

# Model for “Cs1”

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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', A'']**
  - Spin (s): **[0, 1]**
- Max. neighbor: **10**
- Search cell range: **(-2, 3), (-2, 3), (-2, 3)**
- Toroidal priority: **false**

## Group and Unit Cell

- Group: SG No. 6  $C_s^1 Pm$  (b-axis setting) [ monoclinic ]
- Associated point group: PG No. 6  $C_s m$  (b-axis setting) [ monoclinic ]
- Unit cell:  
 $a = 1.00000$ ,  $b = 1.00000$ ,  $c = 1.00000$ ,  $\alpha = 90.0$ ,  $\beta = 90.0$ ,  $\gamma = 90.0$
- Lattice vectors (conventional cell):  
 $\mathbf{a}_1 = [ 1.00000, 0.00000, 0.00000 ]$   
 $\mathbf{a}_2 = [ 0.00000, 1.00000, 0.00000 ]$   
 $\mathbf{a}_3 = [ 0.00000, 0.00000, 1.00000 ]$

## Symmetry Operation

Table 1: Symmetry operation

#	SO	#	SO	#	SO	#	SO
1	{1 0}	2	{m <sub>010</sub>  0}				

Table 2: Harmonics

#	symbol	irrep.	rank	X	multiplicity	component	symmetry
1	$\mathbb{Q}_0(A')$	$A'$	0	$Q, T$	-	-	1
2	$\mathbb{G}_1(A')$	$A'$	1	$G, M$	-	-	$y$
3	$\mathbb{Q}_1(A', 1)$	$A'$	1	$Q, T$	1	-	$x$
4	$\mathbb{Q}_1(A', 2)$	$A'$	1	$Q, T$	2	-	$z$
5	$\mathbb{Q}_2(A', 1)$	$A'$	2	$Q, T$	1	-	$-\frac{x^2}{2} - \frac{y^2}{2} + z^2$
6	$\mathbb{Q}_2(A', 2)$	$A'$	2	$Q, T$	2	-	$\frac{\sqrt{3}(x-y)(x+y)}{2}$
7	$\mathbb{Q}_2(A', 3)$	$A'$	2	$Q, T$	3	-	$\sqrt{3}xz$
8	$\mathbb{G}_3(A', 1)$	$A'$	3	$G, M$	1	-	$\sqrt{15}xyz$
9	$\mathbb{G}_3(A', 2)$	$A'$	3	$G, M$	2	-	$-\frac{y(3x^2-2y^2+3z^2)}{2}$
10	$\mathbb{G}_3(A', 3)$	$A'$	3	$G, M$	3	-	$-\frac{\sqrt{15}y(x-z)(x+z)}{2}$
11	$\mathbb{Q}_3(A', 1)$	$A'$	3	$Q, T$	1	-	$\frac{x(2x^2-3y^2-3z^2)}{2}$
12	$\mathbb{Q}_3(A', 2)$	$A'$	3	$Q, T$	2	-	$-\frac{z(3x^2+3y^2-2z^2)}{2}$
13	$\mathbb{Q}_3(A', 4)$	$A'$	3	$Q, T$	4	-	$\frac{\sqrt{15}z(x-y)(x+y)}{2}$
14	$\mathbb{G}_0(A'')$	$A''$	0	$G, M$	-	-	1
15	$\mathbb{G}_1(A'', 1)$	$A''$	1	$G, M$	1	-	$x$
16	$\mathbb{G}_1(A'', 2)$	$A''$	1	$G, M$	2	-	$z$

