

# 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**

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## 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):
  - $\mathbf{a}_1 = [1.00000, 0.00000, 0.00000]$
  - $\mathbf{a}_2 = [0.00000, 1.00000, 0.00000]$
  - $\mathbf{a}_3 = [0.00000, 0.00000, 1.00000]$

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## Symmetry Operation

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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	$\{m_{010} 0\}$
6	$\{m_{100} 0\}$	7	$\{m_{110} 0\}$	8	$\{m_{1-10} 0\}$				

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## Harmonics

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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	$-y$

*continued ...*

Table 2

#	symbol	irrep.	rank	X	multiplicity	component	symmetry
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	$y$

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**Basis in full matrix**


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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

11 (all 13) SAMBs

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

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

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

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

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

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

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

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

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

- 'A'-'A' bond-cluster

\* bra:  $\langle s, \uparrow |, \langle s, \downarrow |$   
 \* ket:  $|s, \uparrow\rangle, |s, \downarrow\rangle$   
 \* wyckoff: **1a@1a**

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

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

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

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

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#### Atomic SAMB

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

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

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

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

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

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#### Cluster SAMB

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• Site cluster

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

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

- Bond cluster

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

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

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

\*\* Wyckoff: **2a@2c**

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

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

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

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

— Site and Bond —

Table 5: Orbital of each site

#	site	orbital
1	<b>A</b>	$ 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 ( $\mathbf{s}$ )	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,  $|\mathbf{v}|=1.0$  (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,-2,5,-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,  $|\mathbf{v}|=1.0$  (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]	[1,2,3,4,5,6,7,8]	(1,1)	(1,1)	[0,0,1]