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`

- Unit cell:
  $a = 1.0,\ b = 1.0,\ c = 1.0,\ \alpha = 90.0,\ \beta = 90.0,\ \gamma = 120.0$
- Lattice vectors:
  $\boldsymbol{a}_1 = \begin{pmatrix} 1.0 & 0 & 0 \end{pmatrix}$
  $\boldsymbol{a}_2 = \begin{pmatrix} -0.5 & 0.86602540378444 & 0 \end{pmatrix}$
  $\boldsymbol{a}_3 = \begin{pmatrix} 0 & 0 & 1.0 \end{pmatrix}$

Table 1: High-symmetry line: Γ-X.

	symbol	position	symbol	position
	Γ	$\begin{pmatrix} 0 & 0 & 0 \end{pmatrix}$	X	$\begin{pmatrix} \frac{1}{2} & 0 & 0 \end{pmatrix}$

- Kets: dimension = 8

Table 2: Hilbert space for full matrix.

	No.	ket	No.	ket	No.	ket	No.	ket
	1	$(p_x,\uparrow)@\mathrm{A}_1$	2	$(p_x,\downarrow)@\mathrm{A}_1$	3	$(p_y,\uparrow)@\mathrm{A}_1$	4	$(p_y,\downarrow)@\mathrm{A}_1$

- Sites in (primitive) unit cell:

Table 3: Site-clusters.

	site	position	mapping
S_1	A_1	$\begin{pmatrix}\frac{1}{3} & \frac{2}{3} & 0\end{pmatrix}$	[1,2,3,4,5,6]
S_2	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	#	$\boldsymbol{b}@\boldsymbol{c}$	mapping
B_1	b_1	A_1	B_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	A_1	B_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	A_1	B_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:

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

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

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

No. 2 $\hat{\mathbb{Q}}_0^{(A_1)}(1,1)$ $[\mathrm{M}_1, \mathrm{S}_1]$

$$\hat{\mathbb{Z}}_2 = \mathbb{X}_2[\mathbb{Q}_0^{(a,A_1)}(1,1)] \otimes \mathbb{Y}_1[\mathbb{Q}_0^{(s,A_1)}]$$

$$\hat{\mathbb{Z}}_2(\boldsymbol{k}) = \mathbb{X}_2[\mathbb{Q}_0^{(a,A_1)}(1,1)] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_1)}]$$

No. 3 $\hat{\mathbb{Q}}_0^{(A_1)}$ $[\mathrm{M}_1, \mathrm{S}_2]$

$$\hat{\mathbb{Z}}_3 = \mathbb{X}_1[\mathbb{Q}_0^{(a,A_1)}] \otimes \mathbb{Y}_2[\mathbb{Q}_0^{(s,A_1)}]$$

$$\hat{\mathbb{Z}}_3(\boldsymbol{k}) = \mathbb{X}_1[\mathbb{Q}_0^{(a,A_1)}] \otimes \mathbb{U}_2[\mathbb{Q}_0^{(s,A_1)}]$$

No. 4 $\hat{\mathbb{Q}}_0^{(A_1)}(1,1)$ $[\mathrm{M}_1, \mathrm{S}_2]$

$$\hat{\mathbb{Z}}_4 = \mathbb{X}_2[\mathbb{Q}_0^{(a,A_1)}(1,1)] \otimes \mathbb{Y}_2[\mathbb{Q}_0^{(s,A_1)}]$$

$$\hat{\mathbb{Z}}_4(\boldsymbol{k}) = \mathbb{X}_2[\mathbb{Q}_0^{(a,A_1)}(1,1)] \otimes \mathbb{U}_2[\mathbb{Q}_0^{(s,A_1)}]$$

No. 5 $\hat{\mathbb{Q}}_0^{(A_1)}$ $[\mathrm{M}_1, \mathrm{B}_1]$

$$\hat{\mathbb{Z}}_5 = \mathbb{X}_1[\mathbb{Q}_0^{(a,A_1)}] \otimes \mathbb{Y}_3[\mathbb{Q}_0^{(b,A_1)}]$$

$$\hat{\mathbb{Z}}_5(\boldsymbol{k}) = \frac{\sqrt{2}\mathbb{X}_1[\mathbb{Q}_0^{(a,A_1)}] \otimes \mathbb{U}_3[\mathbb{Q}_0^{(u,A_1)}] \otimes \mathbb{F}_1[\mathbb{Q}_0^{(k,A_1)}]}{2} - \frac{\sqrt{2}\mathbb{X}_1[\mathbb{Q}_0^{(a,A_1)}] \otimes \mathbb{U}_4[\mathbb{T}_0^{(u,A_1)}] \otimes \mathbb{F}_4[\mathbb{T}_0^{(k,A_1)}]}{2}$$

