SAMB for "`Cs1`"

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- Group: No. 6 C_s^1 Pm (b-axis setting) [monoclinic]
- Associated point group: No. 4 C_s m (b-axis setting) [monoclinic]

- Generation condition
  - model type: `tight_binding`
  - time-reversal type: `electric`
  - irrep: `[A']`
  - `spinful`

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

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 = 4

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 [1a: m]	A_1	$\begin{pmatrix}0 & 0 & 0\end{pmatrix}$	[1,2]

- Bonds in (primitive) unit cell:

Table 4: Bond-clusters.

	bond	tail	head	n	#	$\boldsymbol{b}@\boldsymbol{c}$	mapping
B_1 [1b: m]	b_1	A_1	A_1	1	1	$\begin{pmatrix}0 & 1 & 0\end{pmatrix}@\begin{pmatrix}0 & \frac{1}{2} & 0\end{pmatrix}$	[1,-2]
B_2 [1a: m]	b_2	A_1	A_1	1	2	$\begin{pmatrix}-1 & 0 & 0\end{pmatrix}@\begin{pmatrix}\frac{1}{2} & 0 & 0\end{pmatrix}$	[1,2]
B_3 [1a: m]	b_3	A_1	A_1	1	3	$\begin{pmatrix}0 & 0 & -1\end{pmatrix}@\begin{pmatrix}0 & 0 & \frac{1}{2}\end{pmatrix}$	[1,2]
B_4 [1a: m]	b_4	A_1	A_1	2	1	$\begin{pmatrix}-1 & 0 & -1\end{pmatrix}@\begin{pmatrix}\frac{1}{2} & 0 & \frac{1}{2}\end{pmatrix}$	[1,2]
B_5 [1b: m]	b_5	A_1	A_1	2	2	$\begin{pmatrix}-1 & 1 & 0\end{pmatrix}@\begin{pmatrix}\frac{1}{2} & \frac{1}{2} & 0\end{pmatrix}$	[1]
	b_6	A_1	A_1	2	2	$\begin{pmatrix}-1 & -1 & 0\end{pmatrix}@\begin{pmatrix}\frac{1}{2} & \frac{1}{2} & 0\end{pmatrix}$	[2]
B_6 [1b: m]	b_7	A_1	A_1	2	3	$\begin{pmatrix}0 & 1 & 1\end{pmatrix}@\begin{pmatrix}0 & \frac{1}{2} & \frac{1}{2}\end{pmatrix}$	[1]
	b_8	A_1	A_1	2	3	$\begin{pmatrix}0 & -1 & 1\end{pmatrix}@\begin{pmatrix}0 & \frac{1}{2} & \frac{1}{2}\end{pmatrix}$	[2]
B_7 [1a: m]	b_9	A_1	A_1	2	4	$\begin{pmatrix}-1 & 0 & 1\end{pmatrix}@\begin{pmatrix}\frac{1}{2} & 0 & \frac{1}{2}\end{pmatrix}$	[1,2]

- SAMB:

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

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

No. 2 $\hat{\mathbb{Q}}_2^{(A',2)}$ $[\mathrm{M}_1, \mathrm{S}_1]$

$\hat{\mathbb{Z}}_2 = \mathbb{X}_2[\mathbb{Q}_2^{(a,A',2)}] \otimes \mathbb{Y}_1[\mathbb{Q}_0^{(s,A')}]$

No. 3 $\hat{\mathbb{Q}}_0^{(A')}(1,1)$ $[\mathrm{M}_1, \mathrm{S}_1]$

$\hat{\mathbb{Z}}_3 = \mathbb{X}_3[\mathbb{Q}_0^{(a,A')}(1,1)] \otimes \mathbb{Y}_1[\mathbb{Q}_0^{(s,A')}]$

No. 4 $\hat{\mathbb{Q}}_2^{(A',3)}(1,-1)$ $[\mathrm{M}_1, \mathrm{S}_1]$

$\hat{\mathbb{Z}}_4 = \mathbb{X}_4[\mathbb{Q}_2^{(a,A',3)}(1,-1)] \otimes \mathbb{Y}_1[\mathbb{Q}_0^{(s,A')}]$

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

$\hat{\mathbb{Z}}_5 = \mathbb{X}_1[\mathbb{Q}_0^{(a,A')}] \otimes \mathbb{Y}_2[\mathbb{Q}_0^{(b,A')}]$

