

SAMB for “C3v”

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- Group: No. 19 $C_{3v} - 1$ $31m$ (31m setting) [trigonal]
- Generation condition
 - model type: **tight_binding**
 - time-reversal type: **electric**
 - irrep: [A1]
 - **spinless**

- Kets: dimension = 12

Table 1: Hilbert space for full matrix.

No.	ket	No.	ket	No.	ket	No.	ket	No.	ket
1	$s@A_1$	2	$s@A_2$	3	$s@A_3$	4	$p_x@B_1$	5	$p_y@B_1$
6	$p_z@B_1$	7	$p_x@B_2$	8	$p_y@B_2$	9	$p_z@B_2$	10	$p_x@B_3$
11	$p_y@B_3$	12	$p_z@B_3$						

- Sites in (primitive) unit cell:

Table 2: Site-clusters.

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

continued ...

Table 2

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

- Bonds in (primitive) unit cell:

Table 3: Bond-clusters.

	bond	tail	head	n	#	$\mathbf{b@c}$	mapping
B ₁ [3b: ..m]	b ₁	A ₂	A ₁	1	1	$\begin{pmatrix} \frac{1}{3} & \frac{1}{6} & 0 \end{pmatrix} @ \begin{pmatrix} 0 & -\frac{1}{12} & 0 \end{pmatrix}$	[1,-5]
	b ₂	A ₃	A ₂	1	1	$\begin{pmatrix} -\frac{1}{6} & \frac{1}{6} & 0 \end{pmatrix} @ \begin{pmatrix} \frac{1}{12} & \frac{1}{12} & 0 \end{pmatrix}$	[2,-4]
	b ₃	A ₃	A ₁	1	1	$\begin{pmatrix} \frac{1}{6} & \frac{1}{3} & 0 \end{pmatrix} @ \begin{pmatrix} -\frac{1}{12} & 0 & 0 \end{pmatrix}$	[-3,6]
B ₂ [6c: 1]	b ₄	B ₁	A ₁	1	1	$\begin{pmatrix} -\frac{1}{2} & \frac{1}{6} & 0 \end{pmatrix} @ \begin{pmatrix} -\frac{5}{12} & -\frac{1}{12} & 0 \end{pmatrix}$	[1]
	b ₅	B ₂	A ₂	1	1	$\begin{pmatrix} -\frac{1}{6} & -\frac{2}{3} & 0 \end{pmatrix} @ \begin{pmatrix} \frac{1}{12} & -\frac{1}{3} & 0 \end{pmatrix}$	[2]
	b ₆	B ₃	A ₃	1	1	$\begin{pmatrix} \frac{2}{3} & \frac{1}{2} & 0 \end{pmatrix} @ \begin{pmatrix} \frac{1}{3} & \frac{5}{12} & 0 \end{pmatrix}$	[3]
	b ₇	B ₁	A ₃	1	1	$\begin{pmatrix} -\frac{2}{3} & -\frac{1}{6} & 0 \end{pmatrix} @ \begin{pmatrix} -\frac{1}{3} & \frac{1}{12} & 0 \end{pmatrix}$	[4]
	b ₈	B ₃	A ₂	1	1	$\begin{pmatrix} \frac{1}{2} & \frac{2}{3} & 0 \end{pmatrix} @ \begin{pmatrix} \frac{5}{12} & \frac{1}{3} & 0 \end{pmatrix}$	[5]
	b ₉	B ₂	A ₁	1	1	$\begin{pmatrix} \frac{1}{6} & -\frac{1}{2} & 0 \end{pmatrix} @ \begin{pmatrix} -\frac{1}{12} & -\frac{5}{12} & 0 \end{pmatrix}$	[6]

- SAMB:

$$\boxed{\text{No. 1}} \quad \hat{\mathbb{Q}}_0^{(A_1)} [\mathbb{M}_1, \mathbb{S}_1]$$

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

$$\boxed{\text{No. 2}} \quad \hat{\mathbb{Q}}_0^{(A_1)} [\mathbb{M}_2, \mathbb{S}_2]$$

$$\hat{\mathbb{Z}}_2 = \mathbb{X}_2[\mathbb{Q}_0^{(a,A_1)}] \otimes \mathbb{U}_2[\mathbb{Q}_0^{(s,A_1)}]$$

$$\boxed{\text{No. 3}} \quad \hat{Q}_2^{(A_1)} [M_2, S_2]$$

$$\hat{Z}_3 = \mathbb{X}_3[Q_2^{(a, A_1)}] \otimes \mathbb{U}_2[Q_0^{(s, A_1)}]$$

