

# Model for “C3v1”

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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.: [ $A_1$ ,  $A_2$ ,  $E$ ]
  - 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.: [ $A_1$ ,  $A_2$ ,  $E$ ]
  - Spin (s): [0, 1]
- Site-cluster selection:
  - Rank: [0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11]
  - Irrep.: [ $A_1$ ,  $A_2$ ,  $E$ ]
- Bond-cluster selection:
  - Type: [Q, G, M, T]
  - Rank: [0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11]
  - Irrep.: [ $A_1$ ,  $A_2$ ,  $E$ ]
- 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. 156  $C_{3v}^1$   $P3m1$  [ trigonal ]
- Associated point group: PG No. 156  $C_{3v}$   $3m$  (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

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Table 1: Symmetry operation

#	SO	#	SO	#	SO	#	SO	#	SO
1	$\{1 0\}$	2	$\{3_{001}^+ 0\}$	3	$\{3_{001}^- 0\}$	4	$\{m_{110} 0\}$	5	$\{m_{100} 0\}$
6	$\{m_{010} 0\}$								

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## Harmonics

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Table 2: Harmonics

#	symbol	irrep.	rank	X	multiplicity	component	symmetry
1	$\mathbb{Q}_0(A_1)$	$A_1$	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	$G, M$	-	-	$z$
9	$\mathbb{G}_2(A_2)$	$A_2$	2	$G, M$	-	-	$-\frac{x^2}{2} - \frac{y^2}{2} + z^2$

*continued ...*

Table 2

#	symbol	irrep.	rank	X	multiplicity	component	symmetry
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	$\frac{\sqrt{15}z(x-y)(x+y)}{2}$
30	$\mathbb{G}_{4,1}(E, 2)$	$E$	4	$G, M$	2	1	$\frac{\sqrt{35}(x^2-2xy-y^2)(x^2+2xy-y^2)}{8}$

continued ...

Table 2

#	symbol	irrep.	rank	X	multiplicity	component	symmetry
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$	$y$
$ p_z\rangle$	$z$

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**SAMB: 60 (all 60)**


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• **A : 'A' site-cluster**

\* 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 : 'B' site-cluster**

\* 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**

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

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

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

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

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

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

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

\* 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**

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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



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

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

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

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

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

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

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

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

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## Atomic SAMB

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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## Cluster SAMB

- Site cluster

\*\* Wyckoff: 1c

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

\*\* Wyckoff: 1b

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

- Bond cluster

\*\* Wyckoff: 3a@3d

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

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

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

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

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

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

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#### Site and Bond

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Table 5: Orbital of each site

#	site	orbital
1	<b>A</b>	$ p_x, \uparrow\rangle,  p_x, \downarrow\rangle,  p_y, \uparrow\rangle,  p_y, \downarrow\rangle$
2	<b>B</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	<b>A</b>	<b>B</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 ( $s$ )	mapping
1	[ 0.33333, 0.66667, 0.00000]	[1,2,3,4,5,6]

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

SL	position ( $s$ )	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,  $|v|=0.57735$  (cartesian)

SL	vector ( $v$ )	center ( $c$ )	mapping	head	tail	$R$ (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]