

# SAMB for “kappaET”

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- Group: No. 32  $C_{2v}^8$   $Pba2$  [ orthorhombic ]
  - Associated point group: No. 7  $C_{2v}$   $mm2$  [ orthorhombic ]
  - Generation condition
    - model type: **tight\_binding**
    - time-reversal type: **electric**
    - irrep: [A1]
    - **spinful**
- 

- Unit cell:
  - $a = 1.0$ ,  $b = 1.2$ ,  $c = 1.0$ ,  $\alpha = 90.0$ ,  $\beta = 90.0$ ,  $\gamma = 90.0$
- Lattice vectors:
  - $\mathbf{a}_1 = (1.0 \ 0 \ 0)$
  - $\mathbf{a}_2 = (0 \ 1.2 \ 0)$
  - $\mathbf{a}_3 = (0 \ 0 \ 1.0)$

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	$(s, \uparrow)@A_1$	2	$(s, \downarrow)@A_1$	3	$(s, \uparrow)@A_2$	4	$(s, \downarrow)@A_2$	5	$(s, \uparrow)@A_3$
6	$(s, \downarrow)@A_3$	7	$(s, \uparrow)@A_4$	8	$(s, \downarrow)@A_4$				

- Sites in (primitive) unit cell:

Table 3: Site-clusters.

	site	position	mapping
$S_1$ [4c: 1]	$A_1$	$\begin{pmatrix} \frac{9}{10} & \frac{1}{20} & 0 \end{pmatrix}$	[1]
	$A_2$	$\begin{pmatrix} \frac{1}{10} & \frac{19}{20} & 0 \end{pmatrix}$	[2]
	$A_3$	$\begin{pmatrix} \frac{2}{5} & \frac{9}{20} & 0 \end{pmatrix}$	[3]
	$A_4$	$\begin{pmatrix} \frac{3}{5} & \frac{11}{20} & 0 \end{pmatrix}$	[4]

- Bonds in (primitive) unit cell:

Table 4: Bond-clusters.

	bond	tail	head	$n$	#	$\mathbf{b@c}$	mapping
$B_1$ [2a: ..2]	$b_1$	$A_2$	$A_1$	1	1	$\begin{pmatrix} \frac{1}{5} & -\frac{1}{10} & 0 \end{pmatrix} @ \begin{pmatrix} 0 & 0 & 0 \end{pmatrix}$	[1,-2]
	$b_2$	$A_4$	$A_3$	1	1	$\begin{pmatrix} \frac{1}{5} & \frac{1}{10} & 0 \end{pmatrix} @ \begin{pmatrix} \frac{1}{2} & \frac{1}{2} & 0 \end{pmatrix}$	[3,-4]
$B_2$ [4c: 1]	$b_3$	$A_4$	$A_1$	2	1	$\begin{pmatrix} -\frac{3}{10} & \frac{1}{2} & 0 \end{pmatrix} @ \begin{pmatrix} \frac{3}{4} & \frac{3}{10} & 0 \end{pmatrix}$	[1]
	$b_4$	$A_3$	$A_2$	2	1	$\begin{pmatrix} \frac{3}{10} & -\frac{1}{2} & 0 \end{pmatrix} @ \begin{pmatrix} \frac{1}{4} & \frac{7}{10} & 0 \end{pmatrix}$	[2]
	$b_5$	$A_3$	$A_2$	2	1	$\begin{pmatrix} \frac{3}{10} & \frac{1}{2} & 0 \end{pmatrix} @ \begin{pmatrix} \frac{1}{4} & \frac{1}{5} & 0 \end{pmatrix}$	[-3]
	$b_6$	$A_4$	$A_1$	2	1	$\begin{pmatrix} -\frac{3}{10} & -\frac{1}{2} & 0 \end{pmatrix} @ \begin{pmatrix} \frac{3}{4} & \frac{4}{5} & 0 \end{pmatrix}$	[-4]
$B_3$ [4c: 1]	$b_7$	$A_3$	$A_1$	3	1	$\begin{pmatrix} \frac{1}{2} & \frac{2}{5} & 0 \end{pmatrix} @ \begin{pmatrix} \frac{3}{20} & \frac{1}{4} & 0 \end{pmatrix}$	[1]

*continued ...*

Table 4

	bond	tail	head	$n$	#	$\mathbf{b@c}$	mapping
	b <sub>8</sub>	A <sub>4</sub>	A <sub>2</sub>	3	1	$\begin{pmatrix} -\frac{1}{2} & -\frac{2}{5} & 0 \end{pmatrix} @ \begin{pmatrix} \frac{17}{20} & \frac{3}{4} & 0 \end{pmatrix}$	[2]
	b <sub>9</sub>	A <sub>3</sub>	A <sub>1</sub>	3	1	$\begin{pmatrix} -\frac{1}{2} & \frac{2}{5} & 0 \end{pmatrix} @ \begin{pmatrix} \frac{13}{20} & \frac{1}{4} & 0 \end{pmatrix}$	[-3]
	b <sub>10</sub>	A <sub>4</sub>	A <sub>2</sub>	3	1	$\begin{pmatrix} \frac{1}{2} & -\frac{2}{5} & 0 \end{pmatrix} @ \begin{pmatrix} \frac{7}{20} & \frac{3}{4} & 0 \end{pmatrix}$	[-4]