No. 6 $\hat{\mathbb{Q}}_0^{(A_1)}(1,1)$ $[\mathrm{M}_1, \mathrm{B}_1]$

$$\hat{\mathbb{Z}}_6 = \mathbb{X}_2[\mathbb{Q}_0^{(a,A_1)}(1,1)] \otimes \mathbb{Y}_3[\mathbb{Q}_0^{(b,A_1)}]$$

$$\hat{\mathbb{Z}}_6(\boldsymbol{k}) = \frac{\sqrt{2}\mathbb{X}_2[\mathbb{Q}_0^{(a,A_1)}(1,1)] \otimes \mathbb{U}_3[\mathbb{Q}_0^{(u,A_1)}] \otimes \mathbb{F}_1[\mathbb{Q}_0^{(k,A_1)}]}{2} - \frac{\sqrt{2}\mathbb{X}_2[\mathbb{Q}_0^{(a,A_1)}(1,1)] \otimes \mathbb{U}_4[\mathbb{T}_0^{(u,A_1)}] \otimes \mathbb{F}_4[\mathbb{T}_0^{(k,A_1)}]}{2}$$

No. 7 $\hat{\mathbb{Q}}_3^{(A_1,2)}$ $[\mathrm{M}_1, \mathrm{B}_1]$

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

$$\hat{\mathbb{Z}}_7(\boldsymbol{k}) = -\frac{\mathbb{X}_3[\mathbb{Q}_{2,0}^{(a,E,2)}] \otimes \mathbb{U}_3[\mathbb{Q}_0^{(u,A_1)}] \otimes \mathbb{F}_2[\mathbb{Q}_{1,0}^{(k,E)}]}{2} + \frac{\mathbb{X}_3[\mathbb{Q}_{2,0}^{(a,E,2)}] \otimes \mathbb{U}_4[\mathbb{T}_0^{(u,A_1)}] \otimes \mathbb{F}_5[\mathbb{T}_{1,0}^{(k,E)}]}{2}$$
$$- \frac{\mathbb{X}_4[\mathbb{Q}_{2,1}^{(a,E,2)}] \otimes \mathbb{U}_3[\mathbb{Q}_0^{(u,A_1)}] \otimes \mathbb{F}_3[\mathbb{Q}_{1,1}^{(k,E)}]}{2} + \frac{\mathbb{X}_4[\mathbb{Q}_{2,1}^{(a,E,2)}] \otimes \mathbb{U}_4[\mathbb{T}_0^{(u,A_1)}] \otimes \mathbb{F}_6[\mathbb{T}_{1,1}^{(k,E)}]}{2}$$

No. 8 $\hat{\mathbb{Q}}_1^{(A_1)}(1,-1)$ $[\mathrm{M}_1, \mathrm{B}_1]$

$$\hat{\mathbb{Z}}_8 = \frac{\sqrt{2}\mathbb{X}_5[\mathbb{Q}_{2,0}^{(a,E,1)}(1,-1)] \otimes \mathbb{Y}_4[\mathbb{Q}_{1,0}^{(b,E)}]}{2} + \frac{\sqrt{2}\mathbb{X}_6[\mathbb{Q}_{2,1}^{(a,E,1)}(1,-1)] \otimes \mathbb{Y}_5[\mathbb{Q}_{1,1}^{(b,E)}]}{2}$$

