Model for "C4v1"

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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, B_1, B_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, B_1, B_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, B_1, B_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, B_1, B_2, E]
- 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):
  $\boldsymbol{a}_1 =$ [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	#	SO
	1	$\{1\|0\}$	2	$\{2_{001}\|0\}$	3	$\{4^{+}_{001}\|0\}$	4	$\{4^{-}_{001}\|0\}$	5	$\{\mathrm{m}_{010}\|0\}$
	6	$\{\mathrm{m}_{100}\|0\}$	7	$\{\mathrm{m}_{110}\|0\}$	8	$\{\mathrm{m}_{1-10}\|0\}$				

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

continued ...

Table 2

#	symbol	irrep.	rank	X	multiplicity	component	symmetry
10	$\mathbb{Q}_{1,1}(E)$	E	1	Q, T	-	1	x
11	$\mathbb{Q}_{1,2}(E)$					2	y

Basis in full matrix

Table 3: dimension = 2

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

Table 4: Atomic basis (orbital part only)

orbital	definition
$\|s\rangle$	1

SAMB: 13 (all 13)

- `A` : '`A`' site-cluster
  * bra: $\langle s,\uparrow|$, $\langle s,\downarrow|$

* ket: $|s,\uparrow\rangle$, $|s,\downarrow\rangle$
* wyckoff: `1a`

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

- `A;A_001_1` : '`A`-'`A`' bond-cluster
  * bra: $\langle s,\uparrow|$, $\langle s,\downarrow|$
  * ket: $|s,\uparrow\rangle$, $|s,\downarrow\rangle$
  * wyckoff: `2a@2c`

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

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

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

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

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

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

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

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

- `A;A_001_2` : '`A`-'`A`' bond-cluster
  * bra: $\langle s,\uparrow|$, $\langle s,\downarrow|$
  * ket: $|s,\uparrow\rangle$, $|s,\downarrow\rangle$
  * wyckoff: `1a@1a`

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

z6 $\mathbb{G}_{1}^{(1,-1;c)}(A_2) = \mathbb{M}_{1}^{(1,-1;a)}(A_2)\mathbb{T}_{0}^{(b)}(A_1)$

z12 $\mathbb{G}_{1,1}^{(1,-1;c)}(E) = \dfrac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E)\mathbb{T}_{0}^{(b)}(A_1)}{2}$

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: $|s,\uparrow\rangle$, $|s,\downarrow\rangle$

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

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

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

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`

y1 $\mathbb{Q}_{0}^{(s)}(A_1) = [1]$

- Bond cluster

** Wyckoff: `1a@1a`

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

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

** Wyckoff: `2a@2c`

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

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

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

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]

Site in Unit Cell

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

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

SL	position ($\boldsymbol{s}$)	mapping
1	[0.00000, 0.00000, 0.00000]	[1,2,3,4,5,6,7,8]

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 (2a@2c), ND, $|\boldsymbol{v}|$= 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,-2,5,-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]