*continued ...*

Table 2

#	symbol	irrep.	rank	X	multiplicity	component	symmetry
17	$\mathbb{Q}_1(A'')$	$A''$	1	$Q, T$	-	-	$y$
18	$\mathbb{G}_2(A'', 1)$	$A''$	2	$G, M$	1	-	$-\frac{x^2}{2} - \frac{y^2}{2} + z^2$
19	$\mathbb{Q}_2(A'', 1)$	$A''$	2	$Q, T$	1	-	$\sqrt{3}yz$
20	$\mathbb{Q}_2(A'', 2)$	$A''$	2	$Q, T$	2	-	$\sqrt{3}xy$
21	$\mathbb{G}_3(A'', 1)$	$A''$	3	$G, M$	1	-	$\frac{x(2x^2 - 3y^2 - 3z^2)}{2}$
22	$\mathbb{G}_3(A'', 3)$	$A''$	3	$G, M$	3	-	$\frac{\sqrt{15}x(y-z)(y+z)}{2}$
23	$\mathbb{G}_3(A'', 4)$	$A''$	3	$G, M$	4	-	$\frac{\sqrt{15}z(x-y)(x+y)}{2}$
24	$\mathbb{Q}_3(A'', 1)$	$A''$	3	$Q, T$	1	-	$\sqrt{15}xyz$
25	$\mathbb{Q}_3(A'', 3)$	$A''$	3	$Q, T$	3	-	$-\frac{\sqrt{15}y(x-z)(x+z)}{2}$

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Basis in full matrix

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Table 3: dimension = 4

#	orbital@atom(SL)	#	orbital@atom(SL)	#	orbital@atom(SL)	#	orbital@atom(SL)
1	$ p_x, \uparrow\rangle @A(1)$	2	$ p_x, \downarrow\rangle @A(1)$	3	$ p_y, \uparrow\rangle @A(1)$	4	$ p_y, \downarrow\rangle @A(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

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70 (all 150) SAMBs

- '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: **1a**

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

$$\boxed{\text{z2}} \quad \mathbb{Q}_2^{(c)}(A', 2) = \mathbb{Q}_2^{(a)}(A', 2)\mathbb{Q}_0^{(s)}(A')$$

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

$$\boxed{\text{z4}} \quad \mathbb{Q}_2^{(1, -1; c)}(A', 3) = \mathbb{Q}_2^{(1, -1; a)}(A', 3)\mathbb{Q}_0^{(s)}(A')$$

$$\boxed{\text{z79}} \quad \mathbb{Q}_2^{(c)}(A'', 2) = \mathbb{Q}_2^{(a)}(A'', 2)\mathbb{Q}_0^{(s)}(A')$$

$$\boxed{\text{z80}} \quad \mathbb{Q}_2^{(1, -1; c)}(A'', 1) = \mathbb{Q}_2^{(1, -1; a)}(A'', 1)\mathbb{Q}_0^{(s)}(A')$$

- 'A'-'A' 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: **1a@1a**

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

$$\boxed{\text{z6}} \quad \mathbb{Q}_2^{(c)}(A', 2) = \mathbb{Q}_2^{(a)}(A', 2)\mathbb{Q}_0^{(b)}(A')$$

$$\boxed{\text{z7}} \quad \mathbb{Q}_2^{(1, -1; c)}(A', 1) = \mathbb{Q}_2^{(1, -1; a)}(A', 1)\mathbb{Q}_0^{(b)}(A')$$

$$\boxed{\text{z8}} \quad \mathbb{Q}_2^{(1, -1; c)}(A', 3) = \mathbb{Q}_2^{(1, -1; a)}(A', 3)\mathbb{Q}_0^{(b)}(A')$$

$$\boxed{\text{z9}} \quad \mathbb{Q}_2^{(c)}(A'', 2) = \mathbb{Q}_2^{(a)}(A'', 2)\mathbb{Q}_0^{(b)}(A')$$

$$\boxed{\text{z10}} \quad \mathbb{Q}_2^{(1, -1; c)}(A'', 1) = \mathbb{Q}_2^{(1, -1; a)}(A'', 1)\mathbb{Q}_0^{(b)}(A')$$

$$\boxed{\text{z11}} \quad \mathbb{G}_1^{(1, -1; c)}(A') = \mathbb{M}_1^{(1, -1; a)}(A')\mathbb{T}_0^{(b)}(A')$$

