

# Model for “C2h1”

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## General Condition

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- Basis type: 1gs
- SAMB selection:
  - Type: [Q, G]
  - Rank: [0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11]
  - Irrep.: [ $A_g$ ,  $B_g$ ,  $A_u$ ,  $B_u$ ]
  - 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.: [ $A_g$ ,  $B_g$ ,  $A_u$ ,  $B_u$ ]
  - Spin (s): [0, 1]
- Site-cluster selection:
  - Rank: [0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11]
  - Irrep.: [ $A_g$ ,  $B_g$ ,  $A_u$ ,  $B_u$ ]
- Bond-cluster selection:
  - Type: [Q, G, M, T]
  - Rank: [0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11]
  - Irrep.: [ $A_g$ ,  $B_g$ ,  $A_u$ ,  $B_u$ ]
- Max. neighbor: 10
- Search cell range: (-2, 3), (-2, 3), (-2, 3)
- Toroidal priority: false

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## Group and Unit Cell

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- Group: SG No. 10  $C_{2h}^1$   $P2/m$  (b-axis setting) [ monoclinic ]
- Associated point group: PG No. 10  $C_{2h}$   $2/m$  (b-axis setting) [ monoclinic ]
- Unit cell:  
 $a = 1.00000, b = 1.20000, c = 1.00000, \alpha = 90.0, \beta = 90.0, \gamma = 90.0$
- Lattice vectors (conventional cell):  
 $\mathbf{a}_1 = [1.00000, 0.00000, 0.00000]$   
 $\mathbf{a}_2 = [0.00000, 1.20000, 0.00000]$   
 $\mathbf{a}_3 = [0.00000, 0.00000, 1.00000]$

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**Symmetry Operation**

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Table 1: Symmetry operation

#	SO	#	SO	#	SO	#	SO	#	SO
1	{1 0}	2	{2 <sub>010</sub>  0}	3	{-1 0}	4	{m <sub>010</sub>  0}		

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**Harmonics**

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Table 2: Harmonics

#	symbol	irrep.	rank	X	multiplicity	component	symmetry
1	$\mathbb{Q}_0(A_g)$	$A_g$	0	$Q, T$	-	-	1
2	$\mathbb{G}_1(A_g)$	$A_g$	1	$G, M$	-	-	$y$
3	$\mathbb{Q}_2(A_g, 3)$	$A_g$	2	$Q, T$	3	-	$\sqrt{3}xz$
4	$\mathbb{G}_0(A_u)$	$A_u$	0	$G, M$	-	-	1
5	$\mathbb{Q}_1(A_u)$	$A_u$	1	$Q, T$	-	-	$y$
6	$\mathbb{G}_2(A_u, 2)$	$A_u$	2	$G, M$	2	-	$\frac{\sqrt{3}(x-y)(x+y)}{2}$
7	$\mathbb{G}_1(B_g, 1)$	$B_g$	1	$G, M$	1	-	$x$
8	$\mathbb{G}_1(B_g, 2)$	$B_g$	1	$G, M$	2	-	$z$
9	$\mathbb{Q}_2(B_g, 1)$	$B_g$	2	$Q, T$	1	-	$\sqrt{3}yz$
10	$\mathbb{Q}_2(B_g, 2)$	$B_g$	2	$Q, T$	2	-	$\sqrt{3}xy$

*continued ...*

Table 2

#	symbol	irrep.	rank	X	multiplicity	component	symmetry
11	$\mathbb{Q}_1(B_u, 1)$	$B_u$	1	$Q, T$	1	-	$x$
12	$\mathbb{Q}_1(B_u, 2)$	$B_u$	1	$Q, T$	2	-	$z$
13	$\mathbb{G}_2(B_u, 2)$	$B_u$	2	$G, M$	2	-	$\sqrt{3}xy$

