Model for "C4v1"

General Condition

- Basis type: `lgs`
- SAMB selection:
  - Type: `[Q, G]`
  - Rank: `[0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11]`
  - Irrep.: $[A_1, A_2, B_1, B_2, E]$
  - 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. 99 C_{4v}^1 $P4mm$ [tetragonal]
- Associated point group: PG No. 99 C_{4v} $4mm$ [tetragonal]
- Unit cell:
  $a = 1.00000$, $b = 1.00000$, $c = 1.00000$, $\alpha = 90.0$, $\beta = 90.0$, $\gamma = 90.0$
- Lattice vectors (conventional cell):
  $a_1 = [1.00000, 0.00000, 0.00000]$
  $a_2 = [0.00000, 1.00000, 0.00000]$
  $a_3 = [0.00000, 0.00000, 1.00000]$

Symmetry Operation

Table 1: Symmetry operation

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

continued ...

Table 1

#	SO	#	SO	#	SO	#	SO	#	SO
6	$\{m_{100}|0\}$	7	$\{m_{110}|0\}$	8	$\{m_{1-10}|0\}$				

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	$\mathbb{G}_0(A_2)$	A_2	0	G, M	-	-	1
4	$\mathbb{G}_1(A_2)$	A_2	1	G, M	-	-	z
5	$\mathbb{G}_2(B_1)$	B_1	2	G, M	-	-	$\sqrt{3}xy$
6	$\mathbb{Q}_2(B_1)$	B_1	2	Q, T	-	-	$\frac{\sqrt{3}(x-y)(x+y)}{2}$
7	$\mathbb{G}_2(B_2)$	B_2	2	G, M	-	-	$\frac{\sqrt{3}(x-y)(x+y)}{2}$
8	$\mathbb{G}_{1,1}(E)$	E	1	G, M	-	1	$-y$
9	$\mathbb{G}_{1,2}(E)$					2	x
10	$\mathbb{Q}_{1,1}(E)$	E	1	Q, T	-	1	x
11	$\mathbb{Q}_{1,2}(E)$					2	y

Table 3: dimension = 2

#	orbital@atom(SL)	#	orbital@atom(SL)
0	$\lvert s, \uparrow \rangle$ @A(1)	1	$\lvert s, \downarrow \rangle$ @A(1)

Table 4: Atomic basis (orbital part only)

orbital	definition
$\lvert s \rangle$	1

▬ **SAMB** ▬

11 (all 13) SAMBs

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

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

- 'A'-'A' bond-cluster
  * bra: $\langle s, \uparrow |$, $\langle s, \downarrow |$
  * ket: $| s, \uparrow \rangle$, $| s, \downarrow \rangle$
  * wyckoff: `2a@2c`

$\boxed{\text{z2}}$ $\quad \mathbb{Q}_0^{(c)}(A_1) = \mathbb{Q}_0^{(a)}(A_1)\mathbb{Q}_0^{(b)}(A_1)$

$\boxed{\text{z3}}$ $\quad \mathbb{Q}_1^{(1,-1;c)}(A_1) = \dfrac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E)\mathbb{T}_{1,1}^{(b)}(E)}{2} + \dfrac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E)\mathbb{T}_{1,2}^{(b)}(E)}{2}$

$\boxed{\text{z5}}$ $\quad \mathbb{G}_0^{(1,-1;c)}(A_2) = -\dfrac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E)\mathbb{T}_{1,2}^{(b)}(E)}{2} + \dfrac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E)\mathbb{T}_{1,1}^{(b)}(E)}{2}$

$\boxed{\text{z7}}$ $\quad \mathbb{Q}_2^{(c)}(B_1) = \mathbb{Q}_0^{(a)}(A_1)\mathbb{Q}_2^{(b)}(B_1)$

$\boxed{\text{z8}}$ $\quad \mathbb{G}_2^{(1,-1;c)}(B_1) = -\dfrac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E)\mathbb{T}_{1,1}^{(b)}(E)}{2} + \dfrac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E)\mathbb{T}_{1,2}^{(b)}(E)}{2}$

$\boxed{\text{z9}}$ $\quad \mathbb{G}_2^{(1,-1;c)}(B_2) = \dfrac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E)\mathbb{T}_{1,2}^{(b)}(E)}{2} + \dfrac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E)\mathbb{T}_{1,1}^{(b)}(E)}{2}$

