

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: Γ -X.

	symbol	position		symbol	position
	Γ	$\begin{pmatrix} 0 & 0 & 0 \end{pmatrix}$		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
	1	$(s, \uparrow)@A_1$	2	$(s, \downarrow)@A_1$

- Sites in (primitive) unit cell:

Table 3: Site-clusters.

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

- Bonds in (primitive) unit cell:

Table 4: Bond-clusters.

bond	tail	head	n	#	$\mathbf{b@c}$	mapping	
B ₁	b ₁	A ₁	A ₁	1	1	$\begin{pmatrix} 1 & 0 & 0 \end{pmatrix} @ \begin{pmatrix} \frac{1}{2} & 0 & 0 \end{pmatrix}$	[1,-2,-3,4]
B ₂	b ₂	A ₁	A ₁	1	2	$\begin{pmatrix} 0 & 0 & 1 \end{pmatrix} @ \begin{pmatrix} 0 & 0 & \frac{1}{2} \end{pmatrix}$	[1,-2,-3,4]
B ₃	b ₃	B ₁	B ₁	1	1	$\begin{pmatrix} 0 & 0 & 1 \end{pmatrix} @ \begin{pmatrix} \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \end{pmatrix}$	[1,-2,-3,4]
B ₄	b ₄	B ₁	B ₁	1	2	$\begin{pmatrix} 1 & 0 & 0 \end{pmatrix} @ \begin{pmatrix} 0 & \frac{1}{2} & 0 \end{pmatrix}$	[1,-2,-3,4]
B ₅	b ₅	A ₁	B ₁	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 ₆	A ₁	B ₁	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 ₇	A ₁	B ₁	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 ₈	A ₁	B ₁	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 ₁	(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
$\mathbb{Q}_0^{(Ag)}$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$
$\mathbb{Q}_1^{(Au)}$	$\frac{1}{2}$	$\frac{1}{2}$	$-\frac{1}{2}$	$-\frac{1}{2}$
$\mathbb{Q}_1^{(Bu,1)}$	$\frac{1}{2}$	$-\frac{1}{2}$	$-\frac{1}{2}$	$\frac{1}{2}$
$\mathbb{Q}_2^{(Bg,2)}$	$\frac{1}{2}$	$-\frac{1}{2}$	$\frac{1}{2}$	$-\frac{1}{2}$