- SAMB:

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

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

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

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

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

$$\begin{aligned} \hat{\mathbb{Z}}_2(\mathbf{k}) = & \frac{\mathbb{X}_1[\mathbb{Q}_0^{(a,A_1)}] \otimes \mathbb{U}_2[\mathbb{Q}_0^{(u,A_1)}] \otimes \mathbb{F}_1[\mathbb{Q}_0^{(k,A_1)}]}{2} + \frac{\mathbb{X}_1[\mathbb{Q}_0^{(a,A_1)}] \otimes \mathbb{U}_3[\mathbb{Q}_2^{(u,A_2)}] \otimes \mathbb{F}_2[\mathbb{Q}_2^{(k,A_2)}]}{2} \\ & - \frac{\mathbb{X}_1[\mathbb{Q}_0^{(a,A_1)}] \otimes \mathbb{U}_4[\mathbb{T}_1^{(u,B_1)}] \otimes \mathbb{F}_3[\mathbb{T}_1^{(k,B_1)}]}{2} - \frac{\mathbb{X}_1[\mathbb{Q}_0^{(a,A_1)}] \otimes \mathbb{U}_5[\mathbb{T}_1^{(u,B_2)}] \otimes \mathbb{F}_4[\mathbb{T}_1^{(k,B_2)}]}{2} \end{aligned}$$

$$\boxed{\text{No. 3}} \quad \hat{\mathbb{Q}}_1^{(A_1)}(1, -1) [\mathbb{M}_1, \mathbb{B}_1]$$

$$\hat{\mathbb{Z}}_3 = -\frac{\sqrt{2}\mathbb{X}_3[\mathbb{M}_1^{(a,B_1)}(1, -1)] \otimes \mathbb{Y}_3[\mathbb{T}_1^{(b,B_1)}]}{2} + \frac{\sqrt{2}\mathbb{X}_4[\mathbb{M}_1^{(a,B_2)}(1, -1)] \otimes \mathbb{Y}_4[\mathbb{T}_1^{(b,B_2)}]}{2}$$

$$\begin{aligned} \hat{\mathbb{Z}}_3(\mathbf{k}) = & -\frac{\sqrt{2}\mathbb{X}_3[\mathbb{M}_1^{(a,B_1)}(1, -1)] \otimes \mathbb{U}_2[\mathbb{Q}_0^{(u,A_1)}] \otimes \mathbb{F}_3[\mathbb{T}_1^{(k,B_1)}]}{4} - \frac{\sqrt{2}\mathbb{X}_3[\mathbb{M}_1^{(a,B_1)}(1, -1)] \otimes \mathbb{U}_3[\mathbb{Q}_2^{(u,A_2)}] \otimes \mathbb{F}_4[\mathbb{T}_1^{(k,B_2)}]}{4} - \frac{\sqrt{2}\mathbb{X}_3[\mathbb{M}_1^{(a,B_1)}(1, -1)] \otimes \mathbb{U}_4[\mathbb{T}_1^{(u,B_1)}] \otimes \mathbb{F}_1[\mathbb{Q}_0^{(k,A_1)}]}{4} \\ & - \frac{\sqrt{2}\mathbb{X}_3[\mathbb{M}_1^{(a,B_1)}(1, -1)] \otimes \mathbb{U}_5[\mathbb{T}_1^{(u,B_2)}] \otimes \mathbb{F}_2[\mathbb{Q}_2^{(k,A_2)}]}{4} + \frac{\sqrt{2}\mathbb{X}_4[\mathbb{M}_1^{(a,B_2)}(1, -1)] \otimes \mathbb{U}_2[\mathbb{Q}_0^{(u,A_1)}] \otimes \mathbb{F}_4[\mathbb{T}_1^{(k,B_2)}]}{4} + \frac{\sqrt{2}\mathbb{X}_4[\mathbb{M}_1^{(a,B_2)}(1, -1)] \otimes \mathbb{U}_3[\mathbb{Q}_2^{(u,A_2)}] \otimes \mathbb{F}_3[\mathbb{T}_1^{(k,B_1)}]}{4} \\ & + \frac{\sqrt{2}\mathbb{X}_4[\mathbb{M}_1^{(a,B_2)}(1, -1)] \otimes \mathbb{U}_4[\mathbb{T}_1^{(u,B_1)}] \otimes \mathbb{F}_2[\mathbb{Q}_2^{(k,A_2)}]}{4} + \frac{\sqrt{2}\mathbb{X}_4[\mathbb{M}_1^{(a,B_2)}(1, -1)] \otimes \mathbb{U}_5[\mathbb{T}_1^{(u,B_2)}] \otimes \mathbb{F}_1[\mathbb{Q}_0^{(k,A_1)}]}{4} \end{aligned}$$

