Model for “Cs1”

Generated on 2026-02-01 11:16:07 by MultiPie 2.0.7

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]`
- 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 $C_{\rm s}^1$ Pm (b-axis setting) [monoclinic]
- Associated point group: PG No. 6 $C_{\rm s}$ 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):
  $\boldsymbol{a}_1 =$ [1.00000, 0.00000, 0.00000]
  $\boldsymbol{a}_2 =$ [0.00000, 1.00000, 0.00000]
  $\boldsymbol{a}_3 =$ [0.00000, 0.00000, 1.00000]

Symmetry Operation

Table 1: Symmetry operation

#	SO	#	SO	#	SO	#	SO
1	$\{1\|0\}$	2	$\{\mathrm{m}_{010}\|0\}$				

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	-	$\frac{x\left(2x^2-3y^2-3z^2\right)}{2}$
12	$\mathbb{Q}_3(A',2)$	A'	3	Q, T	2	-	$-\frac{z\left(3x^2+3y^2-2z^2\right)}{2}$
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	-	$\frac{x\left(2x^2-3y^2-3z^2\right)}{2}$
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	$\lvert p_x, \uparrow\rangle$ @A(1)	1	$\lvert p_x, \downarrow\rangle$ @A(1)	2	$\lvert p_y, \uparrow\rangle$ @A(1)	3	$\lvert p_y, \downarrow\rangle$ @A(1)

Table 4: Atomic basis (orbital part only)

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

SAMB

70 (all 150) SAMBs

- 'A' site-cluster : A
  - * bra: $\langle p_x, \uparrow\rvert$, $\langle p_x, \downarrow\rvert$, $\langle p_y, \uparrow\rvert$, $\langle p_y, \downarrow\rvert$
  - * ket: $\lvert p_x, \uparrow\rangle$, $\lvert p_x, \downarrow\rangle$, $\lvert p_y, \uparrow\rangle$, $\lvert p_y, \downarrow\rangle$
  - * wyckoff: 1a

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

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

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

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

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

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

- '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`

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

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

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

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

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

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

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

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

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

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

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

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

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

$\boxed{\text{z86}}$ $\mathbb{G}_{3}^{(1,-1;c)}(A'',1) = \mathbb{M}_{3}^{(1,-1;a)}(A'',1)\mathbb{T}_{0}^{(b)}(A')$

$\boxed{\text{z87}}$ $\mathbb{G}_{3}^{(1,-1;c)}(A'',3) = \mathbb{M}_{3}^{(1,-1;a)}(A'',3)\mathbb{T}_{0}^{(b)}(A')$

$\boxed{\text{z88}}$ $\mathbb{G}_{3}^{(1,-1;c)}(A'',4) = \mathbb{M}_{3}^{(1,-1;a)}(A'',4)\mathbb{T}_{0}^{(b)}(A')$

* 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`

$\boxed{\text{z13}}$ $\mathbb{Q}_{0}^{(c)}(A') = \mathbb{Q}_{0}^{(a)}(A')\mathbb{Q}_{0}^{(b)}(A')$

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

$\boxed{\text{z15}}$ $\mathbb{Q}_{2}^{(c)}(A',2) = \mathbb{Q}_{2}^{(a)}(A',2)\mathbb{Q}_{0}^{(b)}(A')$

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

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

$\boxed{\text{z18}}$ $\mathbb{Q}_{2}^{(1,-1;c)}(A',1) = \mathbb{Q}_{2}^{(1,-1;a)}(A',1)\mathbb{Q}_{0}^{(b)}(A')$

$\boxed{\text{z19}}$ $\mathbb{Q}_{2}^{(1,-1;c)}(A',3) = \mathbb{Q}_{2}^{(1,-1;a)}(A',3)\mathbb{Q}_{0}^{(b)}(A')$

$\boxed{\text{z20}}$ $\mathbb{Q}_{3}^{(1,-1;c)}(A',1) = -\mathbb{M}_{3}^{(1,-1;a)}(A'',4)\mathbb{T}_{1}^{(b)}(A'')$

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

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

$\boxed{\text{z89}}$ $\mathbb{Q}_{2}^{(c)}(A'',2) = \mathbb{Q}_{2}^{(a)}(A'',2)\mathbb{Q}_{0}^{(b)}(A')$

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

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

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

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

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

- '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`

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Cluster SAMB

- Site cluster

** Wyckoff: `1a`

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

- Bond cluster

** Wyckoff: `1a@1a`

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

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

** Wyckoff: `1b@1b`

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

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

** Wyckoff: `2c@1b`

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

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

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

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

Site and Bond

Table 5: Orbital of each site

#	site	orbital
1	`A`	$\lvert p_x, \uparrow\rangle$, $\lvert p_x, \downarrow\rangle$, $\lvert p_y, \uparrow\rangle$, $\lvert p_y, \downarrow\rangle$

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), m

SL	position ($\boldsymbol{s}$)	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, $|\boldsymbol{v}|$= 1.0 (cartesian)

SL	vector ($\boldsymbol{v}$)	center ($\boldsymbol{c}$)	mapping	head	tail	$\boldsymbol{R}$ (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, $|\boldsymbol{v}|$= 1.0 (cartesian)

SL	vector ($\boldsymbol{v}$)	center ($\boldsymbol{c}$)	mapping	head	tail	$\boldsymbol{R}$ (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, $|\boldsymbol{v}|$= 1.0 (cartesian)

SL	vector ($\boldsymbol{v}$)	center ($\boldsymbol{c}$)	mapping	head	tail	$\boldsymbol{R}$ (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, $|\boldsymbol{v}|$= 1.41421 (cartesian)

SL	vector ($\boldsymbol{v}$)	center ($\boldsymbol{c}$)	mapping	head	tail	$\boldsymbol{R}$ (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, $|\boldsymbol{v}|$= 1.41421 (cartesian)

SL	vector ($\boldsymbol{v}$)	center ($\boldsymbol{c}$)	mapping	head	tail	$\boldsymbol{R}$ (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, $|\boldsymbol{v}|$= 1.41421 (cartesian)

SL	vector ($\boldsymbol{v}$)	center ($\boldsymbol{c}$)	mapping	head	tail	$\boldsymbol{R}$ (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, $|\boldsymbol{v}|$= 1.41421 (cartesian)

SL	vector ($\boldsymbol{v}$)	center ($\boldsymbol{c}$)	mapping	head	tail	$\boldsymbol{R}$ (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]