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— Basis in full matrix —

Table 3: dimension = 4

#	orbital@atom(SL)	#	orbital@atom(SL)	#	orbital@atom(SL)	#	orbital@atom(SL)
0	$ s, \uparrow\rangle @A(1)$	1	$ s, \downarrow\rangle @A(1)$	2	$ s, \uparrow\rangle @B(1)$	3	$ s, \downarrow\rangle @B(1)$

Table 4: Atomic basis (orbital part only)

orbital	definition
$ s\rangle$	1

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— SAMB: 34 (all 34) —

- A : 'A' site-cluster

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

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

- B : 'B' site-cluster
  - \* bra:  $\langle s, \uparrow |$ ,  $\langle s, \downarrow |$
  - \* ket:  $|s, \uparrow \rangle$ ,  $|s, \downarrow \rangle$
  - \* wyckoff: **1e**

$$\boxed{z2} \quad \mathbb{Q}_0^{(c)}(A_g) = \mathbb{Q}_0^{(a)}(A_g)\mathbb{Q}_0^{(s)}(A_g)$$

- A;A\_001\_1 : 'A'-A' bond-cluster
  - \* bra:  $\langle s, \uparrow |$ ,  $\langle s, \downarrow |$
  - \* ket:  $|s, \uparrow \rangle$ ,  $|s, \downarrow \rangle$
  - \* wyckoff: **1a@1d**

$$\boxed{z3} \quad \mathbb{Q}_0^{(c)}(A_g) = \mathbb{Q}_0^{(a)}(A_g)\mathbb{Q}_0^{(b)}(A_g)$$

$$\boxed{z15} \quad \mathbb{Q}_1^{(1,-1;c)}(A_u) = \mathbb{M}_1^{(1,-1;a)}(B_g, 2)\mathbb{T}_1^{(b)}(B_u, 1)$$

$$\boxed{z16} \quad \mathbb{G}_0^{(1,-1;c)}(A_u) = \mathbb{M}_1^{(1,-1;a)}(B_g, 1)\mathbb{T}_1^{(b)}(B_u, 1)$$

$$\boxed{z27} \quad \mathbb{Q}_1^{(1,-1;c)}(B_u, 2) = -\mathbb{M}_1^{(1,-1;a)}(A_g)\mathbb{T}_1^{(b)}(B_u, 1)$$

- A;A\_001\_2 : 'A'-A' bond-cluster
  - \* bra:  $\langle s, \uparrow |$ ,  $\langle s, \downarrow |$
  - \* ket:  $|s, \uparrow \rangle$ ,  $|s, \downarrow \rangle$
  - \* wyckoff: **1a@1c**

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

$$\boxed{z17} \quad \mathbb{Q}_1^{(1,-1;c)}(A_u) = \mathbb{M}_1^{(1,-1;a)}(B_g, 2)\mathbb{T}_1^{(b)}(B_u, 1)$$

$$\boxed{z18} \quad \mathbb{G}_0^{(1,-1;c)}(A_u) = \mathbb{M}_1^{(1,-1;a)}(B_g, 1)\mathbb{T}_1^{(b)}(B_u, 1)$$

$$\boxed{z28} \quad \mathbb{Q}_1^{(1,-1;c)}(B_u, 2) = -\mathbb{M}_1^{(1,-1;a)}(A_g)\mathbb{T}_1^{(b)}(B_u, 1)$$

• B;A\_001\_1 : 'A'-'B' bond-cluster

- \* bra:  $\langle s, \uparrow |$ ,  $\langle s, \downarrow |$
- \* ket:  $|s, \uparrow \rangle$ ,  $|s, \downarrow \rangle$
- \* wyckoff: 4a@4o