$$\hat{\mathbb{Z}}_8(\boldsymbol{k}) = \frac{\mathbb{X}_5[\mathbb{Q}_{2,0}^{(a,E,1)}(1,-1)] \otimes \mathbb{U}_3[\mathbb{Q}_0^{(u,A_1)}] \otimes \mathbb{F}_2[\mathbb{Q}_{1,0}^{(k,E)}]}{2} - \frac{\mathbb{X}_5[\mathbb{Q}_{2,0}^{(a,E,1)}(1,-1)] \otimes \mathbb{U}_4[\mathbb{T}_0^{(u,A_1)}] \otimes \mathbb{F}_5[\mathbb{T}_{1,0}^{(k,E)}]}{2}$$
$$+ \frac{\mathbb{X}_6[\mathbb{Q}_{2,1}^{(a,E,1)}(1,-1)] \otimes \mathbb{U}_3[\mathbb{Q}_0^{(u,A_1)}] \otimes \mathbb{F}_3[\mathbb{Q}_{1,1}^{(k,E)}]}{2} - \frac{\mathbb{X}_6[\mathbb{Q}_{2,1}^{(a,E,1)}(1,-1)] \otimes \mathbb{U}_4[\mathbb{T}_0^{(u,A_1)}] \otimes \mathbb{F}_6[\mathbb{T}_{1,1}^{(k,E)}]}{2}$$

No. 9 $\hat{\mathbb{Q}}_1^{(A_1)}(1,1)$ $[\mathrm{M}_1, \mathrm{B}_1]$

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

$$\hat{\mathbb{Z}}_9(\boldsymbol{k}) = \frac{\mathbb{X}_7[\mathbb{M}_{1,0}^{(a,E)}(1,1)] \otimes \mathbb{U}_3[\mathbb{Q}_0^{(u,A_1)}] \otimes \mathbb{F}_5[\mathbb{T}_{1,0}^{(k,E)}]}{2} + \frac{\mathbb{X}_7[\mathbb{M}_{1,0}^{(a,E)}(1,1)] \otimes \mathbb{U}_4[\mathbb{T}_0^{(u,A_1)}] \otimes \mathbb{F}_2[\mathbb{Q}_{1,0}^{(k,E)}]}{2}$$
$$+ \frac{\mathbb{X}_8[\mathbb{M}_{1,1}^{(a,E)}(1,1)] \otimes \mathbb{U}_3[\mathbb{Q}_0^{(u,A_1)}] \otimes \mathbb{F}_6[\mathbb{T}_{1,1}^{(k,E)}]}{2} + \frac{\mathbb{X}_8[\mathbb{M}_{1,1}^{(a,E)}(1,1)] \otimes \mathbb{U}_4[\mathbb{T}_0^{(u,A_1)}] \otimes \mathbb{F}_3[\mathbb{Q}_{1,1}^{(k,E)}]}{2}$$

No. 10 $\hat{\mathbb{G}}_3^{(A_1)}(1,-1)$ $[\mathrm{M}_1, \mathrm{B}_1]$

$$\hat{\mathbb{Z}}_{10} = \mathbb{X}_{13}[\mathbb{M}_3^{(a,A_1)}(1,-1)] \otimes \mathbb{Y}_6[\mathbb{T}_0^{(b,A_1)}]$$

$$\hat{\mathbb{Z}}_{10}(\boldsymbol{k}) = \frac{\sqrt{2}\mathbb{X}_{13}[\mathbb{M}_3^{(a,A_1)}(1,-1)] \otimes \mathbb{U}_3[\mathbb{Q}_0^{(u,A_1)}] \otimes \mathbb{F}_4[\mathbb{T}_0^{(k,A_1)}]}{2} + \frac{\sqrt{2}\mathbb{X}_{13}[\mathbb{M}_3^{(a,A_1)}(1,-1)] \otimes \mathbb{U}_4[\mathbb{T}_0^{(u,A_1)}] \otimes \mathbb{F}_1[\mathbb{Q}_0^{(k,A_1)}]}{2}$$

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

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

$$\hat{\mathbb{Z}}_{11}(\boldsymbol{k}) = \frac{\mathbb{X}_{11}[\mathbb{M}_{3,0}^{(a,E,2)}(1,-1)] \otimes \mathbb{U}_3[\mathbb{Q}_0^{(u,A_1)}] \otimes \mathbb{F}_5[\mathbb{T}_{1,0}^{(k,E)}]}{2} + \frac{\mathbb{X}_{11}[\mathbb{M}_{3,0}^{(a,E,2)}(1,-1)] \otimes \mathbb{U}_4[\mathbb{T}_0^{(u,A_1)}] \otimes \mathbb{F}_2[\mathbb{Q}_{1,0}^{(k,E)}]}{2}$$
$$+ \frac{\mathbb{X}_{12}[\mathbb{M}_{3,1}^{(a,E,2)}(1,-1)] \otimes \mathbb{U}_3[\mathbb{Q}_0^{(u,A_1)}] \otimes \mathbb{F}_6[\mathbb{T}_{1,1}^{(k,E)}]}{2} + \frac{\mathbb{X}_{12}[\mathbb{M}_{3,1}^{(a,E,2)}(1,-1)] \otimes \mathbb{U}_4[\mathbb{T}_0^{(u,A_1)}] \otimes \mathbb{F}_3[\mathbb{Q}_{1,1}^{(k,E)}]}{2}$$