$$\boxed{\text{z12}} \quad \mathbb{G}_3^{(1, -1; c)}(A', 1) = \mathbb{M}_3^{(1, -1; a)}(A', 1)\mathbb{T}_0^{(b)}(A')$$

$$\boxed{\text{z81}} \quad \mathbb{G}_3^{(1, -1; c)}(A', 2) = \mathbb{M}_3^{(1, -1; a)}(A', 2)\mathbb{T}_0^{(b)}(A')$$

$$\boxed{\text{z82}} \quad \mathbb{G}_3^{(1, -1; c)}(A', 3) = \mathbb{M}_3^{(1, -1; a)}(A', 3)\mathbb{T}_0^{(b)}(A')$$

$$\boxed{\text{z83}} \quad \mathbb{G}_1^{(c)}(A'', 2) = \mathbb{M}_1^{(a)}(A'', 2)\mathbb{T}_0^{(b)}(A')$$

$$\boxed{\text{z84}} \quad \mathbb{G}_1^{(1, -1; c)}(A'', 1) = \mathbb{M}_1^{(1, -1; a)}(A'', 1)\mathbb{T}_0^{(b)}(A')$$

$$\boxed{\text{z85}} \quad \mathbb{G}_1^{(1, -1; c)}(A'', 2) = \mathbb{M}_1^{(1, -1; a)}(A'', 2)\mathbb{T}_0^{(b)}(A')$$

$$\boxed{\text{z86}} \quad \mathbb{G}_3^{(1, -1; c)}(A'', 1) = \mathbb{M}_3^{(1, -1; a)}(A'', 1)\mathbb{T}_0^{(b)}(A')$$

$$\boxed{\text{z87}} \quad \mathbb{G}_3^{(1, -1; c)}(A'', 3) = \mathbb{M}_3^{(1, -1; a)}(A'', 3)\mathbb{T}_0^{(b)}(A')$$

$$\boxed{\text{z88}} \quad \mathbb{G}_3^{(1, -1; c)}(A'', 4) = \mathbb{M}_3^{(1, -1; a)}(A'', 4)\mathbb{T}_0^{(b)}(A')$$

\* common SAMBs

(z5, z23, z47, z55), (z6, z24, z48, z56), (z7, z25, z49, z57), (z8, z26, z50, z58), (z9, z27, z51, z59), (z10, z28, z52, z60), (z11, z29, z53, z61), (z12, z30, z54, z62), (z81, z95, z119, z127), (z82, z96, z120, z128), (z83, z97, z121, z129), (z84, z98, z122, z130), (z85, z99, z123, z131), (z86, z100, z124, z132), (z87, z101, z125, z133), (z88, z102, z126, z134)

• 'A'-'A' 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: **1b@1b**

$$\boxed{\text{z13}} \quad \mathbb{Q}_0^{(c)}(A') = \mathbb{Q}_0^{(a)}(A')\mathbb{Q}_0^{(b)}(A')$$

$$\boxed{\text{z14}} \quad \mathbb{Q}_1^{(c)}(A', 1) = -\mathbb{M}_1^{(a)}(A'', 2)\mathbb{T}_1^{(b)}(A'')$$

$$\boxed{\text{z15}} \quad \mathbb{Q}_2^{(c)}(A', 2) = \mathbb{Q}_2^{(a)}(A', 2)\mathbb{Q}_0^{(b)}(A')$$

$$\boxed{\text{z16}} \quad \mathbb{Q}_1^{(1,-1;c)}(A', 1) = -\mathbb{M}_1^{(1,-1;a)}(A'', 2)\mathbb{T}_1^{(b)}(A'')$$

$$\boxed{\text{z17}} \quad \mathbb{Q}_1^{(1,-1;c)}(A', 2) = \mathbb{M}_1^{(1,-1;a)}(A'', 1)\mathbb{T}_1^{(b)}(A'')$$