No. 6 $\hat{\mathbb{Q}}_2^{(A',2)}$ $[\mathrm{M}_1, \mathrm{B}_1]$

$\hat{\mathbb{Z}}_6 = \mathbb{X}_2[\mathbb{Q}_2^{(a,A',2)}] \otimes \mathbb{Y}_2[\mathbb{Q}_0^{(b,A')}]$

No. 7 $\hat{\mathbb{Q}}_0^{(A')}(1,1)$ $[\mathrm{M}_1, \mathrm{B}_1]$

$\hat{\mathbb{Z}}_7 = \mathbb{X}_3[\mathbb{Q}_0^{(a,A')}(1,1)] \otimes \mathbb{Y}_2[\mathbb{Q}_0^{(b,A')}]$

No. 8 $\hat{\mathbb{Q}}_2^{(A',3)}(1,-1)$ $[\mathrm{M}_1, \mathrm{B}_1]$

$\hat{\mathbb{Z}}_8 = \mathbb{X}_4[\mathbb{Q}_2^{(a,A',3)}(1,-1)] \otimes \mathbb{Y}_2[\mathbb{Q}_0^{(b,A')}]$

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

$\hat{\mathbb{Z}}_9 = -\mathbb{X}_{12}[\mathbb{M}_1^{(a,A'',2)}(1,1)] \otimes \mathbb{Y}_3[\mathbb{T}_1^{(b,A'')}]$

No. 10 $\hat{\mathbb{Q}}_1^{(A',2)}(1,1)$ $[\mathrm{M}_1, \mathrm{B}_1]$

$\hat{\mathbb{Z}}_{10} = \mathbb{X}_{11}[\mathbb{M}_1^{(a,A'',1)}(1,1)] \otimes \mathbb{Y}_3[\mathbb{T}_1^{(b,A'')}]$

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

$\hat{\mathbb{Z}}_{11} = \mathbb{X}_{13}[\mathbb{M}_1^{(a,A'',1)}(1,-1)] \otimes \mathbb{Y}_3[\mathbb{T}_1^{(b,A'')}]$

No. 12 $\hat{\mathbb{G}}_2^{(A',1)}(1,-1)$ $[\mathrm{M}_1, \mathrm{B}_1]$

$\hat{\mathbb{Z}}_{12} = -\mathbb{X}_{15}[\mathbb{M}_3^{(a,A'',4)}(1,-1)] \otimes \mathbb{Y}_3[\mathbb{T}_1^{(b,A'')}]$

No. 13 $\hat{\mathbb{G}}_2^{(A',2)}(1,-1)$ $[\mathrm{M}_1, \mathrm{B}_1]$

$\hat{\mathbb{Z}}_{13} = -\mathbb{X}_{14}[\mathbb{M}_3^{(a,A'',1)}(1,-1)] \otimes \mathbb{Y}_3[\mathbb{T}_1^{(b,A'')}]$

No. 14 $\hat{\mathbb{Q}}_1^{(A',1)}$ $[\mathrm{M}_1, \mathrm{B}_1]$

$\hat{\mathbb{Z}}_{14} = -\mathbb{X}_{16}[\mathbb{M}_1^{(a,A'',2)}] \otimes \mathbb{Y}_3[\mathbb{T}_1^{(b,A'')}]$

No. 15 $\hat{\mathbb{Q}}_0^{(A')}$ $[\mathrm{M}_1, \mathrm{B}_2]$

$\hat{\mathbb{Z}}_{15} = \mathbb{X}_1[\mathbb{Q}_0^{(a,A')}] \otimes \mathbb{Y}_4[\mathbb{Q}_0^{(b,A')}]$

No. 16 $\hat{\mathbb{Q}}_2^{(A',2)}$ $[\mathrm{M}_1, \mathrm{B}_2]$

$\hat{\mathbb{Z}}_{16} = \mathbb{X}_2[\mathbb{Q}_2^{(a,A',2)}] \otimes \mathbb{Y}_4[\mathbb{Q}_0^{(b,A')}]$

No. 17 $\hat{\mathbb{Q}}_0^{(A')}(1,1)$ $[\mathrm{M}_1, \mathrm{B}_2]$

$\hat{\mathbb{Z}}_{17} = \mathbb{X}_3[\mathbb{Q}_0^{(a,A')}(1,1)] \otimes \mathbb{Y}_4[\mathbb{Q}_0^{(b,A')}]$

