

Model for “Cs1”

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General Condition

- Basis type: 1gs
- 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]
- Atomic selection:
 - Type: [Q, G, M, T]
 - Rank: [0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11]
 - Irrep.: [A', A'']
 - Spin (s): [0, 1]
- Site-cluster selection:
 - Rank: [0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11]
 - Irrep.: [A', A'']
- Bond-cluster selection:
 - Type: [Q, G, M, T]
 - Rank: [0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11]
 - Irrep.: [A', A'']
- 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 ₀₁₀ 0}		

 — Harmonics —

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	-	$-\frac{y(3x^2 - 2y^2 + 3z^2)}{2}$

continued ...

Table 2

#	symbol	irrep.	rank	X	multiplicity	component	symmetry
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
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	-	$-\frac{\sqrt{15}y(x-z)(x+z)}{2}$

— Basis in full matrix —

Table 3: dimension = 4

#	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)$

Table 4: Atomic basis (orbital part only)

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

SAMB

70 (all 150) 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: **1a**

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

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

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

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

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

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

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

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

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

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

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

$$\boxed{\text{z9}} \quad \mathbb{G}_1^{(1,-1;c)}(A') = \mathbb{M}_1^{(1,-1;a)}(A')\mathbb{T}_0^{(b)}(A')$$

$$\boxed{\text{z10}} \quad \mathbb{G}_3^{(1,-1;c)}(A', 1) = \mathbb{M}_3^{(1,-1;a)}(A', 1)\mathbb{T}_0^{(b)}(A')$$

$$\boxed{\text{z11}} \quad \mathbb{G}_3^{(1,-1;c)}(A', 2) = \mathbb{M}_3^{(1,-1;a)}(A', 2)\mathbb{T}_0^{(b)}(A')$$

$$\boxed{\text{z12}} \quad \mathbb{G}_3^{(1,-1;c)}(A', 3) = \mathbb{M}_3^{(1,-1;a)}(A', 3)\mathbb{T}_0^{(b)}(A')$$

$$\boxed{\text{z81}} \quad \mathbb{Q}_2^{(c)}(A'', 2) = \mathbb{Q}_2^{(a)}(A'', 2)\mathbb{Q}_0^{(b)}(A')$$

$$\boxed{\text{z82}} \quad \mathbb{Q}_2^{(1,-1;c)}(A'', 1) = \mathbb{Q}_2^{(1,-1;a)}(A'', 1)\mathbb{Q}_0^{(b)}(A')$$

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

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

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

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

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

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

* common SAMBs

(A;A_001_1, A;A_001_3, A;A_002_2, A;A_002_3), (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 : A;A_001_2

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

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

* 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 : 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: 2c@1b

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

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

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

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

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

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

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

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

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

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

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

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

$$\boxed{\text{z43}} \quad \mathbb{G}_1^{(1,-1;c)}(A') = \mathbb{M}_1^{(1,-1;a)}(A')\mathbb{T}_0^{(b)}(A')$$

$$\boxed{\text{z44}} \quad \mathbb{G}_3^{(1,-1;c)}(A', 1) = \mathbb{M}_3^{(1,-1;a)}(A', 1)\mathbb{T}_0^{(b)}(A')$$

$$\boxed{\text{z45}} \quad \mathbb{G}_3^{(1,-1;c)}(A', 2) = \mathbb{M}_3^{(1,-1;a)}(A', 2)\mathbb{T}_0^{(b)}(A')$$

$$\boxed{\text{z46}} \quad \mathbb{G}_3^{(1,-1;c)}(A', 3) = \mathbb{M}_3^{(1,-1;a)}(A', 3)\mathbb{T}_0^{(b)}(A')$$

$$\boxed{\text{z103}} \quad \mathbb{Q}_1^{(c)}(A'', a) = \mathbb{Q}_0^{(a)}(A')\mathbb{Q}_1^{(b)}(A'')$$

$$\boxed{\text{z104}} \quad \mathbb{Q}_1^{(c)}(A'', b) = -\mathbb{Q}_2^{(a)}(A', 2)\mathbb{Q}_1^{(b)}(A'')$$

$$\boxed{\text{z105}} \quad \mathbb{Q}_2^{(c)}(A'', 2) = \mathbb{Q}_2^{(a)}(A'', 2)\mathbb{Q}_0^{(b)}(A')$$