$$\boxed{\text{No. 4}} \quad \hat{\mathbb{G}}_2^{(A_1)}(1, -1) [\mathbb{M}_1, \mathbb{B}_1]$$

$$\hat{\mathbb{Z}}_4 = \frac{\sqrt{2}\mathbb{X}_3[\mathbb{M}_1^{(a, B_1)}(1, -1)] \otimes \mathbb{Y}_3[\mathbb{T}_1^{(b, B_1)}]}{2} + \frac{\sqrt{2}\mathbb{X}_4[\mathbb{M}_1^{(a, B_2)}(1, -1)] \otimes \mathbb{Y}_4[\mathbb{T}_1^{(b, B_2)}]}{2}$$

$$\begin{aligned} \hat{\mathbb{Z}}_4(\mathbf{k}) = & \frac{\sqrt{2}\mathbb{X}_3[\mathbb{M}_1^{(a, B_1)}(1, -1)] \otimes \mathbb{U}_2[\mathbb{Q}_0^{(u, A_1)}] \otimes \mathbb{F}_3[\mathbb{T}_1^{(k, B_1)}]}{4} + \frac{\sqrt{2}\mathbb{X}_3[\mathbb{M}_1^{(a, B_1)}(1, -1)] \otimes \mathbb{U}_3[\mathbb{Q}_2^{(u, A_2)}] \otimes \mathbb{F}_4[\mathbb{T}_1^{(k, B_2)}]}{4} + \frac{\sqrt{2}\mathbb{X}_3[\mathbb{M}_1^{(a, B_1)}(1, -1)] \otimes \mathbb{U}_4[\mathbb{T}_1^{(u, B_1)}] \otimes \mathbb{F}_1[\mathbb{Q}_0^{(k, A_1)}]}{4} \\ & + \frac{\sqrt{2}\mathbb{X}_3[\mathbb{M}_1^{(a, B_1)}(1, -1)] \otimes \mathbb{U}_5[\mathbb{T}_1^{(u, B_2)}] \otimes \mathbb{F}_2[\mathbb{Q}_2^{(k, A_2)}]}{4} + \frac{\sqrt{2}\mathbb{X}_4[\mathbb{M}_1^{(a, B_2)}(1, -1)] \otimes \mathbb{U}_2[\mathbb{Q}_0^{(u, A_1)}] \otimes \mathbb{F}_4[\mathbb{T}_1^{(k, B_2)}]}{4} + \frac{\sqrt{2}\mathbb{X}_4[\mathbb{M}_1^{(a, B_2)}(1, -1)] \otimes \mathbb{U}_3[\mathbb{Q}_2^{(u, A_2)}] \otimes \mathbb{F}_3[\mathbb{T}_1^{(k, B_1)}]}{4} \\ & + \frac{\sqrt{2}\mathbb{X}_4[\mathbb{M}_1^{(a, B_2)}(1, -1)] \otimes \mathbb{U}_4[\mathbb{T}_1^{(u, B_1)}] \otimes \mathbb{F}_2[\mathbb{Q}_2^{(k, A_2)}]}{4} + \frac{\sqrt{2}\mathbb{X}_4[\mathbb{M}_1^{(a, B_2)}(1, -1)] \otimes \mathbb{U}_5[\mathbb{T}_1^{(u, B_2)}] \otimes \mathbb{F}_1[\mathbb{Q}_0^{(k, A_1)}]}{4} \end{aligned}$$

$$\boxed{\text{No. 5}} \quad \hat{\mathbb{Q}}_0^{(A_1)} [\mathbb{M}_1, \mathbb{B}_2]$$

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

$$\hat{\mathbb{Z}}_5(\mathbf{k}) = \frac{\sqrt{2}\mathbb{X}_1[\mathbb{Q}_0^{(a, A_1)}] \otimes \mathbb{U}_6[\mathbb{Q}_0^{(u, A_1)}] \otimes \mathbb{F}_5[\mathbb{Q}_0^{(k, A_1)}]}{2} - \frac{\sqrt{2}\mathbb{X}_1[\mathbb{Q}_0^{(a, A_1)}] \otimes \mathbb{U}_8[\mathbb{T}_1^{(u, B_1)}] \otimes \mathbb{F}_7[\mathbb{T}_1^{(k, B_1)}]}{2}$$

$$\boxed{\text{No. 6}} \quad \hat{\mathbb{Q}}_1^{(A_1)}(1, -1) [\mathbb{M}_1, \mathbb{B}_2]$$

$$\hat{\mathbb{Z}}_6 = -\frac{\sqrt{2}\mathbb{X}_3[\mathbb{M}_1^{(a, B_1)}(1, -1)] \otimes \mathbb{Y}_6[\mathbb{T}_1^{(b, B_1)}]}{2} + \frac{\sqrt{2}\mathbb{X}_4[\mathbb{M}_1^{(a, B_2)}(1, -1)] \otimes \mathbb{Y}_7[\mathbb{T}_1^{(b, B_2)}]}{2}$$

