

# 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:
  - $\mathbf{a}_1 = (1.0 \ 0 \ 0)$
  - $\mathbf{a}_2 = (-0.5 \ 0.86602540378444 \ 0)$
  - $\mathbf{a}_3 = (0 \ 0 \ 1.0)$

Table 1: High-symmetry line:  $\Gamma$ -X.

	symbol	position		symbol	position
	$\Gamma$	$\begin{pmatrix} 0 & 0 & 0 \end{pmatrix}$		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 <sub>1</sub> A <sub>1</sub>	$\begin{pmatrix} \frac{1}{3} & \frac{2}{3} & 0 \end{pmatrix}$	[1,2,3,4,5,6]
S <sub>2</sub> B <sub>1</sub>	$\begin{pmatrix} \frac{2}{3} & \frac{1}{3} & 0 \end{pmatrix}$	[1,2,3,4,5,6]

- Bonds in (primitive) unit cell:

Table 4: Bond-clusters.

bond	tail	head	$n$	#	$\mathbf{b}@c$	mapping
B <sub>1</sub> b <sub>1</sub>	B <sub>1</sub>	A <sub>1</sub>	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 <sub>2</sub>	B <sub>1</sub>	A <sub>1</sub>	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 <sub>3</sub>	B <sub>1</sub>	A <sub>1</sub>	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:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Table 5: Atomic SAMB group.

group	bra	ket
$\mathbb{M}_1$	$(p_x, \uparrow), (p_x, \downarrow), (p_y, \uparrow), (p_y, \downarrow)$	$(p_x, \uparrow), (p_x, \downarrow), (p_y, \uparrow), (p_y, \downarrow)$

Table 6: Atomic SAMB.

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

*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	$A_1$	—	—	$\frac{\sqrt{10}X(X^2-3Y^2)}{4}$
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	$-\sqrt{15}XYZ$

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

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

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

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	$\{m_{100} 0\}$	5	$\{m_{010} 0\}$
6	$\{m_{110} 0\}$								

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