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

$$\boxed{\text{z19}} \quad \mathbb{Q}_2^{(1,-1;c)}(A', 3) = \mathbb{Q}_2^{(1,-1;a)}(A', 3)\mathbb{Q}_0^{(b)}(A')$$

$$\boxed{\text{z20}} \quad \mathbb{Q}_3^{(1,-1;c)}(A', 1) = -\mathbb{M}_3^{(1,-1;a)}(A'', 4)\mathbb{T}_1^{(b)}(A'')$$

$$\boxed{\text{z21}} \quad \mathbb{Q}_3^{(1,-1;c)}(A', 2) = -\frac{\sqrt{6}\mathbb{M}_3^{(1,-1;a)}(A'', 1)\mathbb{T}_1^{(b)}(A'')}{4} - \frac{\sqrt{10}\mathbb{M}_3^{(1,-1;a)}(A'', 3)\mathbb{T}_1^{(b)}(A'')}{4}$$

$$\boxed{\text{z22}} \quad \mathbb{Q}_3^{(1,-1;c)}(A', 4) = \frac{\sqrt{10}\mathbb{M}_3^{(1,-1;a)}(A'', 1)\mathbb{T}_1^{(b)}(A'')}{4} - \frac{\sqrt{6}\mathbb{M}_3^{(1,-1;a)}(A'', 3)\mathbb{T}_1^{(b)}(A'')}{4}$$

$$\boxed{\text{z89}} \quad \mathbb{Q}_2^{(c)}(A'', 2) = \mathbb{Q}_2^{(a)}(A'', 2)\mathbb{Q}_0^{(b)}(A')$$

$$\boxed{\text{z90}} \quad \mathbb{Q}_2^{(1,-1;c)}(A'', 1) = \mathbb{Q}_2^{(1,-1;a)}(A'', 1)\mathbb{Q}_0^{(b)}(A')$$

$$\boxed{\text{z91}} \quad \mathbb{Q}_3^{(1,-1;c)}(A'', 1) = -\mathbb{M}_3^{(1,-1;a)}(A', 3)\mathbb{T}_1^{(b)}(A'')$$

$$\boxed{\text{z92}} \quad \mathbb{Q}_3^{(1,-1;c)}(A'', 3) = \mathbb{M}_3^{(1,-1;a)}(A', 1)\mathbb{T}_1^{(b)}(A'')$$

$$\boxed{\text{z93}} \quad \mathbb{G}_0^{(1,-1;c)}(A'') = \mathbb{M}_1^{(1,-1;a)}(A')\mathbb{T}_1^{(b)}(A'')$$

$$\boxed{\text{z94}} \quad \mathbb{G}_2^{(1,-1;c)}(A'', 1) = -\mathbb{M}_3^{(1,-1;a)}(A', 2)\mathbb{T}_1^{(b)}(A'')$$

• 'A'-'A' 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: 2c@1b

$$\boxed{\text{z31}} \quad \mathbb{Q}_0^{(c)}(A') = \mathbb{Q}_0^{(a)}(A')\mathbb{Q}_0^{(b)}(A')$$

$$\boxed{\text{z32}} \quad \mathbb{Q}_1^{(c)}(A', 1a) = \mathbb{Q}_2^{(a)}(A'', 2)\mathbb{Q}_1^{(b)}(A'')$$

$$\boxed{\text{z33}} \quad \mathbb{Q}_1^{(c)}(A', 1b) = -\mathbb{M}_1^{(a)}(A'', 2)\mathbb{T}_1^{(b)}(A'')$$

