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	#	$\boldsymbol{b}$@$\boldsymbol{c}$	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:

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

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

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

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

$\boxed{\text{No. 3}}$ $\hat{\mathbb{Q}}_2^{(A_1)}$ $[\mathrm{M}_2, \mathrm{S}_2]$

$$\hat{\mathbb{Z}}_3 = \mathbb{X}_3[\mathbb{Q}_2^{(a,A_1)}] \otimes \mathbb{U}_2[\mathbb{Q}_0^{(s,A_1)}]$$

$\boxed{\text{No. 4}}$ $\hat{\mathbb{Q}}_1^{(A_1)}$ $[\mathrm{M}_2, \mathrm{S}_2]$

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

$\boxed{\text{No. 5}}$ $\hat{\mathbb{Q}}_3^{(A_1,2)}$ $[\mathrm{M}_2, \mathrm{S}_2]$

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

$\boxed{\text{No. 6}}$ $\hat{\mathbb{Q}}_0^{(A_1)}$ $[\mathrm{M}_1, \mathrm{B}_1]$

$$\hat{\mathbb{Z}}_6 = \mathbb{X}_1[\mathbb{Q}_0^{(a,A_1)}] \otimes \mathbb{U}_5[\mathbb{Q}_0^{(u,A_1)}]$$

$\boxed{\text{No. 7}}$ $\hat{\mathbb{Q}}_1^{(A_1)}$ $[\mathrm{M}_3, \mathrm{B}_2]$

$$\hat{\mathbb{Z}}_7 = \mathbb{X}_8[\mathbb{Q}_1^{(a,A_1)}] \otimes \mathbb{U}_6[\mathbb{Q}_0^{(u,A_1)}]$$

$\boxed{\text{No. 8}}$ $\hat{\mathbb{Q}}_0^{(A_1)}$ $[\mathrm{M}_3, \mathrm{B}_2]$

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

$\boxed{\text{No. 9}}$ $\hat{\mathbb{Q}}_3^{(A_1,2)}$ $[\mathrm{M}_3, \mathrm{B}_2]$

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

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
$\mathbb{X}_1$	$\mathbb{Q}_0^{(a,A_1)}$	M_1	$\begin{pmatrix} 1 \end{pmatrix}$
$\mathbb{X}_2$	$\mathbb{Q}_0^{(a,A_1)}$	M_2	$\begin{pmatrix} \frac{\sqrt{3}}{3} & 0 & 0 \\ 0 & \frac{\sqrt{3}}{3} & 0 \\ 0 & 0 & \frac{\sqrt{3}}{3} \end{pmatrix}$
$\mathbb{X}_3$	$\mathbb{Q}_2^{(a,A_1)}$	M_2	$\begin{pmatrix} -\frac{\sqrt{6}}{6} & 0 & 0 \\ 0 & -\frac{\sqrt{6}}{6} & 0 \\ 0 & 0 & \frac{\sqrt{6}}{3} \end{pmatrix}$
$\mathbb{X}_4$	$\mathbb{Q}_{2,0}^{(a,E,1)}$	M_2	$\begin{pmatrix} 0 & 0 & \frac{\sqrt{2}}{2} \\ 0 & 0 & 0 \\ \frac{\sqrt{2}}{2} & 0 & 0 \end{pmatrix}$
$\mathbb{X}_5$	$\mathbb{Q}_{2,1}^{(a,E,1)}$	M_2	$\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{2}}{2} \\ 0 & \frac{\sqrt{2}}{2} & 0 \end{pmatrix}$
$\mathbb{X}_6$	$\mathbb{Q}_{2,0}^{(a,E,2)}$	M_2	$\begin{pmatrix} \frac{\sqrt{2}}{2} & 0 & 0 \\ 0 & -\frac{\sqrt{2}}{2} & 0 \\ 0 & 0 & 0 \end{pmatrix}$
$\mathbb{X}_7$	$\mathbb{Q}_{2,1}^{(a,E,2)}$	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	$-\sqrt{3}xy$

- 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	$\frac{1}{2}$
$\mathbb{Q}_{3}^{(A_2)}$	$-\frac{\sqrt{6}}{6}$	$-\frac{\sqrt{6}}{6}$	$-\frac{\sqrt{6}}{6}$	$\frac{\sqrt{6}}{6}$	$\frac{\sqrt{6}}{6}$	$\frac{\sqrt{6}}{6}$