

SAMB for “C3v1”

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- Group: No. 156 C_{3v}^1 $P3m1$ [trigonal]
 - Associated point group: No. 19 C_{3v} $3m1$ (3m1 setting) [trigonal]
 - Generation condition
 - model type: **tight_binding**
 - time-reversal type: **electric**
 - irrep: [A1]
 - **spinful**
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- Unit cell:
 $a = 1.0$, $b = 1.0$, $c = 1.0$, $\alpha = 90.0$, $\beta = 90.0$, $\gamma = 120.0$
- Lattice vectors:
 $\mathbf{a}_1 = (1.0 \ 0 \ 0)$
 $\mathbf{a}_2 = (-0.5 \ 0.86602540378444 \ 0)$
 $\mathbf{a}_3 = (0 \ 0 \ 1.0)$

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 = 8

Table 2: Hilbert space for full matrix.

No.	ket	No.	ket	No.	ket	No.	ket	No.	ket
1	$(p_x, \uparrow)@A_1$	2	$(p_x, \downarrow)@A_1$	3	$(p_y, \uparrow)@A_1$	4	$(p_y, \downarrow)@A_1$	5	$(p_x, \uparrow)@B_1$
6	$(p_x, \downarrow)@B_1$	7	$(p_y, \uparrow)@B_1$	8	$(p_y, \downarrow)@B_1$				

- Sites in (primitive) unit cell:

Table 3: Site-clusters.

	site	position	mapping
S ₁ [1b: 3m.]	A ₁	$\begin{pmatrix} \frac{1}{3} & \frac{2}{3} & 0 \end{pmatrix}$	[1,2,3,4,5,6]
S ₂ [1c: 3m.]	B ₁	$\begin{pmatrix} \frac{2}{3} & \frac{1}{3} & 0 \end{pmatrix}$	[1,2,3,4,5,6]

- Bonds in (primitive) unit cell:

Table 4: Bond-clusters.

	bond	tail	head	n	#	$\mathbf{b}@c$	mapping
B ₁ [3d: .m.]	b ₁	B ₁	A ₁	1	1	$\begin{pmatrix} \frac{1}{3} & \frac{2}{3} & 0 \end{pmatrix} @ \begin{pmatrix} \frac{1}{2} & 0 & 0 \end{pmatrix}$	[1,4]
	b ₂	B ₁	A ₁	1	1	$\begin{pmatrix} -\frac{2}{3} & -\frac{1}{3} & 0 \end{pmatrix} @ \begin{pmatrix} 0 & \frac{1}{2} & 0 \end{pmatrix}$	[2,6]
	b ₃	B ₁	A ₁	1	1	$\begin{pmatrix} \frac{1}{3} & -\frac{1}{3} & 0 \end{pmatrix} @ \begin{pmatrix} \frac{1}{2} & \frac{1}{2} & 0 \end{pmatrix}$	[3,5]

- SAMB:

$$\boxed{\text{No. 1}} \quad \hat{Q}_0^{(A_1)} [M_1, S_1]$$

$$\hat{Z}_1 = \mathbb{X}_1[\mathbb{Q}_0^{(a, A_1)}] \otimes \mathbb{Y}_1[\mathbb{Q}_0^{(s, A_1)}]$$