**z5**  $\mathbb{Q}_0^{(c)}(A_g) = \mathbb{Q}_0^{(a)}(A_g)\mathbb{Q}_0^{(b)}(A_g)$

**z6**  $\mathbb{Q}_0^{(1,-1;c)}(A_g) = \mathbb{M}_1^{(1,-1;a)}(B_g, 1)\mathbb{M}_1^{(b)}(B_g, 1)$

**z7**  $\mathbb{Q}_2^{(1,-1;c)}(A_g, 3) = \mathbb{M}_1^{(1,-1;a)}(B_g, 2)\mathbb{M}_1^{(b)}(B_g, 1)$

**z8**  $\mathbb{G}_1^{(1,-1;c)}(A_g) = \mathbb{M}_1^{(1,-1;a)}(A_g)\mathbb{T}_0^{(b)}(A_g)$

**z11**  $\mathbb{Q}_1^{(c)}(A_u) = \mathbb{Q}_0^{(a)}(A_g)\mathbb{Q}_1^{(b)}(A_u)$

**z12**  $\mathbb{Q}_1^{(1,-1;c)}(A_u) = \mathbb{M}_1^{(1,-1;a)}(B_g, 2)\mathbb{T}_1^{(b)}(B_u, 1)$

**z13**  $\mathbb{G}_0^{(1,-1;c)}(A_u) = \frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(A_g)\mathbb{T}_1^{(b)}(A_u)}{2} + \frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(B_g, 1)\mathbb{T}_1^{(b)}(B_u, 1)}{2}$

**z14**  $\mathbb{G}_2^{(1,-1;c)}(A_u, 2) = -\frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(A_g)\mathbb{T}_1^{(b)}(A_u)}{2} + \frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(B_g, 1)\mathbb{T}_1^{(b)}(B_u, 1)}{2}$

**z19**  $\mathbb{Q}_2^{(c)}(B_g, 1) = \mathbb{Q}_0^{(a)}(A_g)\mathbb{Q}_2^{(b)}(B_g, 1)$

**z20**  $\mathbb{Q}_2^{(1,-1;c)}(B_g, 2) = \mathbb{M}_1^{(1,-1;a)}(A_g)\mathbb{M}_1^{(b)}(B_g, 1)$

**z21**  $\mathbb{G}_1^{(1,-1;c)}(B_g, 1) = \mathbb{M}_1^{(1,-1;a)}(B_g, 1)\mathbb{T}_0^{(b)}(A_g)$

**z22**  $\mathbb{G}_1^{(1,-1;c)}(B_g, 2) = \mathbb{M}_1^{(1,-1;a)}(B_g, 2)\mathbb{T}_0^{(b)}(A_g)$

**z29**  $\mathbb{Q}_1^{(c)}(B_u, 1) = \mathbb{Q}_0^{(a)}(A_g)\mathbb{Q}_1^{(b)}(B_u, 1)$

**z30**  $\mathbb{Q}_1^{(1,-1;c)}(B_u, 1) = -\mathbb{M}_1^{(1,-1;a)}(B_g, 2)\mathbb{T}_1^{(b)}(A_u)$

**z31**  $\mathbb{Q}_1^{(1,-1;c)}(B_u, 2) = -\frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(A_g)\mathbb{T}_1^{(b)}(B_u, 1)}{2} + \frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(B_g, 1)\mathbb{T}_1^{(b)}(A_u)}{2}$

**z32**  $\mathbb{G}_2^{(1,-1;c)}(B_u, 2) = \frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(A_g)\mathbb{T}_1^{(b)}(B_u, 1)}{2} + \frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(B_g, 1)\mathbb{T}_1^{(b)}(A_u)}{2}$

