

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):
 - $\mathbf{a}_1 = [1.00000, 0.00000, 0.00000]$
 - $\mathbf{a}_2 = [0.00000, 1.20000, 0.00000]$
 - $\mathbf{a}_3 = [0.00000, 0.00000, 1.00000]$

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 | - | $\sqrt{3}yz$ |
| 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 | - | $\sqrt{3}xy$ |

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)

- A : 'A' site-cluster

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

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

• **B : 'B' site-cluster**

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

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

• **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**

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

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

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

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

• **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**

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

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

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

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

• **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**

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- **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**

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

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

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

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

- **B;B_001_2** : 'B'-'B' bond-cluster

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

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

* wyckoff: **1a@1h**

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

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

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

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

Atomic SAMB

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

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

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

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

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

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

Cluster SAMB

- Site cluster

** Wyckoff: **1a**

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

** Wyckoff: **1e**

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

- Bond cluster

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

— 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 (<i>s</i>) | 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] |

— 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, $|\mathbf{v}|=1.0$ (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, $|\mathbf{v}|=1.0$ (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] |