$$\begin{aligned} \hat{\mathbb{Z}}_6(\mathbf{k}) = & -\frac{\mathbb{X}_3[\mathbb{M}_1^{(a, B_1)}(1, -1)] \otimes \mathbb{U}_6[\mathbb{Q}_0^{(u, A_1)}] \otimes \mathbb{F}_7[\mathbb{T}_1^{(k, B_1)}]}{2} - \frac{\mathbb{X}_3[\mathbb{M}_1^{(a, B_1)}(1, -1)] \otimes \mathbb{U}_8[\mathbb{T}_1^{(u, B_1)}] \otimes \mathbb{F}_5[\mathbb{Q}_0^{(k, A_1)}]}{2} \\ & + \frac{\mathbb{X}_4[\mathbb{M}_1^{(a, B_2)}(1, -1)] \otimes \mathbb{U}_6[\mathbb{Q}_0^{(u, A_1)}] \otimes \mathbb{F}_8[\mathbb{T}_1^{(k, B_2)}]}{2} + \frac{\mathbb{X}_4[\mathbb{M}_1^{(a, B_2)}(1, -1)] \otimes \mathbb{U}_8[\mathbb{T}_1^{(u, B_1)}] \otimes \mathbb{F}_6[\mathbb{Q}_2^{(k, A_2)}]}{2} \end{aligned}$$

$$\boxed{\text{No. 7}} \quad \hat{\mathbb{G}}_2^{(A_1)}(1, -1) [\mathbb{M}_1, \mathbb{B}_2]$$

$$\hat{\mathbb{Z}}_7 = \frac{\sqrt{2}\mathbb{X}_3[\mathbb{M}_1^{(a, B_1)}(1, -1)] \otimes \mathbb{Y}_6[\mathbb{T}_1^{(b, B_1)}]}{2} + \frac{\sqrt{2}\mathbb{X}_4[\mathbb{M}_1^{(a, B_2)}(1, -1)] \otimes \mathbb{Y}_7[\mathbb{T}_1^{(b, B_2)}]}{2}$$

$$\begin{aligned} \hat{\mathbb{Z}}_7(\mathbf{k}) = & \frac{\mathbb{X}_3[\mathbb{M}_1^{(a, B_1)}(1, -1)] \otimes \mathbb{U}_6[\mathbb{Q}_0^{(u, A_1)}] \otimes \mathbb{F}_7[\mathbb{T}_1^{(k, B_1)}]}{2} + \frac{\mathbb{X}_3[\mathbb{M}_1^{(a, B_1)}(1, -1)] \otimes \mathbb{U}_8[\mathbb{T}_1^{(u, B_1)}] \otimes \mathbb{F}_5[\mathbb{Q}_0^{(k, A_1)}]}{2} \\ & + \frac{\mathbb{X}_4[\mathbb{M}_1^{(a, B_2)}(1, -1)] \otimes \mathbb{U}_6[\mathbb{Q}_0^{(u, A_1)}] \otimes \mathbb{F}_8[\mathbb{T}_1^{(k, B_2)}]}{2} + \frac{\mathbb{X}_4[\mathbb{M}_1^{(a, B_2)}(1, -1)] \otimes \mathbb{U}_8[\mathbb{T}_1^{(u, B_1)}] \otimes \mathbb{F}_6[\mathbb{Q}_2^{(k, A_2)}]}{2} \end{aligned}$$

$$\boxed{\text{No. 8}} \quad \hat{\mathbb{Q}}_2^{(A_1, 2)}(1, -1) [\mathbb{M}_1, \mathbb{B}_2]$$

$$\hat{\mathbb{Z}}_8 = -\mathbb{X}_2[\mathbb{M}_1^{(a, A_2)}(1, -1)] \otimes \mathbb{Y}_8[\mathbb{T}_2^{(b, A_2)}]$$

$$\hat{\mathbb{Z}}_8(\mathbf{k}) = -\frac{\sqrt{2}\mathbb{X}_2[\mathbb{M}_1^{(a, A_2)}(1, -1)] \otimes \mathbb{U}_7[\mathbb{Q}_1^{(u, B_2)}] \otimes \mathbb{F}_7[\mathbb{T}_1^{(k, B_1)}]}{2} - \frac{\sqrt{2}\mathbb{X}_2[\mathbb{M}_1^{(a, A_2)}(1, -1)] \otimes \mathbb{U}_9[\mathbb{T}_2^{(u, A_2)}] \otimes \mathbb{F}_5[\mathbb{Q}_0^{(k, A_1)}]}{2}$$

$$\boxed{\text{No. 9}} \quad \hat{\mathbb{Q}}_0^{(A_1)} [\mathbb{M}_1, \mathbb{B}_3]$$

$$\hat{\mathbb{Z}}_9 = \mathbb{X}_1[\mathbb{Q}_0^{(a, A_1)}] \otimes \mathbb{Y}_9[\mathbb{Q}_0^{(b, A_1)}]$$

$$\hat{\mathbb{Z}}_9(\mathbf{k}) = \frac{\sqrt{2}\mathbb{X}_1[\mathbb{Q}_0^{(a, A_1)}] \otimes \mathbb{U}_{10}[\mathbb{Q}_0^{(u, A_1)}] \otimes \mathbb{F}_9[\mathbb{Q}_0^{(k, A_1)}]}{2} - \frac{\sqrt{2}\mathbb{X}_1[\mathbb{Q}_0^{(a, A_1)}] \otimes \mathbb{U}_{12}[\mathbb{T}_1^{(u, B_2)}] \otimes \mathbb{F}_{12}[\mathbb{T}_1^{(k, B_2)}]}{2}$$