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

$$\boxed{\text{z35}} \quad \mathbb{Q}_1^{(1,-1;c)}(A', 1) = -\mathbb{M}_1^{(1,-1;a)}(A'', 2)\mathbb{T}_1^{(b)}(A'')$$

$$\boxed{\text{z36}} \quad \mathbb{Q}_1^{(1,-1;c)}(A', 2a) = \mathbb{Q}_2^{(1,-1;a)}(A'', 1)\mathbb{Q}_1^{(b)}(A'')$$

$$\boxed{\text{z37}} \quad \mathbb{Q}_1^{(1,-1;c)}(A', 2b) = \mathbb{M}_1^{(1,-1;a)}(A'', 1)\mathbb{T}_1^{(b)}(A'')$$

$$\boxed{\text{z38}} \quad \mathbb{Q}_2^{(1,-1;c)}(A', 1) = \mathbb{Q}_2^{(1,-1;a)}(A', 1)\mathbb{Q}_0^{(b)}(A')$$

$$\boxed{\text{z39}} \quad \mathbb{Q}_2^{(1,-1;c)}(A', 3) = \mathbb{Q}_2^{(1,-1;a)}(A', 3)\mathbb{Q}_0^{(b)}(A')$$

$$\boxed{\text{z40}} \quad \mathbb{Q}_3^{(1,-1;c)}(A', 1) = -\mathbb{M}_3^{(1,-1;a)}(A'', 4)\mathbb{T}_1^{(b)}(A'')$$

$$\boxed{\text{z41}} \quad \mathbb{Q}_3^{(1,-1;c)}(A', 2) = -\frac{\sqrt{6}\mathbb{M}_3^{(1,-1;a)}(A'', 1)\mathbb{T}_1^{(b)}(A'')}{4} - \frac{\sqrt{10}\mathbb{M}_3^{(1,-1;a)}(A'', 3)\mathbb{T}_1^{(b)}(A'')}{4}$$

$$\boxed{\text{z42}} \quad \mathbb{Q}_3^{(1,-1;c)}(A', 4) = \frac{\sqrt{10}\mathbb{M}_3^{(1,-1;a)}(A'', 1)\mathbb{T}_1^{(b)}(A'')}{4} - \frac{\sqrt{6}\mathbb{M}_3^{(1,-1;a)}(A'', 3)\mathbb{T}_1^{(b)}(A'')}{4}$$

$$\boxed{\text{z43}} \quad \mathbb{Q}_1^{(c)}(A'', a) = \mathbb{Q}_0^{(a)}(A')\mathbb{Q}_1^{(b)}(A'')$$

$$\boxed{\text{z44}} \quad \mathbb{Q}_1^{(c)}(A'', b) = -\mathbb{Q}_2^{(a)}(A', 2)\mathbb{Q}_1^{(b)}(A'')$$

$$\boxed{\text{z45}} \quad \mathbb{Q}_2^{(c)}(A'', 2) = \mathbb{Q}_2^{(a)}(A'', 2)\mathbb{Q}_0^{(b)}(A')$$

$$\boxed{\text{z46}} \quad \mathbb{Q}_1^{(1,-1;c)}(A'') = -\mathbb{Q}_2^{(1,-1;a)}(A', 1)\mathbb{Q}_1^{(b)}(A'')$$