$$\boxed{\text{No. 2}} \quad \hat{Q}_0^{(A_1)}(1, 1) [M_1, S_1]$$

$$\hat{Z}_2 = X_2[Q_0^{(a, A_1)}(1, 1)] \otimes Y_1[Q_0^{(s, A_1)}]$$

$$\boxed{\text{No. 3}} \quad \hat{Q}_0^{(A_1)} [M_1, S_2]$$

$$\hat{Z}_3 = X_1[Q_0^{(a, A_1)}] \otimes Y_2[Q_0^{(s, A_1)}]$$

$$\boxed{\text{No. 4}} \quad \hat{Q}_0^{(A_1)}(1, 1) [M_1, S_2]$$

$$\hat{Z}_4 = X_2[Q_0^{(a, A_1)}(1, 1)] \otimes Y_2[Q_0^{(s, A_1)}]$$

$$\boxed{\text{No. 5}} \quad \hat{Q}_0^{(A_1)} [M_1, B_1]$$

$$\hat{Z}_5 = X_1[Q_0^{(a, A_1)}] \otimes Y_3[Q_0^{(b, A_1)}]$$

$$\boxed{\text{No. 6}} \quad \hat{Q}_0^{(A_1)}(1, 1) [M_1, B_1]$$

$$\hat{Z}_6 = X_2[Q_0^{(a, A_1)}(1, 1)] \otimes Y_3[Q_0^{(b, A_1)}]$$

$$\boxed{\text{No. 7}} \quad \hat{Q}_3^{(A_1, 2)} [M_1, B_1]$$

$$\hat{Z}_7 = -\frac{\sqrt{2}X_3[Q_{2,0}^{(a, E, 2)}] \otimes Y_4[Q_{1,0}^{(b, E)}]}{2} - \frac{\sqrt{2}X_4[Q_{2,1}^{(a, E, 2)}] \otimes Y_5[Q_{1,1}^{(b, E)}]}{2}$$

$$\boxed{\text{No. 8}} \quad \hat{Q}_1^{(A_1)}(1, -1) [M_1, B_1]$$

$$\hat{Z}_8 = \frac{\sqrt{2}X_5[Q_{2,0}^{(a, E, 1)}(1, -1)] \otimes Y_4[Q_{1,0}^{(b, E)}]}{2} + \frac{\sqrt{2}X_6[Q_{2,1}^{(a, E, 1)}(1, -1)] \otimes Y_5[Q_{1,1}^{(b, E)}]}{2}$$

$$\boxed{\text{No. 9}} \quad \hat{Q}_1^{(A_1)}(1, 1) [M_1, B_1]$$

$$\hat{Z}_9 = \frac{\sqrt{2}X_7[M_{1,0}^{(a, E)}(1, 1)] \otimes Y_7[T_{1,0}^{(b, E)}]}{2} + \frac{\sqrt{2}X_8[M_{1,1}^{(a, E)}(1, 1)] \otimes Y_8[T_{1,1}^{(b, E)}]}{2}$$

$$\boxed{\text{No. 10}} \quad \hat{G}_3^{(A_1)}(1, -1) [M_1, B_1]$$

$$\hat{Z}_{10} = X_{13}[M_3^{(a, A_1)}(1, -1)] \otimes Y_6[T_0^{(b, A_1)}]$$

$$\boxed{\text{No. 11}} \quad \hat{\mathbb{Q}}_3^{(A_1, 2)}(1, -1) [\text{M}_1, \text{B}_1]$$

$$\hat{\mathbb{Z}}_{11} = \frac{\sqrt{2}\mathbb{X}_{11}[\mathbb{M}_{3,0}^{(a,E,2)}(1, -1)] \otimes \mathbb{Y}_7[\mathbb{T}_{1,0}^{(b,E)}]}{2} + \frac{\sqrt{2}\mathbb{X}_{12}[\mathbb{M}_{3,1}^{(a,E,2)}(1, -1)] \otimes \mathbb{Y}_8[\mathbb{T}_{1,1}^{(b,E)}]}{2}$$

$$\boxed{\text{No. 12}} \quad \hat{\mathbb{Q}}_1^{(A_1)}(1, -1) [\text{M}_1, \text{B}_1]$$

$$\hat{\mathbb{Z}}_{12} = \frac{\sqrt{2}\mathbb{X}_{10}[\mathbb{M}_{1,1}^{(a,E)}(1, -1)] \otimes \mathbb{Y}_8[\mathbb{T}_{1,1}^{(b,E)}]}{2} + \frac{\sqrt{2}\mathbb{X}_9[\mathbb{M}_{1,0}^{(a,E)}(1, -1)] \otimes \mathbb{Y}_7[\mathbb{T}_{1,0}^{(b,E)}]}{2}$$

Table 5: Atomic SAMB group.

group	bra	ket
M ₁	$(p_x, \uparrow), (p_x, \downarrow), (p_y, \uparrow), (p_y, \downarrow)$	$(p_x, \uparrow), (p_x, \downarrow), (p_y, \uparrow), (p_y, \downarrow)$

Table 6: Atomic SAMB.

symbol	type	group	form
\mathbb{X}_1	$\mathbb{Q}_0^{(a, A_1)}$	M ₁	$\begin{pmatrix} \frac{1}{2} & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 \\ 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & \frac{1}{2} \end{pmatrix}$
\mathbb{X}_2	$\mathbb{Q}_0^{(a, A_1)}(1, 1)$	M ₁	$\begin{pmatrix} 0 & 0 & -\frac{i}{2} & 0 \\ 0 & 0 & 0 & \frac{i}{2} \\ \frac{i}{2} & 0 & 0 & 0 \\ 0 & -\frac{i}{2} & 0 & 0 \end{pmatrix}$
\mathbb{X}_3	$\mathbb{Q}_{2,0}^{(a, E, 2)}$	M ₁	$\begin{pmatrix} 0 & 0 & -\frac{1}{2} & 0 \\ 0 & 0 & 0 & -\frac{1}{2} \\ -\frac{1}{2} & 0 & 0 & 0 \\ 0 & -\frac{1}{2} & 0 & 0 \end{pmatrix}$

continued ...