No. 18 $\hat{\mathbb{Q}}_2^{(A',3)}(1,-1)$ $[\mathrm{M}_1, \mathrm{B}_2]$

$\hat{\mathbb{Z}}_{18} = \mathbb{X}_4[\mathbb{Q}_2^{(a,A',3)}(1,-1)] \otimes \mathbb{Y}_4[\mathbb{Q}_0^{(b,A')}]$

No. 19 $\hat{\mathbb{G}}_1^{(A')}(1,1)$ $[\mathrm{M}_1, \mathrm{B}_2]$

$\hat{\mathbb{Z}}_{19} = \mathbb{X}_7[\mathbb{M}_1^{(a,A')}(1,1)] \otimes \mathbb{Y}_5[\mathbb{T}_0^{(b,A')}]$

No. 20 $\hat{\mathbb{G}}_1^{(A')}(1,-1)$ $[\mathrm{M}_1, \mathrm{B}_2]$

$\hat{\mathbb{Z}}_{20} = \mathbb{X}_8[\mathbb{M}_1^{(a,A')}(1,-1)] \otimes \mathbb{Y}_5[\mathbb{T}_0^{(b,A')}]$

No. 21 $\hat{\mathbb{G}}_3^{(A',1)}(1,-1)$ $[\mathrm{M}_1, \mathrm{B}_2]$

$\hat{\mathbb{Z}}_{21} = \mathbb{X}_9[\mathbb{M}_3^{(a,A',1)}(1,-1)] \otimes \mathbb{Y}_5[\mathbb{T}_0^{(b,A')}]$

No. 22 $\hat{\mathbb{G}}_3^{(A',2)}(1,-1)$ $[\mathrm{M}_1, \mathrm{B}_2]$

$\hat{\mathbb{Z}}_{22} = \mathbb{X}_{10}[\mathbb{M}_3^{(a,A',2)}(1,-1)] \otimes \mathbb{Y}_5[\mathbb{T}_0^{(b,A')}]$

No. 23 $\hat{\mathbb{Q}}_0^{(A')}$ $[\mathrm{M}_1, \mathrm{B}_3]$

$\hat{\mathbb{Z}}_{23} = \mathbb{X}_1[\mathbb{Q}_0^{(a,A')}] \otimes \mathbb{Y}_6[\mathbb{Q}_0^{(b,A')}]$

No. 24 $\hat{\mathbb{Q}}_2^{(A',2)}$ $[\mathrm{M}_1, \mathrm{B}_3]$

$\hat{\mathbb{Z}}_{24} = \mathbb{X}_2[\mathbb{Q}_2^{(a,A',2)}] \otimes \mathbb{Y}_6[\mathbb{Q}_0^{(b,A')}]$

No. 25 $\hat{\mathbb{Q}}_0^{(A')}(1,1)$ $[\mathrm{M}_1, \mathrm{B}_3]$

$\hat{\mathbb{Z}}_{25} = \mathbb{X}_3[\mathbb{Q}_0^{(a,A')}(1,1)] \otimes \mathbb{Y}_6[\mathbb{Q}_0^{(b,A')}]$

No. 26 $\hat{\mathbb{Q}}_2^{(A',3)}(1,-1)$ $[\mathrm{M}_1, \mathrm{B}_3]$

$\hat{\mathbb{Z}}_{26} = \mathbb{X}_4[\mathbb{Q}_2^{(a,A',3)}(1,-1)] \otimes \mathbb{Y}_6[\mathbb{Q}_0^{(b,A')}]$

No. 27 $\hat{\mathbb{G}}_1^{(A')}(1,1)$ $[\mathrm{M}_1, \mathrm{B}_3]$

$\hat{\mathbb{Z}}_{27} = \mathbb{X}_7[\mathbb{M}_1^{(a,A')}(1,1)] \otimes \mathbb{Y}_7[\mathbb{T}_0^{(b,A')}]$

No. 28 $\hat{\mathbb{G}}_1^{(A')}(1,-1)$ $[\mathrm{M}_1, \mathrm{B}_3]$

$\hat{\mathbb{Z}}_{28} = \mathbb{X}_8[\mathbb{M}_1^{(a,A')}(1,-1)] \otimes \mathbb{Y}_7[\mathbb{T}_0^{(b,A')}]$