$$\boxed{\text{No. 4}} \quad \hat{Q}_1^{(A_1)} [M_2, S_2]$$

$$\hat{Z}_4 = \frac{\sqrt{2}\mathbb{X}_4[Q_{2,0}^{(a, E, 1)}] \otimes \mathbb{U}_3[Q_{1,0}^{(s, E)}]}{2} + \frac{\sqrt{2}\mathbb{X}_5[Q_{2,1}^{(a, E, 1)}] \otimes \mathbb{U}_4[Q_{1,1}^{(s, E)}]}{2}$$

$$\boxed{\text{No. 5}} \quad \hat{Q}_3^{(A_1, 2)} [M_2, S_2]$$

$$\hat{Z}_5 = \frac{\sqrt{2}\mathbb{X}_6[Q_{2,0}^{(a, E, 2)}] \otimes \mathbb{U}_3[Q_{1,0}^{(s, E)}]}{2} + \frac{\sqrt{2}\mathbb{X}_7[Q_{2,1}^{(a, E, 2)}] \otimes \mathbb{U}_4[Q_{1,1}^{(s, E)}]}{2}$$

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

$$\hat{Z}_6 = \mathbb{X}_1[Q_0^{(a, A_1)}] \otimes \mathbb{U}_5[Q_0^{(u, A_1)}]$$

$$\boxed{\text{No. 7}} \quad \hat{Q}_1^{(A_1)} [M_3, B_2]$$

$$\hat{Z}_7 = \mathbb{X}_8[Q_1^{(a, A_1)}] \otimes \mathbb{U}_6[Q_0^{(u, A_1)}]$$

$$\boxed{\text{No. 8}} \quad \hat{Q}_0^{(A_1)} [M_3, B_2]$$

$$\hat{Z}_8 = \frac{\sqrt{2}\mathbb{X}_{10}[Q_{1,1}^{(a, E)}] \otimes \mathbb{U}_8[Q_{1,1}^{(u, E)}]}{2} + \frac{\sqrt{2}\mathbb{X}_9[Q_{1,0}^{(a, E)}] \otimes \mathbb{U}_7[Q_{1,0}^{(u, E)}]}{2}$$

$$\boxed{\text{No. 9}} \quad \hat{Q}_3^{(A_1, 2)} [M_3, B_2]$$

$$\hat{Z}_9 = \frac{\sqrt{2}\mathbb{X}_{10}[Q_{1,1}^{(a, E)}] \otimes \mathbb{U}_{10}[Q_{2,1}^{(u, E, 2)}]}{2} + \frac{\sqrt{2}\mathbb{X}_9[Q_{1,0}^{(a, E)}] \otimes \mathbb{U}_9[Q_{2,0}^{(u, E, 2)}]}{2}$$

Table 4: Atomic SAMB group.

group	bra	ket
M ₁	s	s
M ₂	p_x, p_y, p_z	p_x, p_y, p_z
M ₃	p_x, p_y, p_z	s

Table 5: Atomic SAMB.

symbol	type	group	form
X ₁	$\mathbb{Q}_0^{(a,A_1)}$	M ₁	$\begin{pmatrix} 1 \end{pmatrix}$
X ₂	$\mathbb{Q}_0^{(a,A_1)}$	M ₂	$\begin{pmatrix} \frac{\sqrt{3}}{3} & 0 & 0 \\ 0 & \frac{\sqrt{3}}{3} & 0 \\ 0 & 0 & \frac{\sqrt{3}}{3} \end{pmatrix}$
X ₃	$\mathbb{Q}_2^{(a,A_1)}$	M ₂	$\begin{pmatrix} -\frac{\sqrt{6}}{6} & 0 & 0 \\ 0 & -\frac{\sqrt{6}}{6} & 0 \\ 0 & 0 & \frac{\sqrt{6}}{3} \end{pmatrix}$
X ₄	$\mathbb{Q}_{2,0}^{(a,E,1)}$	M ₂	$\begin{pmatrix} 0 & 0 & \frac{\sqrt{2}}{2} \\ 0 & 0 & 0 \\ \frac{\sqrt{2}}{2} & 0 & 0 \end{pmatrix}$
X ₅	$\mathbb{Q}_{2,1}^{(a,E,1)}$	M ₂	$\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{2}}{2} \\ 0 & \frac{\sqrt{2}}{2} & 0 \end{pmatrix}$
X ₆	$\mathbb{Q}_{2,0}^{(a,E,2)}$	M ₂	$\begin{pmatrix} \frac{\sqrt{2}}{2} & 0 & 0 \\ 0 & -\frac{\sqrt{2}}{2} & 0 \\ 0 & 0 & 0 \end{pmatrix}$
X ₇	$\mathbb{Q}_{2,1}^{(a,E,2)}$	M ₂	$\begin{pmatrix} 0 & -\frac{\sqrt{2}}{2} & 0 \\ -\frac{\sqrt{2}}{2} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$

continued ...

