Model for "C2h1"

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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_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

Group and Unit Cell

- 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):
  $\boldsymbol{a}_1 =$ [1.00000, 0.00000, 0.00000]
  $\boldsymbol{a}_2 =$ [0.00000, 1.20000, 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	$\{2_{010}\|0\}$	3	$\{-1\|0\}$	4	$\{\mathrm{m}_{010}\|0\}$		

Harmonics

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	-	$\sqrt{3}yz$

continued ...

Table 2

#	symbol	irrep.	rank	X	multiplicity	component	symmetry
10	$\mathbb{Q}_2(B_g, 2)$	B_g	2	Q, T	2	-	$\sqrt{3}xy$
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	-	$\sqrt{3}xy$

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

SAMB

34 (all 34) SAMBs

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

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

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

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

- 'A'-'A' bond-cluster : A;A_001_1
  * bra: $\langle s,\uparrow|$, $\langle s,\downarrow|$
  * ket: $|s,\uparrow\rangle$, $|s,\downarrow\rangle$
  * wyckoff: 1a@1d

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

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

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

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

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

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

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

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

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

- 'A'-'B' bond-cluster : `B;A_001_1`
  * 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 $\mathbb{G}_0^{(1,-1;c)}(A_u) = \dfrac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(A_g)\mathbb{T}_1^{(b)}(A_u)}{2} + \dfrac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(B_g,1)\mathbb{T}_1^{(b)}(B_u,1)}{2}$

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

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' bond-cluster : `B;B_001_1`
  * 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' bond-cluster : `B;B_001_2`
  * 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 $\mathbb{Q}_1^{(1,-1;c)}(B_u,2) = -\mathbb{M}_1^{(1,-1;a)}(A_g)\mathbb{T}_1^{(b)}(B_u,1)$

Atomic SAMB

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

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

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

Cluster SAMB

- Site cluster

** Wyckoff: `1a`

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

** Wyckoff: `1e`

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

- Bond cluster

** Wyckoff: `1a@1d`

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

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

** Wyckoff: `1a@1h`

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

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

** Wyckoff: `1a@1c`

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

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

** Wyckoff: `1a@1b`

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

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

** Wyckoff: `4a@4o`

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

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

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

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

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

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

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

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

Site and Bond

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]

Site in Unit Cell

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

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

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

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

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

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

Table 10: 1-th 'A'-'A' [2] (#2) bond cluster (1a@1c), ND, $|\boldsymbol{v}|$= 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]	(1,1)	(1,1)	[0,0,1]

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

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

SL	vector ($\boldsymbol{v}$)	center ($\boldsymbol{c}$)	mapping	head	tail	$\boldsymbol{R}$ (primitive)
1	[-1.00000, 0.00000, 0.00000]	[0.00000, 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, $|\boldsymbol{v}|$= 1.0 (cartesian)

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