$$\begin{aligned}
\boxed{\text{z103}} \quad & \mathbb{Q}_2^{(1,-1;c)}(A'', 1) = \mathbb{Q}_2^{(1,-1;a)}(A'', 1)\mathbb{Q}_0^{(b)}(A') \\
\boxed{\text{z104}} \quad & \mathbb{Q}_3^{(1,-1;c)}(A'', 1a) = \mathbb{Q}_2^{(1,-1;a)}(A', 3)\mathbb{Q}_1^{(b)}(A'') \\
\boxed{\text{z105}} \quad & \mathbb{Q}_3^{(1,-1;c)}(A'', 1b) = -\mathbb{M}_3^{(1,-1;a)}(A', 3)\mathbb{T}_1^{(b)}(A'') \\
\boxed{\text{z106}} \quad & \mathbb{Q}_3^{(1,-1;c)}(A'', 3) = \mathbb{M}_3^{(1,-1;a)}(A', 1)\mathbb{T}_1^{(b)}(A'') \\
\boxed{\text{z107}} \quad & \mathbb{G}_1^{(1,-1;c)}(A') = \mathbb{M}_1^{(1,-1;a)}(A')\mathbb{T}_0^{(b)}(A') \\
\boxed{\text{z108}} \quad & \mathbb{G}_3^{(1,-1;c)}(A', 1) = \mathbb{M}_3^{(1,-1;a)}(A', 1)\mathbb{T}_0^{(b)}(A') \\
\boxed{\text{z109}} \quad & \mathbb{G}_3^{(1,-1;c)}(A', 2) = \mathbb{M}_3^{(1,-1;a)}(A', 2)\mathbb{T}_0^{(b)}(A') \\
\boxed{\text{z110}} \quad & \mathbb{G}_3^{(1,-1;c)}(A', 3) = \mathbb{M}_3^{(1,-1;a)}(A', 3)\mathbb{T}_0^{(b)}(A') \\
\boxed{\text{z111}} \quad & \mathbb{G}_1^{(c)}(A'', 2) = \mathbb{M}_1^{(a)}(A'', 2)\mathbb{T}_0^{(b)}(A') \\
\boxed{\text{z112}} \quad & \mathbb{G}_0^{(1,-1;c)}(A'') = \mathbb{M}_1^{(1,-1;a)}(A')\mathbb{T}_1^{(b)}(A'') \\
\boxed{\text{z113}} \quad & \mathbb{G}_1^{(1,-1;c)}(A'', 1) = \mathbb{M}_1^{(1,-1;a)}(A'', 1)\mathbb{T}_0^{(b)}(A') \\
\boxed{\text{z114}} \quad & \mathbb{G}_1^{(1,-1;c)}(A'', 2) = \mathbb{M}_1^{(1,-1;a)}(A'', 2)\mathbb{T}_0^{(b)}(A') \\
\boxed{\text{z115}} \quad & \mathbb{G}_2^{(1,-1;c)}(A'', 1) = -\mathbb{M}_3^{(1,-1;a)}(A', 2)\mathbb{T}_1^{(b)}(A'') \\
\boxed{\text{z116}} \quad & \mathbb{G}_3^{(1,-1;c)}(A'', 1) = \mathbb{M}_3^{(1,-1;a)}(A'', 1)\mathbb{T}_0^{(b)}(A') \\
\boxed{\text{z117}} \quad & \mathbb{G}_3^{(1,-1;c)}(A'', 3) = \mathbb{M}_3^{(1,-1;a)}(A'', 3)\mathbb{T}_0^{(b)}(A') \\
\boxed{\text{z118}} \quad & \mathbb{G}_3^{(1,-1;c)}(A'', 4) = \mathbb{M}_3^{(1,-1;a)}(A'', 4)\mathbb{T}_0^{(b)}(A')
\end{aligned}$$

\* common SAMBs

(z31, z63), (z32, z64), (z33, z65), (z34, z66), (z35, z67), (z36, z68), (z37, z69), (z38, z70), (z39, z71), (z40, z72), (z41, z73), (z42, z74), (z43, z75), (z44, z76), (z45, z77), (z46, z78), (z103, z135), (z104, z136), (z105, z137), (z106, z138), (z107, z139), (z108, z140), (z109, z141), (z110, z142), (z111, z143), (z112, z144), (z113, z145), (z114, z146), (z115, z147), (z116, z148), (z117, z149), (z118, z150)



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

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

$$\boxed{\text{x2}} \quad \mathbb{Q}_2^{(a)}(A', 2) = \begin{bmatrix} \frac{1}{2} & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 \\ 0 & 0 & -\frac{1}{2} & 0 \\ 0 & 0 & 0 & -\frac{1}{2} \end{bmatrix}$$

$$\boxed{\text{x3}} \quad \mathbb{Q}_2^{(a)}(A'', 2) = \begin{bmatrix} 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & \frac{1}{2} \\ \frac{1}{2} & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 \end{bmatrix}$$