Table 5

symbol	type	group	form
\mathbb{X}_8	$\mathbb{Q}_1^{(a, A_1)}$	M_3	$\begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$
\mathbb{X}_9	$\mathbb{Q}_{1,0}^{(a, E)}$	M_3	$\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$
\mathbb{X}_{10}	$\mathbb{Q}_{1,1}^{(a, E)}$	M_3	$\begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$

Table 6: Uniform SAMB.

symbol	type	cluster	form
\mathbb{U}_1	$\mathbb{Q}_0^{(s, A_1)}$	S_1	$\begin{pmatrix} \frac{\sqrt{3}}{3} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{3}}{3} & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{3}}{3} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$
\mathbb{U}_2	$\mathbb{Q}_0^{(s, A_1)}$	S_2	$\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{3}}{3} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{3}}{3} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{3}}{3} \end{pmatrix}$

continued ...

Table 6

symbol	type	cluster	form
\mathbb{U}_3	$\mathbb{Q}_{1,0}^{(s,E)}$	S_2	$\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{6}}{3} & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{6}}{6} & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{6}}{6} \end{pmatrix}$
\mathbb{U}_4	$\mathbb{Q}_{1,1}^{(s,E)}$	S_2	$\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{2}}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{2}}{2} \end{pmatrix}$
\mathbb{U}_5	$\mathbb{Q}_0^{(u,A_1)}$	B_1	$\begin{pmatrix} 0 & \frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} & 0 & 0 & 0 \\ \frac{\sqrt{6}}{6} & 0 & \frac{\sqrt{6}}{6} & 0 & 0 & 0 \\ \frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$
\mathbb{U}_6	$\mathbb{Q}_0^{(u,A_1)}$	B_2	$\begin{pmatrix} 0 & 0 & 0 & \frac{\sqrt{3}}{6} & \frac{\sqrt{3}}{6} & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{3}}{6} & \frac{\sqrt{3}}{6} \\ 0 & 0 & 0 & \frac{\sqrt{3}}{6} & 0 & \frac{\sqrt{3}}{6} \\ \frac{\sqrt{3}}{6} & 0 & \frac{\sqrt{3}}{6} & 0 & 0 & 0 \\ \frac{\sqrt{3}}{6} & \frac{\sqrt{3}}{6} & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{3}}{6} & \frac{\sqrt{3}}{6} & 0 & 0 & 0 \end{pmatrix}$
\mathbb{U}_7	$\mathbb{Q}_{1,0}^{(u,E)}$	B_2	$\begin{pmatrix} 0 & 0 & 0 & \frac{\sqrt{2}}{4} & -\frac{\sqrt{2}}{4} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{2}}{4} & 0 & -\frac{\sqrt{2}}{4} \\ \frac{\sqrt{2}}{4} & 0 & \frac{\sqrt{2}}{4} & 0 & 0 & 0 \\ -\frac{\sqrt{2}}{4} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{2}}{4} & 0 & 0 & 0 \end{pmatrix}$

continued ...

Table 6

symbol	type	cluster	form
\mathbb{U}_8	$\mathbb{Q}_{1,1}^{(u,E)}$	B_2	$\begin{pmatrix} 0 & 0 & 0 & -\frac{\sqrt{6}}{12} & \frac{\sqrt{6}}{12} & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{6}}{6} & -\frac{\sqrt{6}}{6} \\ 0 & 0 & 0 & \frac{\sqrt{6}}{12} & 0 & -\frac{\sqrt{6}}{12} \\ -\frac{\sqrt{6}}{12} & 0 & \frac{\sqrt{6}}{12} & 0 & 0 & 0 \\ \frac{\sqrt{6}}{12} & \frac{\sqrt{6}}{6} & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{6}}{6} & -\frac{\sqrt{6}}{12} & 0 & 0 & 0 \end{pmatrix}$
\mathbb{U}_9	$\mathbb{Q}_{2,0}^{(u,E,2)}$	B_2	$\begin{pmatrix} 0 & 0 & 0 & \frac{\sqrt{6}}{12} & \frac{\sqrt{6}}{12} & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{6}}{6} & -\frac{\sqrt{6}}{6} \\ 0 & 0 & 0 & \frac{\sqrt{6}}{12} & 0 & \frac{\sqrt{6}}{12} \\ \frac{\sqrt{6}}{12} & 0 & \frac{\sqrt{6}}{12} & 0 & 0 & 0 \\ \frac{\sqrt{6}}{12} & -\frac{\sqrt{6}}{6} & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{12} & 0 & 0 & 0 \end{pmatrix}$
\mathbb{U}_{10}	$\mathbb{Q}_{2,1}^{(u,E,2)}$	B_2	$\begin{pmatrix} 0 & 0 & 0 & \frac{\sqrt{2}}{4} & \frac{\sqrt{2}}{4} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{2}}{4} & 0 & -\frac{\sqrt{2}}{4} \\ \frac{\sqrt{2}}{4} & 0 & -\frac{\sqrt{2}}{4} & 0 & 0 & 0 \\ \frac{\sqrt{2}}{4} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{2}}{4} & 0 & 0 & 0 \end{pmatrix}$