No. 29 $\hat{\mathbb{G}}_3^{(A',1)}(1,-1)$ $[\mathrm{M}_1, \mathrm{B}_3]$

$\hat{\mathbb{Z}}_{29} = \mathbb{X}_9[\mathbb{M}_3^{(a,A',1)}(1,-1)] \otimes \mathbb{Y}_7[\mathbb{T}_0^{(b,A')}]$

No. 30 $\hat{\mathbb{G}}_3^{(A',2)}(1,-1)$ $[\mathrm{M}_1, \mathrm{B}_3]$

$\hat{\mathbb{Z}}_{30} = \mathbb{X}_{10}[\mathbb{M}_3^{(a,A',2)}(1,-1)] \otimes \mathbb{Y}_7[\mathbb{T}_0^{(b,A')}]$

No. 31 $\hat{\mathbb{Q}}_0^{(A')}$ $[\mathrm{M}_1, \mathrm{B}_4]$

$\hat{\mathbb{Z}}_{31} = \mathbb{X}_1[\mathbb{Q}_0^{(a,A')}] \otimes \mathbb{Y}_8[\mathbb{Q}_0^{(b,A')}]$

No. 32 $\hat{\mathbb{Q}}_2^{(A',2)}$ $[\mathrm{M}_1, \mathrm{B}_4]$

$\hat{\mathbb{Z}}_{32} = \mathbb{X}_2[\mathbb{Q}_2^{(a,A',2)}] \otimes \mathbb{Y}_8[\mathbb{Q}_0^{(b,A')}]$

No. 33 $\hat{\mathbb{Q}}_0^{(A')}(1,1)$ $[\mathrm{M}_1, \mathrm{B}_4]$

$\hat{\mathbb{Z}}_{33} = \mathbb{X}_3[\mathbb{Q}_0^{(a,A')}(1,1)] \otimes \mathbb{Y}_8[\mathbb{Q}_0^{(b,A')}]$

No. 34 $\hat{\mathbb{Q}}_2^{(A',3)}(1,-1)$ $[\mathrm{M}_1, \mathrm{B}_4]$

$\hat{\mathbb{Z}}_{34} = \mathbb{X}_4[\mathbb{Q}_2^{(a,A',3)}(1,-1)] \otimes \mathbb{Y}_8[\mathbb{Q}_0^{(b,A')}]$

No. 35 $\hat{\mathbb{G}}_1^{(A')}(1,1)$ $[\mathrm{M}_1, \mathrm{B}_4]$

$\hat{\mathbb{Z}}_{35} = \mathbb{X}_7[\mathbb{M}_1^{(a,A')}(1,1)] \otimes \mathbb{Y}_9[\mathbb{T}_0^{(b,A')}]$

No. 36 $\hat{\mathbb{G}}_1^{(A')}(1,-1)$ $[\mathrm{M}_1, \mathrm{B}_4]$

$\hat{\mathbb{Z}}_{36} = \mathbb{X}_8[\mathbb{M}_1^{(a,A')}(1,-1)] \otimes \mathbb{Y}_9[\mathbb{T}_0^{(b,A')}]$

No. 37 $\hat{\mathbb{G}}_3^{(A',1)}(1,-1)$ $[\mathrm{M}_1, \mathrm{B}_4]$

$\hat{\mathbb{Z}}_{37} = \mathbb{X}_9[\mathbb{M}_3^{(a,A',1)}(1,-1)] \otimes \mathbb{Y}_9[\mathbb{T}_0^{(b,A')}]$

No. 38 $\hat{\mathbb{G}}_3^{(A',2)}(1,-1)$ $[\mathrm{M}_1, \mathrm{B}_4]$

$\hat{\mathbb{Z}}_{38} = \mathbb{X}_{10}[\mathbb{M}_3^{(a,A',2)}(1,-1)] \otimes \mathbb{Y}_9[\mathbb{T}_0^{(b,A')}]$

No. 39 $\hat{\mathbb{Q}}_0^{(A')}$ $[\mathrm{M}_1, \mathrm{B}_5]$

$\hat{\mathbb{Z}}_{39} = \mathbb{X}_1[\mathbb{Q}_0^{(a,A')}] \otimes \mathbb{Y}_{10}[\mathbb{Q}_0^{(b,A')}]$

No. 40 $\hat{\mathbb{Q}}_2^{(A',2)}$ $[\mathrm{M}_1, \mathrm{B}_5]$

$\hat{\mathbb{Z}}_{40} = \mathbb{X}_2[\mathbb{Q}_2^{(a,A',2)}] \otimes \mathbb{Y}_{10}[\mathbb{Q}_0^{(b,A')}]$

