

# SAMB for “C2h1”

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- Group: No. 10  $C_{2h}^1$   $P2/m$  (b-axis setting) [ monoclinic ]
  - Associated point group: No. 5  $C_{2h}$   $2/m$  (b-axis setting) [ monoclinic ]
  - Generation condition
    - model type: **tight\_binding**
    - time-reversal type: **electric**
    - irrep: [Ag]
    - **spinful**
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- Unit cell:
  - $a = 1.0$ ,  $b = 1.2$ ,  $c = 1.0$ ,  $\alpha = 90.0$ ,  $\beta = 90.0$ ,  $\gamma = 90.0$
- Lattice vectors:
  - $\mathbf{a}_1 = (1.0 \ 0 \ 0)$
  - $\mathbf{a}_2 = (0 \ 1.2 \ 0)$
  - $\mathbf{a}_3 = (0 \ 0 \ 1.0)$

Table 1: High-symmetry line:  $\Gamma$ -X.

	symbol	position		symbol	position
	$\Gamma$	$\begin{pmatrix} 0 & 0 & 0 \end{pmatrix}$		X	$\begin{pmatrix} \frac{1}{2} & 0 & 0 \end{pmatrix}$

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- Kets: dimension = 4

Table 2: Hilbert space for full matrix.

	No.	ket	No.	ket	No.	ket	No.	ket
	1	$(s, \uparrow)@A_1$	2	$(s, \downarrow)@A_1$	3	$(s, \uparrow)@B_1$	4	$(s, \downarrow)@B_1$

- Sites in (primitive) unit cell:

Table 3: Site-clusters.

	site	position	mapping
S <sub>1</sub>	A <sub>1</sub>	$\begin{pmatrix} 0 & 0 & 0 \end{pmatrix}$	[1,2,3,4]
S <sub>2</sub>	B <sub>1</sub>	$\begin{pmatrix} \frac{1}{2} & \frac{1}{2} & 0 \end{pmatrix}$	[1,2,3,4]

- Bonds in (primitive) unit cell:

Table 4: Bond-clusters.

	bond	tail	head	$n$	#	$\mathbf{b@c}$	mapping
B <sub>1</sub>	b <sub>1</sub>	A <sub>1</sub>	A <sub>1</sub>	1	1	$\begin{pmatrix} 1 & 0 & 0 \end{pmatrix} @ \begin{pmatrix} \frac{1}{2} & 0 & 0 \end{pmatrix}$	[1,-2,-3,4]
B <sub>2</sub>	b <sub>2</sub>	A <sub>1</sub>	A <sub>1</sub>	1	2	$\begin{pmatrix} 0 & 0 & 1 \end{pmatrix} @ \begin{pmatrix} 0 & 0 & \frac{1}{2} \end{pmatrix}$	[1,-2,-3,4]
B <sub>3</sub>	b <sub>3</sub>	B <sub>1</sub>	B <sub>1</sub>	1	1	$\begin{pmatrix} 1 & 0 & 0 \end{pmatrix} @ \begin{pmatrix} 0 & \frac{1}{2} & 0 \end{pmatrix}$	[1,-2,-3,4]
B <sub>4</sub>	b <sub>4</sub>	B <sub>1</sub>	B <sub>1</sub>	1	2	$\begin{pmatrix} 0 & 0 & 1 \end{pmatrix} @ \begin{pmatrix} \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \end{pmatrix}$	[1,-2,-3,4]
B <sub>5</sub>	b <sub>5</sub>	B <sub>1</sub>	A <sub>1</sub>	1	1	$\begin{pmatrix} \frac{1}{2} & \frac{1}{2} & 0 \end{pmatrix} @ \begin{pmatrix} \frac{1}{4} & \frac{1}{4} & 0 \end{pmatrix}$	[1]
	b <sub>6</sub>	B <sub>1</sub>	A <sub>1</sub>	1	1	$\begin{pmatrix} -\frac{1}{2} & \frac{1}{2} & 0 \end{pmatrix} @ \begin{pmatrix} \frac{3}{4} & \frac{1}{4} & 0 \end{pmatrix}$	[2]
	b <sub>7</sub>	B <sub>1</sub>	A <sub>1</sub>	1	1	$\begin{pmatrix} -\frac{1}{2} & -\frac{1}{2} & 0 \end{pmatrix} @ \begin{pmatrix} \frac{3}{4} & \frac{3}{4} & 0 \end{pmatrix}$	[3]
	b <sub>8</sub>	B <sub>1</sub>	A <sub>1</sub>	1	1	$\begin{pmatrix} \frac{1}{2} & -\frac{1}{2} & 0 \end{pmatrix} @ \begin{pmatrix} \frac{1}{4} & \frac{3}{4} & 0 \end{pmatrix}$	[4]

