Model for “C2h1”

Generated on 2026-01-20 13:07:23 by MultiPie 2.0.1

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 $C_{2\mathrm{h}}^1$ $P2/m$ (b-axis setting) [monoclinic]
- Associated point group: PG No. 10 $C_{2\mathrm{h}}$ $2/m$ (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	$\{m_{010}\|0\}$		

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	$\lvert s,\uparrow\rangle$ @A(1)	1	$\lvert s,\downarrow\rangle$ @A(1)	2	$\lvert s,\uparrow\rangle$ @B(1)	3	$\lvert s,\downarrow\rangle$ @B(1)

Table 4: Atomic basis (orbital part only)

orbital	definition
$\lvert s\rangle$	1

SAMB

34 (all 34) SAMBs

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- 'A'-'B' bond-cluster
  * bra: $\langle s,\uparrow|$, $\langle s,\downarrow|$
  * ket: $|s,\uparrow\rangle$, $|s,\downarrow\rangle$
  * wyckoff: `4a@4o`

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

$\boxed{\text{z9}}$ $\mathbb{Q}_0^{(c)}(A_g) = \mathbb{Q}_0^{(a)}(A_g)\mathbb{Q}_0^{(b)}(A_g)$

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

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

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

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

$\boxed{\text{z10}}$ $\mathbb{Q}_0^{(c)}(A_g) = \mathbb{Q}_0^{(a)}(A_g)\mathbb{Q}_0^{(b)}(A_g)$

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

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

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

Atomic SAMB

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

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

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

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

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

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

Cluster SAMB

- Site cluster

** Wyckoff: `1e`

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

** Wyckoff: `1a`

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

- Bond cluster

** Wyckoff: `1a@1c`

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

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

** Wyckoff: `1a@1d`

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

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

** Wyckoff: `1a@1h`

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

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

** Wyckoff: `1a@1b`

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

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

** Wyckoff: `4a@4o`

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

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

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

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

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

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

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

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

— Site and Bond

Table 5: Orbital of each site

#	site	orbital
1	`A`	$\lvert s,\uparrow\rangle$, $\lvert s,\downarrow\rangle$
2	`B`	$\lvert s,\uparrow\rangle$, $\lvert s,\downarrow\rangle$

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]