No. 41 $\hat{\mathbb{Q}}_1^{(A',1)}$ $[\mathrm{M}_1, \mathrm{B}_5]$

$\hat{\mathbb{Z}}_{41} = \mathbb{X}_5[\mathbb{Q}_2^{(a,A'',2)}] \otimes \mathbb{Y}_{11}[\mathbb{Q}_1^{(b,A'')}]$

No. 42 $\hat{\mathbb{Q}}_0^{(A')}(1,1)$ $[\mathrm{M}_1, \mathrm{B}_5]$

$\hat{\mathbb{Z}}_{42} = \mathbb{X}_3[\mathbb{Q}_0^{(a,A')}(1,1)] \otimes \mathbb{Y}_{10}[\mathbb{Q}_0^{(b,A')}]$

No. 43 $\hat{\mathbb{Q}}_2^{(A',3)}(1,-1)$ $[\mathrm{M}_1, \mathrm{B}_5]$

$\hat{\mathbb{Z}}_{43} = \mathbb{X}_4[\mathbb{Q}_2^{(a,A',3)}(1,-1)] \otimes \mathbb{Y}_{10}[\mathbb{Q}_0^{(b,A')}]$

No. 44 $\hat{\mathbb{Q}}_1^{(A',2)}(1,-1)$ $[\mathrm{M}_1, \mathrm{B}_5]$

$\hat{\mathbb{Z}}_{44} = \mathbb{X}_6[\mathbb{Q}_2^{(a,A'',1)}(1,-1)] \otimes \mathbb{Y}_{11}[\mathbb{Q}_1^{(b,A'')}]$

No. 45 $\hat{\mathbb{G}}_1^{(A')}(1,1)$ $[\mathrm{M}_1, \mathrm{B}_5]$

$\hat{\mathbb{Z}}_{45} = \mathbb{X}_7[\mathbb{M}_1^{(a,A')}(1,1)] \otimes \mathbb{Y}_{12}[\mathbb{T}_0^{(b,A')}]$

No. 46 $\hat{\mathbb{Q}}_1^{(A',1)}(1,1)$ $[\mathrm{M}_1, \mathrm{B}_5]$

$\hat{\mathbb{Z}}_{46} = -\mathbb{X}_{12}[\mathbb{M}_1^{(a,A'',2)}(1,1)] \otimes \mathbb{Y}_{13}[\mathbb{T}_1^{(b,A'')}]$

No. 47 $\hat{\mathbb{Q}}_1^{(A',2)}(1,1)$ $[\mathrm{M}_1, \mathrm{B}_5]$

$\hat{\mathbb{Z}}_{47} = \mathbb{X}_{11}[\mathbb{M}_1^{(a,A'',1)}(1,1)] \otimes \mathbb{Y}_{13}[\mathbb{T}_1^{(b,A'')}]$

No. 48 $\hat{\mathbb{G}}_1^{(A')}(1,-1)$ $[\mathrm{M}_1, \mathrm{B}_5]$

$\hat{\mathbb{Z}}_{48} = \mathbb{X}_{8}[\mathbb{M}_1^{(a,A')}(1,-1)] \otimes \mathbb{Y}_{12}[\mathbb{T}_0^{(b,A')}]$

No. 49 $\hat{\mathbb{Q}}_1^{(A',2)}(1,-1)$ $[\mathrm{M}_1, \mathrm{B}_5]$

$\hat{\mathbb{Z}}_{49} = \mathbb{X}_{13}[\mathbb{M}_1^{(a,A'',1)}(1,-1)] \otimes \mathbb{Y}_{13}[\mathbb{T}_1^{(b,A'')}]$

No. 50 $\hat{\mathbb{G}}_3^{(A',1)}(1,-1)$ $[\mathrm{M}_1, \mathrm{B}_5]$

$\hat{\mathbb{Z}}_{50} = \mathbb{X}_{9}[\mathbb{M}_3^{(a,A',1)}(1,-1)] \otimes \mathbb{Y}_{12}[\mathbb{T}_0^{(b,A')}]$