- SAMB:

$$\boxed{\text{No. 1}} \quad \hat{\mathbb{Q}}_0^{(A_g)} [\mathbf{M}_1, \mathbf{S}_1]$$

$$\hat{\mathbb{Z}}_1 = \mathbb{X}_1[\mathbb{Q}_0^{(a, A_g)}] \otimes \mathbb{Y}_1[\mathbb{Q}_0^{(s, A_g)}]$$

$$\hat{\mathbb{Z}}_1(\mathbf{k}) = \mathbb{X}_1[\mathbb{Q}_0^{(a, A_g)}] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s, A_g)}]$$

$$\boxed{\text{No. 2}} \quad \hat{\mathbb{Q}}_0^{(A_g)} [\mathbf{M}_1, \mathbf{S}_2]$$

$$\hat{\mathbb{Z}}_2 = \mathbb{X}_1[\mathbb{Q}_0^{(a, A_g)}] \otimes \mathbb{Y}_2[\mathbb{Q}_0^{(s, A_g)}]$$

$$\hat{\mathbb{Z}}_2(\mathbf{k}) = \mathbb{X}_1[\mathbb{Q}_0^{(a, A_g)}] \otimes \mathbb{U}_2[\mathbb{Q}_0^{(s, A_g)}]$$

$$\boxed{\text{No. 3}} \quad \hat{\mathbb{Q}}_0^{(A_g)} [\mathbf{M}_1, \mathbf{B}_1]$$

$$\hat{\mathbb{Z}}_3 = \mathbb{X}_1[\mathbb{Q}_0^{(a, A_g)}] \otimes \mathbb{Y}_3[\mathbb{Q}_0^{(b, A_g)}]$$

$$\hat{\mathbb{Z}}_3(\mathbf{k}) = \mathbb{X}_1[\mathbb{Q}_0^{(a, A_g)}] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s, A_g)}] \otimes \mathbb{F}_1[\mathbb{Q}_0^{(k, A_g)}]$$

$$\boxed{\text{No. 4}} \quad \hat{\mathbb{Q}}_0^{(A_g)} [\mathbf{M}_1, \mathbf{B}_2]$$

$$\hat{\mathbb{Z}}_4 = \mathbb{X}_1[\mathbb{Q}_0^{(a, A_g)}] \otimes \mathbb{Y}_4[\mathbb{Q}_0^{(b, A_g)}]$$

$$\hat{\mathbb{Z}}_4(\mathbf{k}) = \mathbb{X}_1[\mathbb{Q}_0^{(a, A_g)}] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s, A_g)}] \otimes \mathbb{F}_2[\mathbb{Q}_0^{(k, A_g)}]$$

$$\boxed{\text{No. 5}} \quad \hat{\mathbb{Q}}_0^{(A_g)} [\mathbf{M}_1, \mathbf{B}_3]$$

$$\hat{\mathbb{Z}}_5 = \mathbb{X}_1[\mathbb{Q}_0^{(a, A_g)}] \otimes \mathbb{Y}_5[\mathbb{Q}_0^{(b, A_g)}]$$

$$\hat{\mathbb{Z}}_5(\mathbf{k}) = \mathbb{X}_1[\mathbb{Q}_0^{(a, A_g)}] \otimes \mathbb{U}_2[\mathbb{Q}_0^{(s, A_g)}] \otimes \mathbb{F}_3[\mathbb{Q}_0^{(k, A_g)}]$$

$$\boxed{\text{No. 6}} \quad \hat{\mathbb{Q}}_0^{(A_g)} [\mathbf{M}_1, \mathbf{B}_4]$$