$$\boxed{\text{z106}} \quad \mathbb{Q}_1^{(1,-1;c)}(A'') = -\mathbb{Q}_2^{(1,-1;a)}(A', 1)\mathbb{Q}_1^{(b)}(A'')$$

$$\boxed{\text{z107}} \quad \mathbb{Q}_2^{(1,-1;c)}(A'', 1) = \mathbb{Q}_2^{(1,-1;a)}(A'', 1)\mathbb{Q}_0^{(b)}(A')$$

$$\boxed{\text{z108}} \quad \mathbb{Q}_3^{(1,-1;c)}(A'', 1a) = \mathbb{Q}_2^{(1,-1;a)}(A', 3)\mathbb{Q}_1^{(b)}(A'')$$

$$\boxed{\text{z109}} \quad \mathbb{Q}_3^{(1,-1;c)}(A'', 1b) = -\mathbb{M}_3^{(1,-1;a)}(A', 3)\mathbb{T}_1^{(b)}(A'')$$

$$\boxed{\text{z110}} \quad \mathbb{Q}_3^{(1,-1;c)}(A'', 3) = \mathbb{M}_3^{(1,-1;a)}(A', 1)\mathbb{T}_1^{(b)}(A'')$$

$$\boxed{\text{z111}} \quad \mathbb{G}_1^{(c)}(A'', 2) = \mathbb{M}_1^{(a)}(A'', 2)\mathbb{T}_0^{(b)}(A')$$

$$\boxed{\text{z112}} \quad \mathbb{G}_0^{(1,-1;c)}(A'') = \mathbb{M}_1^{(1,-1;a)}(A')\mathbb{T}_1^{(b)}(A'')$$

$$\boxed{\text{z113}} \quad \mathbb{G}_1^{(1,-1;c)}(A'', 1) = \mathbb{M}_1^{(1,-1;a)}(A'', 1)\mathbb{T}_0^{(b)}(A')$$

$$\boxed{\text{z114}} \quad \mathbb{G}_1^{(1,-1;c)}(A'', 2) = \mathbb{M}_1^{(1,-1;a)}(A'', 2)\mathbb{T}_0^{(b)}(A')$$

$$\boxed{\text{z115}} \quad \mathbb{G}_2^{(1,-1;c)}(A'', 1) = -\mathbb{M}_3^{(1,-1;a)}(A', 2)\mathbb{T}_1^{(b)}(A'')$$

$$\boxed{\text{z116}} \quad \mathbb{G}_3^{(1,-1;c)}(A'', 1) = \mathbb{M}_3^{(1,-1;a)}(A'', 1)\mathbb{T}_0^{(b)}(A')$$

$$\boxed{\text{z117}} \quad \mathbb{G}_3^{(1,-1;c)}(A'', 3) = \mathbb{M}_3^{(1,-1;a)}(A'', 3)\mathbb{T}_0^{(b)}(A')$$

$$\boxed{\text{z118}} \quad \mathbb{G}_3^{(1,-1;c)}(A'', 4) = \mathbb{M}_3^{(1,-1;a)}(A'', 4)\mathbb{T}_0^{(b)}(A')$$

* common SAMBs

(A;A_002_1, A;A_002_4), (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)

Atomic SAMB

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

— Cluster SAMB —

- Site cluster

** Wyckoff: **1a**

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

- Bond cluster

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

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

$$\boxed{y3} \quad \mathbb{T}_1^{(s)}(A'') = [i]$$

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

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

$$\boxed{y5} \quad \mathbb{T}_0^{(s)}(A') = [i]$$

** Wyckoff: 2c@1b

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

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

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

$$\boxed{y9} \quad \mathbb{T}_1^{(s)}(A'') = \left[\frac{\sqrt{2}i}{2}, -\frac{\sqrt{2}i}{2} \right]$$

Site and Bond

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$

Table 6: Neighbor and bra-ket of each bond

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

— Site in Unit Cell —

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

Table 7: 'A' (#1) site cluster (**1a**), \mathbf{m}

SL	position (\mathbf{s})	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 (\mathbf{v})	center (\mathbf{c})	mapping	head	tail	\mathbf{R} (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 (\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]	(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]