No. 51 $\hat{\mathbb{G}}_3^{(A',2)}(1,-1)$ $[\mathrm{M}_1, \mathrm{B}_5]$

$\hat{\mathbb{Z}}_{51} = \mathbb{X}_{10}[\mathbb{M}_3^{(a,A',2)}(1,-1)] \otimes \mathbb{Y}_{12}[\mathbb{T}_0^{(b,A')}]$

No. 52 $\hat{\mathbb{G}}_2^{(A',1)}(1,-1)$ $[\mathrm{M}_1, \mathrm{B}_5]$

$\hat{\mathbb{Z}}_{52} = -\mathbb{X}_{15}[\mathbb{M}_3^{(a,A'',4)}(1,-1)] \otimes \mathbb{Y}_{13}[\mathbb{T}_1^{(b,A'')}]$

No. 53 $\hat{\mathbb{G}}_2^{(A',2)}(1,-1)$ $[\mathrm{M}_1, \mathrm{B}_5]$

$\hat{\mathbb{Z}}_{53} = -\mathbb{X}_{14}[\mathbb{M}_3^{(a,A'',1)}(1,-1)] \otimes \mathbb{Y}_{13}[\mathbb{T}_1^{(b,A'')}]$

No. 54 $\hat{\mathbb{Q}}_1^{(A',1)}$ $[\mathrm{M}_1, \mathrm{B}_5]$

$\hat{\mathbb{Z}}_{54} = -\mathbb{X}_{16}[\mathbb{M}_1^{(a,A'',2)}] \otimes \mathbb{Y}_{13}[\mathbb{T}_1^{(b,A'')}]$

No. 55 $\hat{\mathbb{Q}}_0^{(A')}$ $[\mathrm{M}_1, \mathrm{B}_6]$

$\hat{\mathbb{Z}}_{55} = \mathbb{X}_1[\mathbb{Q}_0^{(a,A')}] \otimes \mathbb{Y}_{14}[\mathbb{Q}_0^{(b,A')}]$

No. 56 $\hat{\mathbb{Q}}_2^{(A',2)}$ $[\mathrm{M}_1, \mathrm{B}_6]$

$\hat{\mathbb{Z}}_{56} = \mathbb{X}_2[\mathbb{Q}_2^{(a,A',2)}] \otimes \mathbb{Y}_{14}[\mathbb{Q}_0^{(b,A')}]$

No. 57 $\hat{\mathbb{Q}}_1^{(A',1)}$ $[\mathrm{M}_1, \mathrm{B}_6]$

$\hat{\mathbb{Z}}_{57} = \mathbb{X}_5[\mathbb{Q}_2^{(a,A'',2)}] \otimes \mathbb{Y}_{15}[\mathbb{Q}_1^{(b,A'')}]$

No. 58 $\hat{\mathbb{Q}}_0^{(A')}(1,1)$ $[\mathrm{M}_1, \mathrm{B}_6]$

$\hat{\mathbb{Z}}_{58} = \mathbb{X}_3[\mathbb{Q}_0^{(a,A')}(1,1)] \otimes \mathbb{Y}_{14}[\mathbb{Q}_0^{(b,A')}]$

No. 59 $\hat{\mathbb{Q}}_2^{(A',3)}(1,-1)$ $[\mathrm{M}_1, \mathrm{B}_6]$

$\hat{\mathbb{Z}}_{59} = \mathbb{X}_4[\mathbb{Q}_2^{(a,A',3)}(1,-1)] \otimes \mathbb{Y}_{14}[\mathbb{Q}_0^{(b,A')}]$

No. 60 $\hat{\mathbb{Q}}_1^{(A',2)}(1,-1)$ $[\mathrm{M}_1, \mathrm{B}_6]$

$\hat{\mathbb{Z}}_{60} = \mathbb{X}_6[\mathbb{Q}_2^{(a,A'',1)}(1,-1)] \otimes \mathbb{Y}_{15}[\mathbb{Q}_1^{(b,A'')}]$

No. 61 $\hat{\mathbb{G}}_1^{(A')}(1,1)$ $[\mathrm{M}_1, \mathrm{B}_6]$

$\hat{\mathbb{Z}}_{61} = \mathbb{X}_7[\mathbb{M}_1^{(a,A')}(1,1)] \otimes \mathbb{Y}_{16}[\mathbb{T}_0^{(b,A')}]$