Table 7: Polar harmonics.

No.	symbol	rank	irrep.	mul.	comp.	form
1	$\mathbb{Q}_0^{(A_1)}$	0	A_1	—	—	1
2	$\mathbb{Q}_1^{(A_1)}$	1	A_1	—	—	z
3	$\mathbb{Q}_{1,0}^{(E)}$	1	E	—	0	x
4	$\mathbb{Q}_{1,1}^{(E)}$	1	E	—	1	y
5	$\mathbb{Q}_2^{(A_1)}$	2	A_1	—	—	$-\frac{x^2}{2} - \frac{y^2}{2} + z^2$
6	$\mathbb{Q}_{2,0}^{(E,1)}$	2	E	1	0	$\sqrt{3}xz$

continued ...

Table 7

No.	symbol	rank	irrep.	mul.	comp.	form
7	$\mathbb{Q}_{2,1}^{(E,1)}$	2	E	1	1	$\sqrt{3}yz$
8	$\mathbb{Q}_{2,0}^{(E,2)}$	2	E	2	0	$\frac{\sqrt{3}(x-y)(x+y)}{2}$
9	$\mathbb{Q}_{2,1}^{(E,2)}$	2	E	2	1	$-\sqrt{3}xy$
10	$\mathbb{Q}_3^{(A_2)}$	3	A_2	—	—	$\frac{\sqrt{10}y(3x^2-y^2)}{4}$

-
- Group info.: Generator = 3_{001}^+ , m_{1-10}

Table 8: Conjugacy class.

rep. SO	symmetry operations
1	1
3_{001}^+	3_{001}^+ , 3_{001}^-
m_{120}	m_{120} , m_{210} , m_{1-10}

Table 9: Symmetry operations.

No.	SO	No.	SO	No.	SO	No.	SO	No.	SO
1	1	2	3_{001}^+	3	3_{001}^-	4	m_{120}	5	m_{210}
6	m_{1-10}								

Table 10: Character table.

	1	3_{001}^+	m_{120}
A_1	1	1	1
A_2	1	1	-1
E	2	-1	0

Table 11: Parity conversion.

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

Table 12: 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 13: Anti-symmetric product, $[\Gamma \otimes \Gamma']_-$.

A_1	A_2	E
-	-	A_2

Table 14: Virtual-cluster sites.

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

Table 15: Virtual-cluster basis.

symbol	1	2	3	4	5	6
$\mathbb{Q}_0^{(A_1)}$	$\frac{\sqrt{6}}{6}$	$\frac{\sqrt{6}}{6}$	$\frac{\sqrt{6}}{6}$	$\frac{\sqrt{6}}{6}$	$\frac{\sqrt{6}}{6}$	$\frac{\sqrt{6}}{6}$
$\mathbb{Q}_{1,0}^{(E)}$	$\frac{1}{2}$	0	$-\frac{1}{2}$	$\frac{1}{2}$	0	$-\frac{1}{2}$
$\mathbb{Q}_{1,1}^{(E)}$	$-\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{3}$	$-\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$	$-\frac{\sqrt{3}}{3}$	$\frac{\sqrt{3}}{6}$
$\mathbb{Q}_{2,0}^{(E,2)}$	$\frac{\sqrt{3}}{6}$	$-\frac{\sqrt{3}}{3}$	$\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$	$-\frac{\sqrt{3}}{3}$	$\frac{\sqrt{3}}{6}$
$\mathbb{Q}_{2,1}^{(E,2)}$	$\frac{1}{2}$	0	$-\frac{1}{2}$	$-\frac{1}{2}$	0	$\frac{1}{2}$
$\mathbb{Q}_3^{(A_2)}$	$-\frac{\sqrt{6}}{6}$	$-\frac{\sqrt{6}}{6}$	$-\frac{\sqrt{6}}{6}$	$\frac{\sqrt{6}}{6}$	$\frac{\sqrt{6}}{6}$	$\frac{\sqrt{6}}{6}$