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

$$\hat{\mathbb{Z}}_{10} = -\frac{\sqrt{2}\mathbb{X}_3[\mathbb{M}_1^{(a, B_1)}(1, -1)] \otimes \mathbb{Y}_{10}[\mathbb{T}_1^{(b, B_1)}]}{2} + \frac{\sqrt{2}\mathbb{X}_4[\mathbb{M}_1^{(a, B_2)}(1, -1)] \otimes \mathbb{Y}_{11}[\mathbb{T}_1^{(b, B_2)}]}{2}$$

$$\begin{aligned} \hat{\mathbb{Z}}_{10}(\mathbf{k}) = & -\frac{\mathbb{X}_3[\mathbb{M}_1^{(a, B_1)}(1, -1)] \otimes \mathbb{U}_{10}[\mathbb{Q}_0^{(u, A_1)}] \otimes \mathbb{F}_{11}[\mathbb{T}_1^{(k, B_1)}]}{2} - \frac{\mathbb{X}_3[\mathbb{M}_1^{(a, B_1)}(1, -1)] \otimes \mathbb{U}_{12}[\mathbb{T}_1^{(u, B_2)}] \otimes \mathbb{F}_{10}[\mathbb{Q}_2^{(k, A_2)}]}{2} \\ & + \frac{\mathbb{X}_4[\mathbb{M}_1^{(a, B_2)}(1, -1)] \otimes \mathbb{U}_{10}[\mathbb{Q}_0^{(u, A_1)}] \otimes \mathbb{F}_{12}[\mathbb{T}_1^{(k, B_2)}]}{2} + \frac{\mathbb{X}_4[\mathbb{M}_1^{(a, B_2)}(1, -1)] \otimes \mathbb{U}_{12}[\mathbb{T}_1^{(u, B_2)}] \otimes \mathbb{F}_9[\mathbb{Q}_0^{(k, A_1)}]}{2} \end{aligned}$$

$$\boxed{\text{No. 11}} \quad \hat{\mathbb{G}}_2^{(A_1)}(1, -1) [\mathbb{M}_1, \mathbb{B}_3]$$

$$\hat{\mathbb{Z}}_{11} = \frac{\sqrt{2}\mathbb{X}_3[\mathbb{M}_1^{(a, B_1)}(1, -1)] \otimes \mathbb{Y}_{10}[\mathbb{T}_1^{(b, B_1)}]}{2} + \frac{\sqrt{2}\mathbb{X}_4[\mathbb{M}_1^{(a, B_2)}(1, -1)] \otimes \mathbb{Y}_{11}[\mathbb{T}_1^{(b, B_2)}]}{2}$$

$$\begin{aligned} \hat{\mathbb{Z}}_{11}(\mathbf{k}) = & \frac{\mathbb{X}_3[\mathbb{M}_1^{(a, B_1)}(1, -1)] \otimes \mathbb{U}_{10}[\mathbb{Q}_0^{(u, A_1)}] \otimes \mathbb{F}_{11}[\mathbb{T}_1^{(k, B_1)}]}{2} + \frac{\mathbb{X}_3[\mathbb{M}_1^{(a, B_1)}(1, -1)] \otimes \mathbb{U}_{12}[\mathbb{T}_1^{(u, B_2)}] \otimes \mathbb{F}_{10}[\mathbb{Q}_2^{(k, A_2)}]}{2} \\ & + \frac{\mathbb{X}_4[\mathbb{M}_1^{(a, B_2)}(1, -1)] \otimes \mathbb{U}_{10}[\mathbb{Q}_0^{(u, A_1)}] \otimes \mathbb{F}_{12}[\mathbb{T}_1^{(k, B_2)}]}{2} + \frac{\mathbb{X}_4[\mathbb{M}_1^{(a, B_2)}(1, -1)] \otimes \mathbb{U}_{12}[\mathbb{T}_1^{(u, B_2)}] \otimes \mathbb{F}_9[\mathbb{Q}_0^{(k, A_1)}]}{2} \end{aligned}$$

$$\boxed{\text{No. 12}} \quad \hat{\mathbb{Q}}_2^{(A_1, 2)}(1, -1) [\mathbb{M}_1, \mathbb{B}_3]$$

$$\hat{\mathbb{Z}}_{12} = -\mathbb{X}_2[\mathbb{M}_1^{(a, A_2)}(1, -1)] \otimes \mathbb{Y}_{12}[\mathbb{T}_2^{(b, A_2)}]$$

$$\hat{\mathbb{Z}}_{12}(\mathbf{k}) = -\frac{\sqrt{2}\mathbb{X}_2[\mathbb{M}_1^{(a, A_2)}(1, -1)] \otimes \mathbb{U}_{11}[\mathbb{Q}_1^{(u, B_1)}] \otimes \mathbb{F}_{12}[\mathbb{T}_1^{(k, B_2)}]}{2} - \frac{\sqrt{2}\mathbb{X}_2[\mathbb{M}_1^{(a, A_2)}(1, -1)] \otimes \mathbb{U}_{13}[\mathbb{T}_2^{(u, A_2)}] \otimes \mathbb{F}_9[\mathbb{Q}_0^{(k, A_1)}]}{2}$$