$$\hat{\mathbb{Z}}_6 = \mathbb{X}_1[\mathbb{Q}_0^{(a, A_g)}] \otimes \mathbb{Y}_6[\mathbb{Q}_0^{(b, A_g)}]$$

$$\hat{\mathbb{Z}}_6(\mathbf{k}) = \mathbb{X}_1[\mathbb{Q}_0^{(a,A_g)}] \otimes \mathbb{U}_2[\mathbb{Q}_0^{(s,A_g)}] \otimes \mathbb{F}_4[\mathbb{Q}_0^{(k,A_g)}]$$

$$\boxed{\text{No. 7}} \quad \hat{\mathbb{Q}}_0^{(A_g)} [\text{M}_1, \text{B}_5]$$

$$\hat{\mathbb{Z}}_7 = \mathbb{X}_1[\mathbb{Q}_0^{(a,A_g)}] \otimes \mathbb{Y}_7[\mathbb{Q}_0^{(b,A_g)}]$$

$$\hat{\mathbb{Z}}_7(\mathbf{k}) = \mathbb{X}_1[\mathbb{Q}_0^{(a,A_g)}] \otimes \mathbb{U}_3[\mathbb{Q}_0^{(u,A_g)}] \otimes \mathbb{F}_5[\mathbb{Q}_0^{(k,A_g)}]$$

$$\boxed{\text{No. 8}} \quad \hat{\mathbb{G}}_1^{(A_g)}(1, -1) [\text{M}_1, \text{B}_5]$$

$$\hat{\mathbb{Z}}_8 = \mathbb{X}_2[\mathbb{M}_1^{(a,A_g)}(1, -1)] \otimes \mathbb{Y}_8[\mathbb{T}_0^{(b,A_g)}]$$

$$\hat{\mathbb{Z}}_8(\mathbf{k}) = \mathbb{X}_2[\mathbb{M}_1^{(a,A_g)}(1, -1)] \otimes \mathbb{U}_4[\mathbb{T}_0^{(u,A_g)}] \otimes \mathbb{F}_5[\mathbb{Q}_0^{(k,A_g)}]$$

$$\boxed{\text{No. 9}} \quad \hat{\mathbb{G}}_1^{(A_g)}(1, -1) [\text{M}_1, \text{B}_5]$$

$$\hat{\mathbb{Z}}_9 = \mathbb{X}_3[\mathbb{M}_1^{(a,B_g,1)}(1, -1)] \otimes \mathbb{Y}_9[\mathbb{T}_2^{(b,B_g,2)}]$$

$$\hat{\mathbb{Z}}_9(\mathbf{k}) = \mathbb{X}_3[\mathbb{M}_1^{(a,B_g,1)}(1, -1)] \otimes \mathbb{U}_4[\mathbb{T}_0^{(u,A_g)}] \otimes \mathbb{F}_6[\mathbb{Q}_2^{(k,B_g,2)}]$$

$$\boxed{\text{No. 10}} \quad \hat{\mathbb{Q}}_2^{(A_g,2)}(1, -1) [\text{M}_1, \text{B}_5]$$

$$\hat{\mathbb{Z}}_{10} = -\mathbb{X}_4[\mathbb{M}_1^{(a,B_g,2)}(1, -1)] \otimes \mathbb{Y}_9[\mathbb{T}_2^{(b,B_g,2)}]$$

$$\hat{\mathbb{Z}}_{10}(\mathbf{k}) = -\mathbb{X}_4[\mathbb{M}_1^{(a,B_g,2)}(1, -1)] \otimes \mathbb{U}_4[\mathbb{T}_0^{(u,A_g)}] \otimes \mathbb{F}_6[\mathbb{Q}_2^{(k,B_g,2)}]$$

Table 5: Atomic SAMB group.

group	bra	ket
M <sub>1</sub>	(s, ↑), (s, ↓)	(s, ↑), (s, ↓)

Table 6: Atomic SAMB.