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

$$\boxed{\text{x5}} \quad \mathbb{Q}_2^{(1,-1;a)}(A', 3) = \begin{bmatrix} 0 & 0 & 0 & -\frac{i}{2} \\ 0 & 0 & -\frac{i}{2} & 0 \\ 0 & \frac{i}{2} & 0 & 0 \\ \frac{i}{2} & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x6}} \quad \mathbb{Q}_2^{(1,-1;a)}(A'', 1) = \begin{bmatrix} 0 & 0 & 0 & -\frac{1}{2} \\ 0 & 0 & \frac{1}{2} & 0 \\ 0 & \frac{1}{2} & 0 & 0 \\ -\frac{1}{2} & 0 & 0 & 0 \end{bmatrix}$$

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

$$\boxed{\text{x8}} \quad \mathbb{M}_1^{(1,-1;a)}(A') = \begin{bmatrix} 0 & -\frac{i}{2} & 0 & 0 \\ \frac{i}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{i}{2} \\ 0 & 0 & \frac{i}{2} & 0 \end{bmatrix}$$

$$\boxed{\text{x9}} \quad \mathbb{M}_3^{(1,-1;a)}(A', 1) = \begin{bmatrix} 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & -\frac{1}{2} \\ \frac{1}{2} & 0 & 0 & 0 \\ 0 & -\frac{1}{2} & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x10}} \quad \mathbb{M}_3^{(1,-1;a)}(A', 2) = \begin{bmatrix} 0 & \frac{3\sqrt{13}i}{26} & 0 & -\frac{\sqrt{13}}{13} \\ -\frac{3\sqrt{13}i}{26} & 0 & -\frac{\sqrt{13}}{13} & 0 \\ 0 & -\frac{\sqrt{13}}{13} & 0 & -\frac{3\sqrt{13}i}{26} \\ -\frac{\sqrt{13}}{13} & 0 & \frac{3\sqrt{13}i}{26} & 0 \end{bmatrix}$$

$$\boxed{\text{x11}} \quad \mathbb{M}_3^{(1,-1;a)}(A', 3) = \begin{bmatrix} 0 & -\frac{\sqrt{13}i}{13} & 0 & -\frac{3\sqrt{13}}{26} \\ \frac{\sqrt{13}i}{13} & 0 & -\frac{3\sqrt{13}}{26} & 0 \\ 0 & -\frac{3\sqrt{13}}{26} & 0 & \frac{\sqrt{13}i}{13} \\ -\frac{3\sqrt{13}}{26} & 0 & -\frac{\sqrt{13}i}{13} & 0 \end{bmatrix}$$

$$\boxed{\text{x12}} \quad \mathbb{M}_1^{(1,-1;a)}(A'', 1) = \begin{bmatrix} 0 & \frac{1}{2} & 0 & 0 \\ \frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2} \\ 0 & 0 & \frac{1}{2} & 0 \end{bmatrix}$$

$$\boxed{\text{x13}} \quad \mathbb{M}_1^{(1,-1;a)}(A'', 2) = \begin{bmatrix} \frac{1}{2} & 0 & 0 & 0 \\ 0 & -\frac{1}{2} & 0 & 0 \\ 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & -\frac{1}{2} \end{bmatrix}$$

$$\boxed{\text{x14}} \quad \mathbb{M}_3^{(1,-1;a)}(A'', 1) = \begin{bmatrix} 0 & \frac{3\sqrt{13}}{26} & 0 & \frac{\sqrt{13}i}{13} \\ \frac{3\sqrt{13}}{26} & 0 & -\frac{\sqrt{13}i}{13} & 0 \\ 0 & \frac{\sqrt{13}i}{13} & 0 & -\frac{3\sqrt{13}}{26} \\ -\frac{\sqrt{13}i}{13} & 0 & -\frac{3\sqrt{13}}{26} & 0 \end{bmatrix}$$