Table 5: Atomic SAMB group.

group	bra	ket
M <sub>1</sub>	$(s, \uparrow), (s, \downarrow)$	$(s, \uparrow), (s, \downarrow)$

Table 6: Atomic SAMB.

symbol	type	group	form
X <sub>1</sub>	$\mathbb{Q}_0^{(a, A_1)}$	M <sub>1</sub>	$\begin{pmatrix} \frac{\sqrt{2}}{2} & 0 \\ 0 & \frac{\sqrt{2}}{2} \end{pmatrix}$
X <sub>2</sub>	$\mathbb{M}_1^{(a, A_2)}(1, -1)$	M <sub>1</sub>	$\begin{pmatrix} \frac{\sqrt{2}}{2} & 0 \\ 0 & -\frac{\sqrt{2}}{2} \end{pmatrix}$
X <sub>3</sub>	$\mathbb{M}_1^{(a, B_1)}(1, -1)$	M <sub>1</sub>	$\begin{pmatrix} 0 & -\frac{\sqrt{2}i}{2} \\ \frac{\sqrt{2}i}{2} & 0 \end{pmatrix}$
X <sub>4</sub>	$\mathbb{M}_1^{(a, B_2)}(1, -1)$	M <sub>1</sub>	$\begin{pmatrix} 0 & \frac{\sqrt{2}}{2} \\ \frac{\sqrt{2}}{2} & 0 \end{pmatrix}$

Table 7: Cluster SAMB.

symbol	type	cluster	form
Y <sub>1</sub>	$\mathbb{Q}_0^{(s, A_1)}$	S <sub>1</sub>	$\begin{pmatrix} \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \end{pmatrix}$
Y <sub>2</sub>	$\mathbb{Q}_0^{(b, A_1)}$	B <sub>1</sub>	$\begin{pmatrix} \frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2} \end{pmatrix}$
Y <sub>3</sub>	$\mathbb{T}_1^{(b, B_1)}$	B <sub>1</sub>	$\begin{pmatrix} \frac{\sqrt{2}i}{2} & \frac{\sqrt{2}i}{2} \end{pmatrix}$
Y <sub>4</sub>	$\mathbb{T}_1^{(b, B_2)}$	B <sub>1</sub>	$\begin{pmatrix} \frac{\sqrt{2}i}{2} & -\frac{\sqrt{2}i}{2} \end{pmatrix}$
Y <sub>5</sub>	$\mathbb{Q}_0^{(b, A_1)}$	B <sub>2</sub>	$\begin{pmatrix} \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \end{pmatrix}$
Y <sub>6</sub>	$\mathbb{T}_1^{(b, B_1)}$	B <sub>2</sub>	$\begin{pmatrix} \frac{i}{2} & -\frac{i}{2} & -\frac{i}{2} & \frac{i}{2} \end{pmatrix}$
Y <sub>7</sub>	$\mathbb{T}_1^{(b, B_2)}$	B <sub>2</sub>	$\begin{pmatrix} \frac{i}{2} & -\frac{i}{2} & \frac{i}{2} & -\frac{i}{2} \end{pmatrix}$

*continued ...*

Table 7

symbol	type	cluster	form
$\mathbb{Y}_8$	$\mathbb{T}_2^{(b,A_2)}$	$B_2$	$\begin{pmatrix} \frac{i}{2} & \frac{i}{2} & \frac{i}{2} & \frac{i}{2} \end{pmatrix}$
$\mathbb{Y}_9$	$\mathbb{Q}_0^{(b,A_1)}$	$B_3$	$\begin{pmatrix} \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \end{pmatrix}$
$\mathbb{Y}_{10}$	$\mathbb{T}_1^{(b,B_1)}$	$B_3$	$\begin{pmatrix} \frac{i}{2} & -\frac{i}{2} & -\frac{i}{2} & \frac{i}{2} \end{pmatrix}$
$\mathbb{Y}_{11}$	$\mathbb{T}_1^{(b,B_2)}$	$B_3$	$\begin{pmatrix} \frac{i}{2} & -\frac{i}{2} & \frac{i}{2} & -\frac{i}{2} \end{pmatrix}$
$\mathbb{Y}_{12}$	$\mathbb{T}_2^{(b,A_2)}$	$B_3$	$\begin{pmatrix} \frac{i}{2} & \frac{i}{2} & \frac{i}{2} & \frac{i}{2} \end{pmatrix}$