symbol	type	group	form
$\mathbb{X}_1$	$\mathbb{Q}_0^{(a, A_g)}$	$M_1$	$\begin{pmatrix} \frac{\sqrt{2}}{2} & 0 \\ 0 & \frac{\sqrt{2}}{2} \end{pmatrix}$
$\mathbb{X}_2$	$\mathbb{M}_1^{(a, A_g)}(1, -1)$	$M_1$	$\begin{pmatrix} 0 & -\frac{\sqrt{2}i}{2} \\ \frac{\sqrt{2}i}{2} & 0 \end{pmatrix}$
$\mathbb{X}_3$	$\mathbb{M}_1^{(a, B_g, 1)}(1, -1)$	$M_1$	$\begin{pmatrix} 0 & \frac{\sqrt{2}}{2} \\ \frac{\sqrt{2}}{2} & 0 \end{pmatrix}$
$\mathbb{X}_4$	$\mathbb{M}_1^{(a, B_g, 2)}(1, -1)$	$M_1$	$\begin{pmatrix} \frac{\sqrt{2}}{2} & 0 \\ 0 & -\frac{\sqrt{2}}{2} \end{pmatrix}$

Table 7: Cluster SAMB.

symbol	type	cluster	form
$\mathbb{Y}_1$	$\mathbb{Q}_0^{(s, A_g)}$	$S_1$	$\begin{pmatrix} 1 \end{pmatrix}$
$\mathbb{Y}_2$	$\mathbb{Q}_0^{(s, A_g)}$	$S_2$	$\begin{pmatrix} 1 \end{pmatrix}$
$\mathbb{Y}_3$	$\mathbb{Q}_0^{(b, A_g)}$	$B_1$	$\begin{pmatrix} 1 \end{pmatrix}$
$\mathbb{Y}_4$	$\mathbb{Q}_0^{(b, A_g)}$	$B_2$	$\begin{pmatrix} 1 \end{pmatrix}$
$\mathbb{Y}_5$	$\mathbb{Q}_0^{(b, A_g)}$	$B_3$	$\begin{pmatrix} 1 \end{pmatrix}$
$\mathbb{Y}_6$	$\mathbb{Q}_0^{(b, A_g)}$	$B_4$	$\begin{pmatrix} 1 \end{pmatrix}$
$\mathbb{Y}_7$	$\mathbb{Q}_0^{(b, A_g)}$	$B_5$	$\begin{pmatrix} \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \end{pmatrix}$
$\mathbb{Y}_8$	$\mathbb{T}_0^{(b, A_g)}$	$B_5$	$\begin{pmatrix} \frac{i}{2} & \frac{i}{2} & \frac{i}{2} & \frac{i}{2} \end{pmatrix}$
$\mathbb{Y}_9$	$\mathbb{T}_2^{(b, B_g, 2)}$	$B_5$	$\begin{pmatrix} \frac{i}{2} & -\frac{i}{2} & \frac{i}{2} & -\frac{i}{2} \end{pmatrix}$

Table 8: Uniform SAMB.

symbol	type	cluster	form
$\mathbb{U}_1$	$\mathbb{Q}_0^{(s, A_g)}$	$S_1$	$\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$
$\mathbb{U}_2$	$\mathbb{Q}_0^{(s, A_g)}$	$S_2$	$\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$
$\mathbb{U}_3$	$\mathbb{Q}_0^{(u, A_g)}$	$B_5$	$\begin{pmatrix} 0 & \frac{\sqrt{2}}{2} \\ \frac{\sqrt{2}}{2} & 0 \end{pmatrix}$
$\mathbb{U}_4$	$\mathbb{T}_0^{(u, A_g)}$	$B_5$	$\begin{pmatrix} 0 & -\frac{\sqrt{2}i}{2} \\ \frac{\sqrt{2}i}{2} & 0 \end{pmatrix}$

Table 9: Structure SAMB.

symbol	type	cluster	form
$\mathbb{F}_1$	$\mathbb{Q}_0^{(k, A_g)}$	$B_1$	$\sqrt{2}c_{001}$
$\mathbb{F}_2$	$\mathbb{Q}_0^{(k, A_g)}$	$B_2$	$\sqrt{2}c_{002}$
$\mathbb{F}_3$	$\mathbb{Q}_0^{(k, A_g)}$	$B_3$	$\sqrt{2}c_{003}$
$\mathbb{F}_4$	$\mathbb{Q}_0^{(k, A_g)}$	$B_4$	$\sqrt{2}c_{004}$
$\mathbb{F}_5$	$\mathbb{Q}_0^{(k, A_g)}$	$B_5$	$c_{005} + c_{006}$
$\mathbb{F}_6$	$\mathbb{Q}_2^{(k, B_g, 2)}$	$B_5$	$c_{005} - c_{006}$

Table 10: Polar harmonics.