Table 6

symbol	type	group	form
\mathbb{X}_4	$\mathbb{Q}_{2,1}^{(a,E,2)}$	M_1	$\begin{pmatrix} -\frac{1}{2} & 0 & 0 & 0 \\ 0 & -\frac{1}{2} & 0 & 0 \\ 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & \frac{1}{2} \end{pmatrix}$
\mathbb{X}_5	$\mathbb{Q}_{2,0}^{(a,E,1)}(1, -1)$	M_1	$\begin{pmatrix} 0 & 0 & 0 & -\frac{i}{2} \\ 0 & 0 & -\frac{i}{2} & 0 \\ 0 & \frac{i}{2} & 0 & 0 \\ \frac{i}{2} & 0 & 0 & 0 \end{pmatrix}$
\mathbb{X}_6	$\mathbb{Q}_{2,1}^{(a,E,1)}(1, -1)$	M_1	$\begin{pmatrix} 0 & 0 & 0 & -\frac{1}{2} \\ 0 & 0 & \frac{1}{2} & 0 \\ 0 & \frac{1}{2} & 0 & 0 \\ -\frac{1}{2} & 0 & 0 & 0 \end{pmatrix}$
\mathbb{X}_7	$\mathbb{M}_{1,0}^{(a,E)}(1, 1)$	M_1	$\begin{pmatrix} 0 & -\frac{\sqrt{19}i}{19} & 0 & -\frac{3\sqrt{19}}{38} \\ \frac{\sqrt{19}i}{19} & 0 & -\frac{3\sqrt{19}}{38} & 0 \\ 0 & -\frac{3\sqrt{19}}{38} & 0 & \frac{2\sqrt{19}i}{19} \\ -\frac{3\sqrt{19}}{38} & 0 & -\frac{2\sqrt{19}i}{19} & 0 \end{pmatrix}$
\mathbb{X}_8	$\mathbb{M}_{1,1}^{(a,E)}(1, 1)$	M_1	$\begin{pmatrix} 0 & \frac{2\sqrt{19}}{19} & 0 & -\frac{3\sqrt{19}i}{38} \\ \frac{2\sqrt{19}}{19} & 0 & \frac{3\sqrt{19}i}{38} & 0 \\ 0 & -\frac{3\sqrt{19}i}{38} & 0 & -\frac{\sqrt{19}}{19} \\ \frac{3\sqrt{19}i}{38} & 0 & -\frac{\sqrt{19}}{19} & 0 \end{pmatrix}$
\mathbb{X}_9	$\mathbb{M}_{1,0}^{(a,E)}(1, -1)$	M_1	$\begin{pmatrix} 0 & \frac{7\sqrt{38}i}{76} & 0 & \frac{\sqrt{38}}{76} \\ -\frac{7\sqrt{38}i}{76} & 0 & \frac{\sqrt{38}}{76} & 0 \\ 0 & \frac{\sqrt{38}}{76} & 0 & \frac{5\sqrt{38}i}{76} \\ \frac{\sqrt{38}}{76} & 0 & -\frac{5\sqrt{38}i}{76} & 0 \end{pmatrix}$
\mathbb{X}_{10}	$\mathbb{M}_{1,1}^{(a,E)}(1, -1)$	M_1	$\begin{pmatrix} 0 & \frac{5\sqrt{38}}{76} & 0 & \frac{\sqrt{38}i}{76} \\ \frac{5\sqrt{38}}{76} & 0 & -\frac{\sqrt{38}i}{76} & 0 \\ 0 & \frac{\sqrt{38}i}{76} & 0 & \frac{7\sqrt{38}}{76} \\ -\frac{\sqrt{38}i}{76} & 0 & \frac{7\sqrt{38}}{76} & 0 \end{pmatrix}$
\mathbb{X}_{11}	$\mathbb{M}_{3,0}^{(a,E,2)}(1, -1)$	M_1	$\begin{pmatrix} \frac{1}{2} & 0 & 0 & 0 \\ 0 & -\frac{1}{2} & 0 & 0 \\ 0 & 0 & -\frac{1}{2} & 0 \\ 0 & 0 & 0 & \frac{1}{2} \end{pmatrix}$

continued ...

