

# 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 <sub>1</sub> [3b: ..m]	A <sub>1</sub>	$\begin{pmatrix} -\frac{1}{6} & -\frac{1}{6} & 0 \end{pmatrix}$	[1,6]
	A <sub>2</sub>	$\begin{pmatrix} \frac{1}{6} & 0 & 0 \end{pmatrix}$	[2,5]
	A <sub>3</sub>	$\begin{pmatrix} 0 & \frac{1}{6} & 0 \end{pmatrix}$	[3,4]

*continued ...*

Table 2

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

- Bonds in (primitive) unit cell:

Table 3: Bond-clusters.

	bond	tail	head	$n$	#	$\mathbf{b@c}$	mapping
B <sub>1</sub> [3b: ..m]	b <sub>1</sub>	A <sub>2</sub>	A <sub>1</sub>	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 <sub>2</sub>	A <sub>3</sub>	A <sub>2</sub>	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 <sub>3</sub>	A <sub>3</sub>	A <sub>1</sub>	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 <sub>2</sub> [6c: 1]	b <sub>4</sub>	B <sub>1</sub>	A <sub>1</sub>	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 <sub>5</sub>	B <sub>2</sub>	A <sub>2</sub>	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 <sub>6</sub>	B <sub>3</sub>	A <sub>3</sub>	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 <sub>7</sub>	B <sub>1</sub>	A <sub>3</sub>	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 <sub>8</sub>	B <sub>3</sub>	A <sub>2</sub>	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 <sub>9</sub>	B <sub>2</sub>	A <sub>1</sub>	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:

$$\boxed{\text{No. 1}} \quad \hat{\mathbb{Q}}_0^{(A_1)} [\mathbb{M}_1, S_1]$$

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

$$\boxed{\text{No. 2}} \quad \hat{\mathbb{Q}}_0^{(A_1)} [\mathbb{M}_2, S_2]$$

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

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

$$\hat{Z}_3 = X_3[Q_2^{(a, A_1)}] \otimes U_2[Q_0^{(s, A_1)}]$$

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

$$\hat{Z}_4 = \frac{\sqrt{2}X_4[Q_{2,0}^{(a, E, 1)}] \otimes U_3[Q_{1,0}^{(s, E)}]}{2} + \frac{\sqrt{2}X_5[Q_{2,1}^{(a, E, 1)}] \otimes U_4[Q_{1,1}^{(s, E)}]}{2}$$

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

$$\hat{Z}_5 = \frac{\sqrt{2}X_6[Q_{2,0}^{(a, E, 2)}] \otimes U_3[Q_{1,0}^{(s, E)}]}{2} + \frac{\sqrt{2}X_7[Q_{2,1}^{(a, E, 2)}] \otimes U_4[Q_{1,1}^{(s, E)}]}{2}$$

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

$$\hat{Z}_6 = X_1[Q_0^{(a, A_1)}] \otimes U_5[Q_0^{(u, A_1)}]$$

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

$$\hat{Z}_7 = X_8[Q_1^{(a, A_1)}] \otimes U_6[Q_0^{(u, A_1)}]$$

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

$$\hat{Z}_8 = \frac{\sqrt{2}X_{10}[Q_{1,1}^{(a, E)}] \otimes U_8[Q_{1,1}^{(u, E)}]}{2} + \frac{\sqrt{2}X_9[Q_{1,0}^{(a, E)}] \otimes U_7[Q_{1,0}^{(u, E)}]}{2}$$

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

$$\hat{Z}_9 = \frac{\sqrt{2}X_{10}[Q_{1,1}^{(a, E)}] \otimes U_{10}[Q_{2,1}^{(u, E, 2)}]}{2} + \frac{\sqrt{2}X_9[Q_{1,0}^{(a, E)}] \otimes U_9[Q_{2,0}^{(u, E, 2)}]}{2}$$

Table 4: Atomic SAMB group.

group	bra	ket
M <sub>1</sub>	$s$	$s$
M <sub>2</sub>	$p_x, p_y, p_z$	$p_x, p_y, p_z$
M <sub>3</sub>	$p_x, p_y, p_z$	$s$

Table 5: Atomic SAMB.

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

*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	$-\sqrt{3}xy$

- 
- 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	$\frac{1}{2}$
$\mathbb{Q}_3^{(A_2)}$	$-\frac{\sqrt{6}}{6}$	$-\frac{\sqrt{6}}{6}$	$-\frac{\sqrt{6}}{6}$	$\frac{\sqrt{6}}{6}$	$\frac{\sqrt{6}}{6}$	$\frac{\sqrt{6}}{6}$