Table 8: Uniform SAMB.

symbol	type	cluster	form
$\mathbb{U}_1$	$\mathbb{Q}_0^{(s,A_1)}$	$S_1$	$\begin{pmatrix} \frac{1}{2} & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 \\ 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & \frac{1}{2} \end{pmatrix}$
$\mathbb{U}_2$	$\mathbb{Q}_0^{(u,A_1)}$	$B_1$	$\begin{pmatrix} 0 & \frac{1}{2} & 0 & 0 \\ \frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2} \\ 0 & 0 & \frac{1}{2} & 0 \end{pmatrix}$
$\mathbb{U}_3$	$\mathbb{Q}_2^{(u,A_2)}$	$B_1$	$\begin{pmatrix} 0 & \frac{1}{2} & 0 & 0 \\ \frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{1}{2} \\ 0 & 0 & -\frac{1}{2} & 0 \end{pmatrix}$
$\mathbb{U}_4$	$\mathbb{T}_1^{(u,B_1)}$	$B_1$	$\begin{pmatrix} 0 & -\frac{i}{2} & 0 & 0 \\ \frac{i}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{i}{2} \\ 0 & 0 & \frac{i}{2} & 0 \end{pmatrix}$
$\mathbb{U}_5$	$\mathbb{T}_1^{(u,B_2)}$	$B_1$	$\begin{pmatrix} 0 & -\frac{i}{2} & 0 & 0 \\ \frac{i}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{i}{2} \\ 0 & 0 & -\frac{i}{2} & 0 \end{pmatrix}$

continued ...

Table 8

symbol	type	cluster	form
$\mathbb{U}_6$	$\mathbb{Q}_0^{(u,A_1)}$	$B_2$	$\begin{pmatrix} 0 & 0 & 0 & \frac{1}{2} \\ 0 & 0 & \frac{1}{2} & 0 \\ 0 & \frac{1}{2} & 0 & 0 \\ \frac{1}{2} & 0 & 0 & 0 \end{pmatrix}$
$\mathbb{U}_7$	$\mathbb{Q}_1^{(u,B_2)}$	$B_2$	$\begin{pmatrix} 0 & 0 & 0 & \frac{1}{2} \\ 0 & 0 & -\frac{1}{2} & 0 \\ 0 & -\frac{1}{2} & 0 & 0 \\ \frac{1}{2} & 0 & 0 & 0 \end{pmatrix}$
$\mathbb{U}_8$	$\mathbb{T}_1^{(u,B_1)}$	$B_2$	$\begin{pmatrix} 0 & 0 & 0 & -\frac{i}{2} \\ 0 & 0 & \frac{i}{2} & 0 \\ 0 & -\frac{i}{2} & 0 & 0 \\ \frac{i}{2} & 0 & 0 & 0 \end{pmatrix}$
$\mathbb{U}_9$	$\mathbb{T}_2^{(u,A_2)}$	$B_2$	$\begin{pmatrix} 0 & 0 & 0 & -\frac{i}{2} \\ 0 & 0 & -\frac{i}{2} & 0 \\ 0 & \frac{i}{2} & 0 & 0 \\ \frac{i}{2} & 0 & 0 & 0 \end{pmatrix}$
$\mathbb{U}_{10}$	$\mathbb{Q}_0^{(u,A_1)}$	$B_3$	$\begin{pmatrix} 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & \frac{1}{2} \\ \frac{1}{2} & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 \end{pmatrix}$
$\mathbb{U}_{11}$	$\mathbb{Q}_1^{(u,B_1)}$	$B_3$	$\begin{pmatrix} 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & -\frac{1}{2} \\ \frac{1}{2} & 0 & 0 & 0 \\ 0 & -\frac{1}{2} & 0 & 0 \end{pmatrix}$
$\mathbb{U}_{12}$	$\mathbb{T}_1^{(u,B_2)}$	$B_3$	$\begin{pmatrix} 0 & 0 & -\frac{i}{2} & 0 \\ 0 & 0 & 0 & \frac{i}{2} \\ \frac{i}{2} & 0 & 0 & 0 \\ 0 & -\frac{i}{2} & 0 & 0 \end{pmatrix}$
$\mathbb{U}_{13}$	$\mathbb{T}_2^{(u,A_2)}$	$B_3$	$\begin{pmatrix} 0 & 0 & -\frac{i}{2} & 0 \\ 0 & 0 & 0 & -\frac{i}{2} \\ \frac{i}{2} & 0 & 0 & 0 \\ 0 & \frac{i}{2} & 0 & 0 \end{pmatrix}$



Table 9: Structure SAMB.