Table 6

symbol	type	group	form
\mathbb{X}_{12}	$\mathbb{M}_{3,1}^{(a,E,2)}(1,-1)$	M_1	$\begin{pmatrix} 0 & 0 & -\frac{1}{2} & 0 \\ 0 & 0 & 0 & \frac{1}{2} \\ -\frac{1}{2} & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 \end{pmatrix}$
\mathbb{X}_{13}	$\mathbb{M}_3^{(a,A_1)}(1,-1)$	M_1	$\begin{pmatrix} 0 & \frac{\sqrt{2}}{4} & 0 & \frac{\sqrt{2}i}{4} \\ \frac{\sqrt{2}}{4} & 0 & -\frac{\sqrt{2}i}{4} & 0 \\ 0 & \frac{\sqrt{2}i}{4} & 0 & -\frac{\sqrt{2}}{4} \\ -\frac{\sqrt{2}i}{4} & 0 & -\frac{\sqrt{2}}{4} & 0 \end{pmatrix}$

Table 7: Cluster SAMB.

symbol	type	cluster	form
\mathbb{Y}_1	$\mathbb{Q}_0^{(s,A_1)}$	S_1	$\begin{pmatrix} 1 \end{pmatrix}$
\mathbb{Y}_2	$\mathbb{Q}_0^{(s,A_1)}$	S_2	$\begin{pmatrix} 1 \end{pmatrix}$
\mathbb{Y}_3	$\mathbb{Q}_0^{(b,A_1)}$	B_1	$\begin{pmatrix} \frac{\sqrt{3}}{3} & \frac{\sqrt{3}}{3} & \frac{\sqrt{3}}{3} \end{pmatrix}$
\mathbb{Y}_4	$\mathbb{Q}_{1,0}^{(b,E)}$	B_1	$\begin{pmatrix} 0 & \frac{\sqrt{2}}{2} & -\frac{\sqrt{2}}{2} \end{pmatrix}$
\mathbb{Y}_5	$\mathbb{Q}_{1,1}^{(b,E)}$	B_1	$\begin{pmatrix} -\frac{\sqrt{6}}{3} & \frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} \end{pmatrix}$
\mathbb{Y}_6	$\mathbb{T}_0^{(b,A_1)}$	B_1	$\begin{pmatrix} \frac{\sqrt{3}i}{3} & \frac{\sqrt{3}i}{3} & \frac{\sqrt{3}i}{3} \end{pmatrix}$
\mathbb{Y}_7	$\mathbb{T}_{1,0}^{(b,E)}$	B_1	$\begin{pmatrix} 0 & \frac{\sqrt{2}i}{2} & -\frac{\sqrt{2}i}{2} \end{pmatrix}$
\mathbb{Y}_8	$\mathbb{T}_{1,1}^{(b,E)}$	B_1	$\begin{pmatrix} -\frac{\sqrt{6}i}{3} & \frac{\sqrt{6}i}{6} & \frac{\sqrt{6}i}{6} \end{pmatrix}$

Table 8: Polar harmonics.

No.	symbol	rank	irrep.	mul.	comp.	form
1	$\mathbb{Q}_0^{(A_1)}$	0	A_1	—	—	1
2	$\mathbb{Q}_{1,0}^{(E)}$	1	E	—	0	x
3	$\mathbb{Q}_{1,1}^{(E)}$	1	E	—	1	y
4	$\mathbb{Q}_{2,0}^{(E,1)}$	2	E	1	0	$\sqrt{3}xz$
5	$\mathbb{Q}_{2,1}^{(E,1)}$	2	E	1	1	$\sqrt{3}yz$
6	$\mathbb{Q}_{2,0}^{(E,2)}$	2	E	2	0	$-\sqrt{3}xy$
7	$\mathbb{Q}_{2,1}^{(E,2)}$	2	E	2	1	$-\frac{\sqrt{3}(x-y)(x+y)}{2}$

Table 9: Axial harmonics.