No. 62 $\hat{\mathbb{Q}}_1^{(A',1)}(1,1)$ $[\mathrm{M}_1, \mathrm{B}_6]$

$\hat{\mathbb{Z}}_{62} = -\mathbb{X}_{12}[\mathbb{M}_1^{(a,A'',2)}(1,1)] \otimes \mathbb{Y}_{17}[\mathbb{T}_1^{(b,A'')}]$

No. 63 $\hat{\mathbb{Q}}_1^{(A',2)}(1,1)$ $[\mathrm{M}_1, \mathrm{B}_6]$

$\hat{\mathbb{Z}}_{63} = \mathbb{X}_{11}[\mathbb{M}_1^{(a,A'',1)}(1,1)] \otimes \mathbb{Y}_{17}[\mathbb{T}_1^{(b,A'')}]$

No. 64 $\hat{\mathbb{G}}_1^{(A')}(1,-1)\ [\mathrm{M}_1,\mathrm{B}_6]$

$\hat{\mathbb{Z}}_{64} = \mathbb{X}_8[\mathbb{M}_1^{(a,A')}(1,-1)] \otimes \mathbb{Y}_{16}[\mathbb{T}_0^{(b,A')}]$

No. 65 $\hat{\mathbb{Q}}_1^{(A',2)}(1,-1)\ [\mathrm{M}_1,\mathrm{B}_6]$

$\hat{\mathbb{Z}}_{65} = \mathbb{X}_{13}[\mathbb{M}_1^{(a,A'',1)}(1,-1)] \otimes \mathbb{Y}_{17}[\mathbb{T}_1^{(b,A'')}]$

No. 66 $\hat{\mathbb{G}}_3^{(A',1)}(1,-1)\ [\mathrm{M}_1,\mathrm{B}_6]$

$\hat{\mathbb{Z}}_{66} = \mathbb{X}_9[\mathbb{M}_3^{(a,A',1)}(1,-1)] \otimes \mathbb{Y}_{16}[\mathbb{T}_0^{(b,A')}]$

No. 67 $\hat{\mathbb{G}}_3^{(A',2)}(1,-1)\ [\mathrm{M}_1,\mathrm{B}_6]$

$\hat{\mathbb{Z}}_{67} = \mathbb{X}_{10}[\mathbb{M}_3^{(a,A',2)}(1,-1)] \otimes \mathbb{Y}_{16}[\mathbb{T}_0^{(b,A')}]$

No. 68 $\hat{\mathbb{G}}_2^{(A',1)}(1,-1)\ [\mathrm{M}_1,\mathrm{B}_6]$

$\hat{\mathbb{Z}}_{68} = -\mathbb{X}_{15}[\mathbb{M}_3^{(a,A'',4)}(1,-1)] \otimes \mathbb{Y}_{17}[\mathbb{T}_1^{(b,A'')}]$

No. 69 $\hat{\mathbb{G}}_2^{(A',2)}(1,-1)\ [\mathrm{M}_1,\mathrm{B}_6]$

$\hat{\mathbb{Z}}_{69} = -\mathbb{X}_{14}[\mathbb{M}_3^{(a,A'',1)}(1,-1)] \otimes \mathbb{Y}_{17}[\mathbb{T}_1^{(b,A'')}]$

No. 70 $\hat{\mathbb{Q}}_1^{(A',1)}\ [\mathrm{M}_1,\mathrm{B}_6]$

$\hat{\mathbb{Z}}_{70} = -\mathbb{X}_{16}[\mathbb{M}_1^{(a,A'',2)}] \otimes \mathbb{Y}_{17}[\mathbb{T}_1^{(b,A'')}]$

No. 71 $\hat{\mathbb{Q}}_0^{(A')}\ [\mathrm{M}_1,\mathrm{B}_7]$

$\hat{\mathbb{Z}}_{71} = \mathbb{X}_1[\mathbb{Q}_0^{(a,A')}] \otimes \mathbb{Y}_{18}[\mathbb{Q}_0^{(b,A')}]$

No. 72 $\hat{\mathbb{Q}}_2^{(A',2)}\ [\mathrm{M}_1,\mathrm{B}_7]$

$\hat{\mathbb{Z}}_{72} = \mathbb{X}_2[\mathbb{Q}_2^{(a,A',2)}] \otimes \mathbb{Y}_{18}[\mathbb{Q}_0^{(b,A')}]$

No. 73 $\hat{\mathbb{Q}}_0^{(A')}(1,1)$ $[\mathrm{M}_1, \mathrm{B}_7]$

$\hat{\mathbb{Z}}_{73} = \mathbb{X}_3[\mathbb{Q}_0^{(a,A')}(1,1)] \otimes \mathbb{Y}_{18}[\mathbb{Q}_0^{(b,A')}]$