- B;B\_001\_1 : 'B-'B' bond-cluster

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

**[z9]**  $\mathbb{Q}_0^{(c)}(A_g) = \mathbb{Q}_0^{(a)}(A_g)\mathbb{Q}_0^{(b)}(A_g)$

**[z23]**  $\mathbb{Q}_1^{(1,-1;c)}(A_u) = \mathbb{M}_1^{(1,-1;a)}(B_g, 2)\mathbb{T}_1^{(b)}(B_u, 1)$

**[z24]**  $\mathbb{G}_0^{(1,-1;c)}(A_u) = \mathbb{M}_1^{(1,-1;a)}(B_g, 1)\mathbb{T}_1^{(b)}(B_u, 1)$

**[z33]**  $\mathbb{Q}_1^{(1,-1;c)}(B_u, 2) = -\mathbb{M}_1^{(1,-1;a)}(A_g)\mathbb{T}_1^{(b)}(B_u, 1)$

- B;B\_001\_2 : 'B-'B' bond-cluster

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

**[z10]**  $\mathbb{Q}_0^{(c)}(A_g) = \mathbb{Q}_0^{(a)}(A_g)\mathbb{Q}_0^{(b)}(A_g)$

**[z25]**  $\mathbb{Q}_1^{(1,-1;c)}(A_u) = \mathbb{M}_1^{(1,-1;a)}(B_g, 2)\mathbb{T}_1^{(b)}(B_u, 1)$

**[z26]**  $\mathbb{G}_0^{(1,-1;c)}(A_u) = \mathbb{M}_1^{(1,-1;a)}(B_g, 1)\mathbb{T}_1^{(b)}(B_u, 1)$

**[z34]**  $\mathbb{Q}_1^{(1,-1;c)}(B_u, 2) = -\mathbb{M}_1^{(1,-1;a)}(A_g)\mathbb{T}_1^{(b)}(B_u, 1)$

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## Atomic SAMB

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

**[x1]**  $\mathbb{Q}_0^{(a)}(A_g) = \begin{bmatrix} \frac{\sqrt{2}}{2} & 0 \\ 0 & \frac{\sqrt{2}}{2} \end{bmatrix}$

**[x2]**  $\mathbb{M}_1^{(1,-1;a)}(A_g) = \begin{bmatrix} 0 & -\frac{\sqrt{2}i}{2} \\ \frac{\sqrt{2}i}{2} & 0 \end{bmatrix}$

$$\boxed{x3} \quad \mathbb{M}_1^{(1, -1; a)}(B_g, 1) = \begin{bmatrix} 0 & \frac{\sqrt{2}}{2} \\ \frac{\sqrt{2}}{2} & 0 \end{bmatrix}$$

$$\boxed{x4} \quad \mathbb{M}_1^{(1, -1; a)}(B_g, 2) = \begin{bmatrix} \frac{\sqrt{2}}{2} & 0 \\ 0 & -\frac{\sqrt{2}}{2} \end{bmatrix}$$

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### — Cluster SAMB —

- Site cluster

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

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

\*\* Wyckoff: **1e**

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

- Bond cluster

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

$$\boxed{y3} \quad \mathbb{Q}_0^{(s)}(A_g) = [1]$$

$$\boxed{y4} \quad \mathbb{T}_1^{(s)}(B_u, 1) = [i]$$

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

$$\boxed{y5} \quad \mathbb{Q}_0^{(s)}(A_g) = [1]$$

$$\boxed{y6} \quad \mathbb{T}_1^{(s)}(B_u, 1) = [i]$$

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

$$\boxed{y7} \quad \mathbb{Q}_0^{(s)}(A_g) = [1]$$

$$\boxed{y8} \quad \mathbb{T}_1^{(s)}(B_u, 1) = [i]$$

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

$$\boxed{y9} \quad \mathbb{Q}_0^{(s)}(A_g) = [1]$$

$$\boxed{y10} \quad \mathbb{T}_1^{(s)}(B_u, 1) = [i]$$

\*\* Wyckoff: **4a@4o**

$$\boxed{y11} \quad \mathbb{Q}_0^{(s)}(A_g) = \left[ \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \right]$$

$$\boxed{y12} \quad \mathbb{T}_0^{(s)}(A_g) = \left[ \frac{i}{2}, \frac{i}{2}, \frac{i}{2}, \frac{i}{2} \right]$$

$$\boxed{y13} \quad \mathbb{Q}_1^{(s)}(A_u) = \left[ \frac{1}{2}, \frac{1}{2}, -\frac{1}{2}, -\frac{1}{2} \right]$$