$$\boxed{\text{x15}} \quad \mathbb{M}_3^{(1,-1;a)}(A'', 3) = \begin{bmatrix} 0 & \frac{\sqrt{13}}{13} & 0 & -\frac{3\sqrt{13}i}{26} \\ \frac{\sqrt{13}}{13} & 0 & \frac{3\sqrt{13}i}{26} & 0 \\ 0 & -\frac{3\sqrt{13}i}{26} & 0 & -\frac{\sqrt{13}}{13} \\ \frac{3\sqrt{13}i}{26} & 0 & -\frac{\sqrt{13}}{13} & 0 \end{bmatrix}$$

$$\boxed{\text{x16}} \quad \mathbb{M}_3^{(1,-1;a)}(A'',4) = \begin{bmatrix} \frac{1}{2} & 0 & 0 & 0 \\ 0 & -\frac{1}{2} & 0 & 0 \\ 0 & 0 & -\frac{1}{2} & 0 \\ 0 & 0 & 0 & \frac{1}{2} \end{bmatrix}$$

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## Cluster SAMB

- Site cluster

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

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

- Bond cluster

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

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

$$\boxed{\text{y3}} \quad \mathbb{T}_0^{(s)}(A') = [i]$$

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

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

$$\boxed{\text{y5}} \quad \mathbb{T}_1^{(s)}(A'') = [i]$$

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

$$\boxed{\text{y6}} \quad \mathbb{Q}_0^{(s)}(A') = \left[ \frac{\sqrt{2}}{2}, \frac{\sqrt{2}}{2} \right]$$

$$\boxed{\text{y7}} \quad \mathbb{T}_0^{(s)}(A') = \left[ \frac{\sqrt{2}i}{2}, \frac{\sqrt{2}i}{2} \right]$$

$$\boxed{\text{y8}} \quad \mathbb{Q}_1^{(s)}(A'') = \left[ \frac{\sqrt{2}}{2}, -\frac{\sqrt{2}}{2} \right]$$

y9

$$\mathbb{T}_1^{(s)}(A'') = \left[ \frac{\sqrt{2}i}{2}, -\frac{\sqrt{2}i}{2} \right]$$

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**Site and Bond**


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Table 5: Orbital of each site

#	site	orbital
1	<b>A</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>A</b>	<b>[1,2]</b>	<b>[p]</b>	<b>[p]</b>

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**Site in Unit Cell**


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

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

SL	position ( <b>s</b> )	mapping
1	[ 0.00000, 0.00000, 0.00000]	[1,2]

## 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 (**1a@1a**), D,  $|\mathbf{v}|=1.0$  (cartesian)

SL	vector ( <b>v</b> )	center ( <b>c</b> )	mapping	head	tail	<b>R</b> (primitive)
1	[-1.00000, 0.00000, 0.00000]	[ 0.50000, 0.00000, 0.00000]	[1,2]	(1,1)	(1,1)	[1,0,0]

Table 9: 1-th 'A'-'A' [2] (#2) bond cluster (**1b@1b**), ND,  $|\mathbf{v}|=1.0$  (cartesian)

SL	vector ( <b>v</b> )	center ( <b>c</b> )	mapping	head	tail	<b>R</b> (primitive)
1	[ 0.00000,-1.00000, 0.00000]	[ 0.00000, 0.50000, 0.00000]	[1,-2]	(1,1)	(1,1)	[0,1,0]

Table 10: 1-th 'A'-'A' [3] (#3) bond cluster (1a@1a), D,  $|\mathbf{v}|=1.0$  (cartesian)

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

Table 11: 2-th 'A'-'A' [1] (#4) bond cluster (2c@1b), D,  $|\mathbf{v}|=1.41421$  (cartesian)

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

Table 12: 2-th 'A'-'A' [2] (#5) bond cluster (1a@1a), D,  $|\mathbf{v}|=1.41421$  (cartesian)

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

Table 13: 2-th 'A'-'A' [3] (#6) bond cluster (**1a@1a**), D,  $|\mathbf{v}|= 1.41421$  (cartesian)

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

Table 14: 2-th 'A'-'A' [4] (#7) bond cluster (**2c@1b**), D,  $|\mathbf{v}|= 1.41421$  (cartesian)

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