No.	symbol	rank	irrep.	mul.	comp.	form
1	$\mathbb{G}_{1,0}^{(E)}$	1	E	—	0	$-Y$
2	$\mathbb{G}_{1,1}^{(E)}$	1	E	—	1	X
3	$\mathbb{G}_3^{(A_1)}$	3	A_1	—	—	$\frac{\sqrt{10}X(X^2-3Y^2)}{4}$
4	$\mathbb{G}_{3,0}^{(E,2)}$	3	E	2	0	$\frac{\sqrt{15}Z(X-Y)(X+Y)}{2}$
5	$\mathbb{G}_{3,1}^{(E,2)}$	3	E	2	1	$-\sqrt{15}XYZ$

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- Group info.: Generator = $\{3_{001}^+|0\}$, $\{m_{110}|0\}$

Table 10: Conjugacy class (point-group part).

rep. SO	symmetry operations
$\{1 0\}$	$\{1 0\}$
$\{3_{001}^+ 0\}$	$\{3_{001}^+ 0\}$, $\{3_{001}^- 0\}$

continued ...

Table 10

rep. SO	symmetry operations
$\{\mathbf{m}_{100} 0\}$	$\{\mathbf{m}_{100} 0\}, \{\mathbf{m}_{010} 0\}, \{\mathbf{m}_{110} 0\}$

Table 11: Symmetry operations.

No.	SO	No.	SO	No.	SO	No.	SO	No.	SO
1	$\{1 0\}$	2	$\{3_{001}^+ 0\}$	3	$\{3_{001}^- 0\}$	4	$\{\mathbf{m}_{100} 0\}$	5	$\{\mathbf{m}_{010} 0\}$
6	$\{\mathbf{m}_{110} 0\}$								

Table 12: Character table (point-group part).

	1	3_{001}^+	\mathbf{m}_{100}
A_1	1	1	1
A_2	1	1	-1
E	2	-1	0

Table 13: Parity conversion.

\leftrightarrow	\leftrightarrow	\leftrightarrow
$A_1 (A_2)$	$A_2 (A_1)$	$E (E)$

Table 14: Symmetric product, $[\Gamma \otimes \Gamma']_+$.

	A_1	A_2	E
A_1	A_1	A_2	E
A_2		A_1	E
E			$A_1 + E$

Table 15: Anti-symmetric product, $[\Gamma \otimes \Gamma']_-$.

A_1	A_2	E
$-$	$-$	A_2

Table 16: Virtual-cluster sites.

No.	position	No.	position	No.	position	No.	position
1	$\begin{pmatrix} -1 & -1 & 0 \end{pmatrix}$	2	$\begin{pmatrix} 1 & 0 & 0 \end{pmatrix}$	3	$\begin{pmatrix} 0 & 1 & 0 \end{pmatrix}$	4	$\begin{pmatrix} 0 & -1 & 0 \end{pmatrix}$
5	$\begin{pmatrix} -1 & 0 & 0 \end{pmatrix}$	6	$\begin{pmatrix} 1 & 1 & 0 \end{pmatrix}$				

Table 17: Virtual-cluster basis.

symbol	1	2	3	4	5	6
$\mathbb{Q}_0^{(A_1)}$	$\frac{\sqrt{6}}{6}$	$\frac{\sqrt{6}}{6}$	$\frac{\sqrt{6}}{6}$	$\frac{\sqrt{6}}{6}$	$\frac{\sqrt{6}}{6}$	$\frac{\sqrt{6}}{6}$
$\mathbb{Q}_{1,0}^{(E)}$	$-\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{3}$	$-\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$	$-\frac{\sqrt{3}}{3}$	$\frac{\sqrt{3}}{6}$
$\mathbb{Q}_{1,1}^{(E)}$	$-\frac{1}{2}$	0	$\frac{1}{2}$	$-\frac{1}{2}$	0	$\frac{1}{2}$
$\mathbb{Q}_{2,0}^{(E,2)}$	$-\frac{1}{2}$	0	$\frac{1}{2}$	$\frac{1}{2}$	0	$-\frac{1}{2}$

continued ...

Table 17

symbol	1	2	3	4	5	6
$\mathbb{Q}_{2,1}^{(E,2)}$	$\frac{\sqrt{3}}{6}$	$-\frac{\sqrt{3}}{3}$	$\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$	$-\frac{\sqrt{3}}{3}$	$\frac{\sqrt{3}}{6}$
$\mathbb{Q}_3^{(A_2)}$	$\frac{\sqrt{6}}{6}$	$\frac{\sqrt{6}}{6}$	$\frac{\sqrt{6}}{6}$	$-\frac{\sqrt{6}}{6}$	$-\frac{\sqrt{6}}{6}$	$-\frac{\sqrt{6}}{6}$