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

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

$$\hat{\mathbb{Z}}_{12}(\boldsymbol{k}) = \frac{\mathbb{X}_{10}[\mathbb{M}_{1,1}^{(a,E)}(1,-1)] \otimes \mathbb{U}_3[\mathbb{Q}_0^{(u,A_1)}] \otimes \mathbb{F}_6[\mathbb{T}_{1,1}^{(k,E)}]}{2} + \frac{\mathbb{X}_{10}[\mathbb{M}_{1,1}^{(a,E)}(1,-1)] \otimes \mathbb{U}_4[\mathbb{T}_0^{(u,A_1)}] \otimes \mathbb{F}_3[\mathbb{Q}_{1,1}^{(k,E)}]}{2}$$
$$+ \frac{\mathbb{X}_9[\mathbb{M}_{1,0}^{(a,E)}(1,-1)] \otimes \mathbb{U}_3[\mathbb{Q}_0^{(u,A_1)}] \otimes \mathbb{F}_5[\mathbb{T}_{1,0}^{(k,E)}]}{2} + \frac{\mathbb{X}_9[\mathbb{M}_{1,0}^{(a,E)}(1,-1)] \otimes \mathbb{U}_4[\mathbb{T}_0^{(u,A_1)}] \otimes \mathbb{F}_2[\mathbb{Q}_{1,0}^{(k,E)}]}{2}$$

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	$\begin{pmatrix} 0 & 0 & -\frac{i}{2} & 0 \\ 0 & 0 & 0 & \frac{i}{2} \\ \frac{i}{2} & 0 & 0 & 0 \\ 0 & -\frac{i}{2} & 0 & 0 \end{pmatrix}$

continued ...

Table 6

symbol	type	group	form
$\mathbb{X}_3$	$\mathbb{Q}_{2,0}^{(a,E,2)}$	M_1	$\begin{pmatrix} 0 & 0 & -\frac{1}{2} & 0 \\ 0 & 0 & 0 & -\frac{1}{2} \\ -\frac{1}{2} & 0 & 0 & 0 \\ 0 & -\frac{1}{2} & 0 & 0 \end{pmatrix}$
$\mathbb{X}_4$	$\mathbb{Q}_{2,1}^{(a,E,2)}$	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	$\begin{pmatrix} 0 & \frac{5\sqrt{38}}{76} & 0 & \frac{\sqrt{38}i}{76} \\ \frac{5\sqrt{38}}{76} & 0 & -\frac{\sqrt{38}i}{76} & 0 \\ 0 & \frac{\sqrt{38}i}{76} & 0 & \frac{7\sqrt{38}}{76} \\ -\frac{\sqrt{38}i}{76} & 0 & \frac{7\sqrt{38}}{76} & 0 \end{pmatrix}$

continued ...

Table 6

symbol	type	group	form
$\mathbb{X}_{11}$	$\mathbb{M}_{3,0}^{(a,E,2)}(1,-1)$	M_1	$\begin{pmatrix} \frac{1}{2} & 0 & 0 & 0 \\ 0 & -\frac{1}{2} & 0 & 0 \\ 0 & 0 & -\frac{1}{2} & 0 \\ 0 & 0 & 0 & \frac{1}{2} \end{pmatrix}$
$\mathbb{X}_{12}$	$\mathbb{M}_{3,1}^{(a,E,2)}(1,-1)$	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: Uniform SAMB.