symbol	type	cluster	form
$\mathbb{F}_1$	$\mathbb{Q}_0^{(k,A_1)}$	$B_1$	$c_{001} + c_{002}$
$\mathbb{F}_2$	$\mathbb{Q}_2^{(k,A_2)}$	$B_1$	$c_{001} - c_{002}$
$\mathbb{F}_3$	$\mathbb{T}_1^{(k,B_1)}$	$B_1$	$s_{001} + s_{002}$
$\mathbb{F}_4$	$\mathbb{T}_1^{(k,B_2)}$	$B_1$	$s_{001} - s_{002}$
$\mathbb{F}_5$	$\mathbb{Q}_0^{(k,A_1)}$	$B_2$	$c_{003} + c_{005}$
$\mathbb{F}_6$	$\mathbb{Q}_2^{(k,A_2)}$	$B_2$	$c_{003} - c_{005}$
$\mathbb{F}_7$	$\mathbb{T}_1^{(k,B_1)}$	$B_2$	$s_{003} - s_{005}$
$\mathbb{F}_8$	$\mathbb{T}_1^{(k,B_2)}$	$B_2$	$s_{003} + s_{005}$
$\mathbb{F}_9$	$\mathbb{Q}_0^{(k,A_1)}$	$B_3$	$c_{007} + c_{009}$
$\mathbb{F}_{10}$	$\mathbb{Q}_2^{(k,A_2)}$	$B_3$	$c_{007} - c_{009}$
$\mathbb{F}_{11}$	$\mathbb{T}_1^{(k,B_1)}$	$B_3$	$s_{007} - s_{009}$
$\mathbb{F}_{12}$	$\mathbb{T}_1^{(k,B_2)}$	$B_3$	$s_{007} + s_{009}$

Table 10: Polar harmonics.

No.	symbol	rank	irrep.	mul.	comp.	form
1	$\mathbb{Q}_0^{(A_1)}$	0	$A_1$	—	—	1
2	$\mathbb{Q}_1^{(B_1)}$	1	$B_1$	—	—	$x$
3	$\mathbb{Q}_1^{(B_2)}$	1	$B_2$	—	—	$y$
4	$\mathbb{Q}_2^{(A_2)}$	2	$A_2$	—	—	$\sqrt{3}xy$

Table 11: Axial harmonics.

No.	symbol	rank	irrep.	mul.	comp.	form
1	$\mathbb{G}_1^{(A_2)}$	1	$A_2$	—	—	$Z$
2	$\mathbb{G}_1^{(B_1)}$	1	$B_1$	—	—	$Y$
3	$\mathbb{G}_1^{(B_2)}$	1	$B_2$	—	—	$X$

- 
- Group info.: Generator =  $\{2_{001}|0\}$ ,  $\{\mathbf{m}_{010}|\frac{1}{2}\frac{1}{2}0\}$

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

rep. SO	symmetry operations
$\{1 0\}$	$\{1 0\}$
$\{2_{001} 0\}$	$\{2_{001} 0\}$
$\{\mathbf{m}_{010} \frac{1}{2}\frac{1}{2}0\}$	$\{\mathbf{m}_{010} \frac{1}{2}\frac{1}{2}0\}$
$\{\mathbf{m}_{100} \frac{1}{2}\frac{1}{2}0\}$	$\{\mathbf{m}_{100} \frac{1}{2}\frac{1}{2}0\}$

Table 13: Symmetry operations.

No.	SO	No.	SO	No.	SO	No.	SO	No.	SO
1	$\{1 0\}$	2	$\{2_{001} 0\}$	3	$\{\mathbf{m}_{010} \frac{1}{2}\frac{1}{2}0\}$	4	$\{\mathbf{m}_{100} \frac{1}{2}\frac{1}{2}0\}$		

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

	1	2 <sub>001</sub>	m <sub>010</sub>	m <sub>100</sub>
$A_1$	1	1	1	1
$A_2$	1	1	-1	-1
$B_1$	1	-1	1	-1
$B_2$	1	-1	-1	1

Table 15: Parity conversion.

$\leftrightarrow$	$\leftrightarrow$	$\leftrightarrow$	$\leftrightarrow$
$A_1 (A_2)$	$B_2 (B_1)$	$B_1 (B_2)$	$A_2 (A_1)$

Table 16: Symmetric product,  $[\Gamma \otimes \Gamma']_+$ .

	$A_1$	$A_2$	$B_1$	$B_2$
$A_1$	$A_1$	$A_2$	$B_1$	$B_2$
$A_2$		$A_1$	$B_2$	$B_1$
$B_1$			$A_1$	$A_2$
$B_2$				$A_1$

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

$A_1$	$A_2$	$B_1$	$B_2$
-	-	-	-

Table 18: Virtual-cluster sites.

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

Table 19: Virtual-cluster basis.

symbol	1	2	3	4
$Q_0^{(A1)}$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$
$Q_1^{(B1)}$	$\frac{1}{2}$	$-\frac{1}{2}$	$\frac{1}{2}$	$-\frac{1}{2}$
$Q_1^{(B2)}$	$\frac{1}{2}$	$-\frac{1}{2}$	$-\frac{1}{2}$	$\frac{1}{2}$
$Q_2^{(A2)}$	$\frac{1}{2}$	$\frac{1}{2}$	$-\frac{1}{2}$	$-\frac{1}{2}$