No.	symbol	rank	irrep.	mul.	comp.	form
1	$\mathbb{Q}_0^{(A_g)}$	0	$A_g$	—	—	1

*continued ...*

Table 10

No.	symbol	rank	irrep.	mul.	comp.	form
2	$\mathbb{Q}_2^{(B_g,2)}$	2	$B_g$	2	—	$\sqrt{3}xy$

Table 11: Axial harmonics.

No.	symbol	rank	irrep.	mul.	comp.	form
1	$\mathbb{G}_1^{(A_g)}$	1	$A_g$	—	—	$Y$
2	$\mathbb{G}_1^{(B_g,1)}$	1	$B_g$	1	—	$X$
3	$\mathbb{G}_1^{(B_g,2)}$	1	$B_g$	2	—	$Z$

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- Group info.: Generator =  $\{2_{010}|0\}$ ,  $\{-1|0\}$

Table 12: Conjugacy class (point-group part).

rep. SO	symmetry operations
$\{1 0\}$	$\{1 0\}$
$\{2_{010} 0\}$	$\{2_{010} 0\}$
$\{-1 0\}$	$\{-1 0\}$
$\{m_{010} 0\}$	$\{m_{010} 0\}$

Table 13: Symmetry operations.

	No.	SO	No.	SO	No.	SO	No.	SO	No.	SO
	1	$\{1 0\}$	2	$\{2_{010} 0\}$	3	$\{-1 0\}$	4	$\{m_{010} 0\}$		

Table 14: Character table (point-group part).

	1	$2_{010}$	$-1$	$m_{010}$
$A_g$	1	1	1	1
$B_g$	1	-1	1	-1
$A_u$	1	1	-1	-1
$B_u$	1	-1	-1	1

Table 15: Parity conversion.

$\leftrightarrow$	$\leftrightarrow$	$\leftrightarrow$	$\leftrightarrow$
$A_g (A_u)$	$B_g (B_u)$	$A_u (A_g)$	$B_u (B_g)$

Table 16: Symmetric product,  $[\Gamma \otimes \Gamma']_+$ .

	$A_g$	$B_g$	$A_u$	$B_u$
$A_g$	$A_g$	$B_g$	$A_u$	$B_u$
$B_g$		$A_g$	$B_u$	$A_u$
$A_u$			$A_g$	$B_g$
$B_u$				$A_g$



Table 17: Anti-symmetric product,  $[\Gamma \otimes \Gamma]_-$ .

$A_g$	$B_g$	$A_u$	$B_u$
—	—	—	—

Table 18: Virtual-cluster sites.

No.	position	No.	position	No.	position	No.	position
1	$\begin{pmatrix} 1 & 1 & 0 \end{pmatrix}$	2	$\begin{pmatrix} -1 & 1 & 0 \end{pmatrix}$	3	$\begin{pmatrix} -1 & -1 & 0 \end{pmatrix}$	4	$\begin{pmatrix} 1 & -1 & 0 \end{pmatrix}$

Table 19: Virtual-cluster basis.

symbol	1	2	3	4
$\mathbb{Q}_0^{(Ag)}$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$
$\mathbb{Q}_1^{(Au)}$	$\frac{1}{2}$	$\frac{1}{2}$	$-\frac{1}{2}$	$-\frac{1}{2}$
$\mathbb{Q}_1^{(Bu,1)}$	$\frac{1}{2}$	$-\frac{1}{2}$	$-\frac{1}{2}$	$\frac{1}{2}$
$\mathbb{Q}_2^{(Bg,2)}$	$\frac{1}{2}$	$-\frac{1}{2}$	$\frac{1}{2}$	$-\frac{1}{2}$