symbol	type	cluster	form
$\mathbb{U}_1$	$\mathbb{Q}_0^{(s,A_1)}$	S_1	$\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$
$\mathbb{U}_2$	$\mathbb{Q}_0^{(s,A_1)}$	S_2	$\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$
$\mathbb{U}_3$	$\mathbb{Q}_0^{(u,A_1)}$	B_1	$\begin{pmatrix} 0 & \frac{\sqrt{2}}{2} \\ \frac{\sqrt{2}}{2} & 0 \end{pmatrix}$
$\mathbb{U}_4$	$\mathbb{T}_0^{(u,A_1)}$	B_1	$\begin{pmatrix} 0 & \frac{\sqrt{2}i}{2} \\ -\frac{\sqrt{2}i}{2} & 0 \end{pmatrix}$

Table 9: Structure SAMB.

symbol	type	cluster	form
$\mathbb{F}_1$	$\mathbb{Q}_0^{(k,A_1)}$	B_1	$\frac{\sqrt{6}c_{001}}{3} + \frac{\sqrt{6}c_{002}}{3} + \frac{\sqrt{6}c_{003}}{3}$
$\mathbb{F}_2$	$\mathbb{Q}_{1,0}^{(k,E)}$	B_1	$c_{002} - c_{003}$
$\mathbb{F}_3$	$\mathbb{Q}_{1,1}^{(k,E)}$	B_1	$-\frac{2\sqrt{3}c_{001}}{3} + \frac{\sqrt{3}c_{002}}{3} + \frac{\sqrt{3}c_{003}}{3}$
$\mathbb{F}_4$	$\mathbb{T}_0^{(k,A_1)}$	B_1	$\frac{\sqrt{6}s_{001}}{3} + \frac{\sqrt{6}s_{002}}{3} + \frac{\sqrt{6}s_{003}}{3}$
$\mathbb{F}_5$	$\mathbb{T}_{1,0}^{(k,E)}$	B_1	$s_{002} - s_{003}$
$\mathbb{F}_6$	$\mathbb{T}_{1,1}^{(k,E)}$	B_1	$-\frac{2\sqrt{3}s_{001}}{3} + \frac{\sqrt{3}s_{002}}{3} + \frac{\sqrt{3}s_{003}}{3}$

Table 10: Polar harmonics.

No.	symbol	rank	irrep.	mul.	comp.	form
1	$\mathbb{Q}_0^{(A_1)}$	0	A_1	–	–	1

continued ...

Table 10

No.	symbol	rank	irrep.	mul.	comp.	form
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 11: 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	–	–	$\frac{\sqrt{10}X\left(X^2-3Y^2\right)}{4}$
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	$-\sqrt{15}XYZ$

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

Table 12: Conjugacy class (point-group part).

rep. SO	symmetry operations
$\{1|0\}$	$\{1|0\}$
$\{3^{+}_{001}|0\}$	$\{3^{+}_{001}|0\},\ \{3^{-}_{001}|0\}$
$\{\mathrm{m}_{100}|0\}$	$\{\mathrm{m}_{100}|0\},\ \{\mathrm{m}_{010}|0\},\ \{\mathrm{m}_{110}|0\}$

Table 13: Symmetry operations.

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

Table 14: Character table (point-group part).

	1	3^{+}_{001}	m_{100}
A_1	1	1	1
A_2	1	1	-1
E	2	-1	0

Table 15: Parity conversion.

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

Table 16: 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 17: Anti-symmetric product, $[\Gamma \otimes \Gamma]_-$.

	A_1	A_2	E
	$-$	$-$	A_2

Table 18: Virtual-cluster sites.

No.	position	No.	position	No.	position	No.	position
1	$\begin{pmatrix}-1 & -1 & 0\end{pmatrix}$	2	$\begin{pmatrix}1 & 0 & 0\end{pmatrix}$	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 19: 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	$-\frac{1}{2}$
$\mathbb{Q}_{2,1}^{(E,2)}$	$\frac{\sqrt{3}}{6}$	$-\frac{\sqrt{3}}{3}$	$\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$	$-\frac{\sqrt{3}}{3}$	$\frac{\sqrt{3}}{6}$
$\mathbb{Q}_3^{(A_2)}$	$\frac{\sqrt{6}}{6}$	$\frac{\sqrt{6}}{6}$	$\frac{\sqrt{6}}{6}$	$-\frac{\sqrt{6}}{6}$	$-\frac{\sqrt{6}}{6}$	$-\frac{\sqrt{6}}{6}$