$\boxed{\text{z10}}$ $\quad \mathbb{Q}_{1,1}^{(1,-1;c)}(E) = -\dfrac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(A_2)\mathbb{T}_{1,2}^{(b)}(E)}{2}$

$\boxed{\text{z11}}$ $\quad \mathbb{Q}_{1,2}^{(1,-1;c)}(E) = \dfrac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(A_2)\mathbb{T}_{1,1}^{(b)}(E)}{2}$

- 'A'-'A' bond-cluster
  * bra: $\langle s, \uparrow |$, $\langle s, \downarrow |$
  * ket: $| s, \uparrow \rangle$, $| s, \downarrow \rangle$
  * wyckoff: `1a@1a`

$\boxed{\text{z4}}$ $\quad \mathbb{Q}_0^{(c)}(A_1) = \mathbb{Q}_0^{(a)}(A_1)\mathbb{Q}_0^{(b)}(A_1)$

$\boxed{\text{z6}}$ $\quad \mathbb{G}_1^{(1,-1;c)}(A_2) = \mathbb{M}_1^{(1,-1;a)}(A_2)\mathbb{T}_0^{(b)}(A_1)$

$\boxed{\text{z12}}$ $\quad \mathbb{G}_{1,1}^{(1,-1;c)}(E) = \dfrac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E)\mathbb{T}_0^{(b)}(A_1)}{2}$

$\boxed{\text{z13}}$ $\mathbb{G}_{1,2}^{(1,-1;c)}(E) = \dfrac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E)\mathbb{T}_0^{(b)}(A_1)}{2}$

──── **Atomic SAMB** ────────────────────────────────

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

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

$\boxed{\text{x2}}$ $\mathbb{M}_1^{(1,-1;a)}(A_2) = \begin{bmatrix} \frac{\sqrt{2}}{2} & 0 \\ 0 & -\frac{\sqrt{2}}{2} \end{bmatrix}$

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

$\boxed{\text{x4}}$ $\mathbb{M}_{1,2}^{(1,-1;a)}(E) = \begin{bmatrix} 0 & \frac{\sqrt{2}}{2} \\ \frac{\sqrt{2}}{2} & 0 \end{bmatrix}$

──── **Cluster SAMB** ────────────────────────────────

- Site cluster

** Wyckoff: `1a`

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

- Bond cluster

** Wyckoff: `1a@1a`

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

$\boxed{\text{y3}}$ $\mathbb{T}_0^{(s)}(A_1) = [i]$

** Wyckoff: `2a@2c`

$\boxed{\text{y4}}$ $\mathbb{Q}_0^{(s)}(A_1) = \left[\dfrac{\sqrt{2}}{2}, \ \dfrac{\sqrt{2}}{2} \right]$

$\boxed{\text{y5}}$ $\mathbb{Q}_2^{(s)}(B_1) = \left[\dfrac{\sqrt{2}}{2}, \ -\dfrac{\sqrt{2}}{2} \right]$

$\boxed{\text{y6}}$ $\mathbb{T}_{1,1}^{(s)}(E) = [i, \, 0]$

$\boxed{\text{y7}}$ $\mathbb{T}_{1,2}^{(s)}(E) = [0, \, i]$

── **Site and Bond** ──────────────────────────

Table 5: Orbital of each site

#	site	orbital
1	A	$|s,\uparrow\rangle, |s,\downarrow\rangle$

Table 6: Neighbor and bra-ket of each bond

#	head	tail	neighbor	head (bra)	tail (ket)
1	A	A	[1]	[s]	[s]

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

Table 7: 'A' (#1) site cluster (1a), 4mm

SL	position (s)	mapping
1	[0.00000, 0.00000, 0.00000]	[1,2,3,4,5,6,7,8]

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 (2a@2c), ND, $|v|=$ 1.0 (cartesian)

SL	vector (v)	center (c)	mapping	head	tail	R (primitive)
1	[-1.00000, 0.00000, 0.00000]	[0.50000, 0.00000, 0.00000]	[1,-2,5,-6]	(1,1)	(1,1)	[1,0,0]
2	[0.00000,-1.00000, 0.00000]	[0.00000, 0.50000, 0.00000]	[3,-4,-7,8]	(1,1)	(1,1)	[0,1,0]

Table 9: 1-th 'A'-'A' [2] (#2) 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]`	`[1,2,3,4,5,6,7,8]`	`(1,1)`	`(1,1)`	`[0,0,1]`