ \frac{\sqrt{2}i}{4} & 0 & \frac{\sqrt{2}}{4} & 0 \\ 0 & \frac{\sqrt{2}}{4} & 0 & \frac{\sqrt{2}i}{4} \\ \frac{\sqrt{2}}{4} & 0 & -\frac{\sqrt{2}i}{4} & 0 \end{bmatrix}$$

$$\boxed{x11} \quad \mathbb{M}_{1,1}^{(1,-1;a)}(E) = \begin{bmatrix} 0 & \frac{i}{2} & 0 & 0 \\ -\frac{i}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{i}{2} \\ 0 & 0 & -\frac{i}{2} & 0 \end{bmatrix}$$

$$\boxed{x12} \quad \mathbb{M}_{1,2}^{(1,-1;a)}(E) = \begin{bmatrix} 0 & \frac{1}{2} & 0 & 0 \\ \frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2} \\ 0 & 0 & \frac{1}{2} & 0 \end{bmatrix}$$

$$\boxed{x13} \quad \mathbb{M}_{3,1}^{(1,-1;a)}(E, 1) = \begin{bmatrix} 0 & \frac{\sqrt{2}i}{4} & 0 & \frac{\sqrt{2}}{4} \\ -\frac{\sqrt{2}i}{4} & 0 & \frac{\sqrt{2}}{4} & 0 \\ 0 & \frac{\sqrt{2}}{4} & 0 & -\frac{\sqrt{2}i}{4} \\ \frac{\sqrt{2}}{4} & 0 & \frac{\sqrt{2}i}{4} & 0 \end{bmatrix}$$

$$\boxed{x14} \quad \mathbb{M}_{3,2}^{(1,-1;a)}(E, 1) = \begin{bmatrix} 0 & -\frac{\sqrt{2}}{4} & 0 & \frac{\sqrt{2}i}{4} \\ -\frac{\sqrt{2}}{4} & 0 & -\frac{\sqrt{2}i}{4} & 0 \\ 0 & \frac{\sqrt{2}i}{4} & 0 & \frac{\sqrt{2}}{4} \\ -\frac{\sqrt{2}i}{4} & 0 & \frac{\sqrt{2}}{4} & 0 \end{bmatrix}$$

$$\boxed{x15} \quad \mathbb{M}_{3,1}^{(1,-1;a)}(E, 2) = \begin{bmatrix} -\frac{1}{2} & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 \\ 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & -\frac{1}{2} \end{bmatrix}$$

$$\boxed{x16} \quad \mathbb{M}_{3,2}^{(1,-1;a)}(E, 2) = \begin{bmatrix} 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & -\frac{1}{2} \\ \frac{1}{2} & 0 & 0 & 0 \\ 0 & -\frac{1}{2} & 0 & 0 \end{bmatrix}$$

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— Cluster SAMB —

- Site cluster

\*\* Wyckoff: **1b**

$$\boxed{y1} \quad \mathbb{Q}_0^{(s)}(A_1) = [1]$$

\*\* Wyckoff: **1c**

$$\boxed{y2} \quad \mathbb{Q}_0^{(s)}(A_1) = [1]$$

- Bond cluster

\*\* Wyckoff: **3a@3d**

$$\boxed{y3} \quad \mathbb{Q}_0^{(s)}(A_1) = \left[ \frac{\sqrt{3}}{3}, \frac{\sqrt{3}}{3}, \frac{\sqrt{3}}{3} \right]$$

$$\boxed{y4} \quad \mathbb{T}_0^{(s)}(A_1) = \left[ \frac{\sqrt{3}i}{3}, \frac{\sqrt{3}i}{3}, \frac{\sqrt{3}i}{3} \right]$$

$$\boxed{y5} \quad \mathbb{Q}_{1,1}^{(s)}(E) = \left[ \frac{\sqrt{2}}{2}, 0, -\frac{\sqrt{2}}{2} \right]$$

$$\boxed{y6} \quad \mathbb{Q}_{1,2}^{(s)}(E) = \left[ -\frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{3}, -\frac{\sqrt{6}}{6} \right]$$

$$\boxed{y7} \quad \mathbb{T}_{1,1}^{(s)}(E) = \left[ \frac{\sqrt{2}i}{2}, 0, -\frac{\sqrt{2}i}{2} \right]$$

$$\boxed{y8} \quad \mathbb{T}_{1,2}^{(s)}(E) = \left[ -\frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{3}, -\frac{\sqrt{6}i}{6} \right]$$

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**Site and Bond**

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Table 5: Orbital of each site

#	site	orbital
1	A	$ p_x, \uparrow\rangle,  p_x, \downarrow\rangle,  p_y, \uparrow\rangle,  p_y, \downarrow\rangle$
2	B	$ 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	B	[1]	[p]	[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 (1b), 3m.

SL	position ( $\mathbf{s}$ )	mapping
1	[ 0.33333, 0.66667, 0.00000]	[1,2,3,4,5,6]

Table 8: 'B' (#2) site cluster (1c), 3m.

SL	position ( $\mathbf{s}$ )	mapping
1	[ 0.66667, 0.33333, 0.00000]	[1,2,3,4,5,6]

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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 9: 1-th 'A'-'B' [1] (#1) bond cluster (3a@3d), D,  $|\mathbf{v}|=0.57735$  (cartesian)

SL	vector ( $\mathbf{v}$ )	center ( $\mathbf{c}$ )	mapping	head	tail	$\mathbf{R}$ (primitive)
1	[-0.33333, 0.33333, 0.00000]	[ 0.50000, 0.50000, 0.00000]	[1,4]	(1,1)	(1,1)	[0,0,0]
2	[-0.33333, -0.66667, 0.00000]	[ 0.50000, 0.00000, 0.00000]	[2,6]	(1,1)	(1,1)	[0,1,0]
3	[ 0.66667, 0.33333, 0.00000]	[ 0.00000, 0.50000, 0.00000]	[3,5]	(1,1)	(1,1)	[-1,0,0]