$$\boxed{y14} \quad \mathbb{T}_1^{(s)}(A_u) = \left[ \frac{i}{2}, \frac{i}{2}, -\frac{i}{2}, -\frac{i}{2} \right]$$

$$\boxed{y15} \quad \mathbb{M}_1^{(s)}(B_g, 1) = \left[ \frac{i}{2}, -\frac{i}{2}, \frac{i}{2}, -\frac{i}{2} \right]$$

$$\boxed{y16} \quad \mathbb{Q}_2^{(s)}(B_g, 1) = \left[ \frac{1}{2}, -\frac{1}{2}, \frac{1}{2}, -\frac{1}{2} \right]$$

$$\boxed{y17} \quad \mathbb{Q}_1^{(s)}(B_u, 1) = \left[ \frac{1}{2}, -\frac{1}{2}, -\frac{1}{2}, \frac{1}{2} \right]$$

$$\boxed{y18} \quad \mathbb{T}_1^{(s)}(B_u, 1) = \left[ \frac{i}{2}, -\frac{i}{2}, -\frac{i}{2}, \frac{i}{2} \right]$$

Table 5: Orbital of each site

#	site	orbital
1	A	$ s, \uparrow\rangle,  s, \downarrow\rangle$
2	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]
2	A	B	[1]	[s]	[s]
3	B	B	[1]	[s]	[s]

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— Site in Unit Cell —————

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

Table 7: 'A' (#1) site cluster (1a), 2/m

SL	position ( $s$ )	mapping
1	[ 0.00000, 0.00000, 0.00000 ]	[1,2,3,4]

Table 8: 'B' (#2) site cluster (1e), 2/m

SL	position ( $s$ )	mapping
1	[ 0.50000, 0.50000, 0.00000]	[1,2,3,4]

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— Bond in Unit Cell —

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Bonds in (conventional) cell (no plus set): tail, head = (SL, plus set), (N)D = (non)directional (listed up to 5th neighbor at most)

Table 9: 1-th 'A'-'A' [1] (#1) bond cluster (1a@1d), 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,-3,4]	(1,1)	(1,1)	[1,0,0]

Table 10: 1-th 'A'-'A' [2] (#2) bond cluster (1a@1c), ND,  $|v|=1.0$  (cartesian)

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

Table 11: 1-th 'A'-'B' [1] (#3) bond cluster (4a@4o), D,  $|\mathbf{v}|=0.78102$  (cartesian)

SL	vector ( $\mathbf{v}$ )	center ( $\mathbf{c}$ )	mapping	head	tail	$\mathbf{R}$ (primitive)
1	[-0.50000, -0.50000, 0.00000]	[ 0.25000, 0.25000, 0.00000]	[1]	(1,1)	(1,1)	[0,0,0]
2	[ 0.50000, -0.50000, 0.00000]	[ 0.75000, 0.25000, 0.00000]	[2]	(1,1)	(1,1)	[-1,0,0]
3	[ 0.50000, 0.50000, 0.00000]	[ 0.75000, 0.75000, 0.00000]	[3]	(1,1)	(1,1)	[-1,-1,0]
4	[-0.50000, 0.50000, 0.00000]	[ 0.25000, 0.75000, 0.00000]	[4]	(1,1)	(1,1)	[0,-1,0]

Table 12: 1-th 'B'-'B' [1] (#4) bond cluster (1a@1b), 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]	[ 0.00000, 0.50000, 0.00000]	[1,-2,-3,4]	(1,1)	(1,1)	[1,0,0]

Table 13: 1-th 'B'-'B' [2] (#5) bond cluster (1a@1h), ND,  $|\mathbf{v}|=1.0$  (cartesian)

SL	vector ( $\mathbf{v}$ )	center ( $\mathbf{c}$ )	mapping	head	tail	$\mathbf{R}$ (primitive)
1	[ 0.00000, 0.00000, -1.00000]	[ 0.50000, 0.50000, 0.50000]	[1,-2,-3,4]	(1,1)	(1,1)	[0,0,1]