No. 74 $\hat{\mathbb{Q}}_2^{(A',3)}(1,-1)$ $[\mathrm{M}_1, \mathrm{B}_7]$

$\hat{\mathbb{Z}}_{74} = \mathbb{X}_4[\mathbb{Q}_2^{(a,A',3)}(1,-1)] \otimes \mathbb{Y}_{18}[\mathbb{Q}_0^{(b,A')}]$

No. 75 $\hat{\mathbb{G}}_1^{(A')}(1,1)$ $[\mathrm{M}_1, \mathrm{B}_7]$

$\hat{\mathbb{Z}}_{75} = \mathbb{X}_7[\mathbb{M}_1^{(a,A')}(1,1)] \otimes \mathbb{Y}_{19}[\mathbb{T}_0^{(b,A')}]$

No. 76 $\hat{\mathbb{G}}_1^{(A')}(1,-1)$ $[\mathrm{M}_1, \mathrm{B}_7]$

$\hat{\mathbb{Z}}_{76} = \mathbb{X}_8[\mathbb{M}_1^{(a,A')}(1,-1)] \otimes \mathbb{Y}_{19}[\mathbb{T}_0^{(b,A')}]$

No. 77 $\hat{\mathbb{G}}_3^{(A',1)}(1,-1)$ $[\mathrm{M}_1, \mathrm{B}_7]$

$\hat{\mathbb{Z}}_{77} = \mathbb{X}_9[\mathbb{M}_3^{(a,A',1)}(1,-1)] \otimes \mathbb{Y}_{19}[\mathbb{T}_0^{(b,A')}]$

No. 78 $\hat{\mathbb{G}}_3^{(A',2)}(1,-1)$ $[\mathrm{M}_1, \mathrm{B}_7]$

$\hat{\mathbb{Z}}_{78} = \mathbb{X}_{10}[\mathbb{M}_3^{(a,A',2)}(1,-1)] \otimes \mathbb{Y}_{19}[\mathbb{T}_0^{(b,A')}]$

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
$\mathbb{X}_1$	$\mathbb{Q}_0^{(a,A')}$	M_1	$\begin{pmatrix} \frac{1}{2} & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 \\ 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & \frac{1}{2} \end{pmatrix}$
$\mathbb{X}_2$	$\mathbb{Q}_2^{(a,A',2)}$	M_1	$\begin{pmatrix} \frac{1}{2} & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 \\ 0 & 0 & -\frac{1}{2} & 0 \\ 0 & 0 & 0 & -\frac{1}{2} \end{pmatrix}$
$\mathbb{X}_3$	$\mathbb{Q}_0^{(a,A')}(1,1)$	M_1	$\begin{pmatrix} 0 & 0 & -\frac{i}{2} & 0 \\ 0 & 0 & 0 & \frac{i}{2} \\ \frac{i}{2} & 0 & 0 & 0 \\ 0 & -\frac{i}{2} & 0 & 0 \end{pmatrix}$
$\mathbb{X}_4$	$\mathbb{Q}_2^{(a,A',3)}(1,-1)$	M_1	$\begin{pmatrix} 0 & 0 & 0 & -\frac{i}{2} \\ 0 & 0 & -\frac{i}{2} & 0 \\ 0 & \frac{i}{2} & 0 & 0 \\ \frac{i}{2} & 0 & 0 & 0 \end{pmatrix}$
$\mathbb{X}_5$	$\mathbb{Q}_2^{(a,A'',2)}$	M_1	$\begin{pmatrix} 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & \frac{1}{2} \\ \frac{1}{2} & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 \end{pmatrix}$
$\mathbb{X}_6$	$\mathbb{Q}_2^{(a,A'',1)}(1,-1)$	M_1	$\begin{pmatrix} 0 & 0 & 0 & -\frac{1}{2} \\ 0 & 0 & \frac{1}{2} & 0 \\ 0 & \frac{1}{2} & 0 & 0 \\ -\frac{1}{2} & 0 & 0 & 0 \end{pmatrix}$
$\mathbb{X}_7$	$\mathbb{M}_1^{(a,A')}(1,1)$	M_1	$\begin{pmatrix} 0 & \frac{\sqrt{19}i}{19} & 0 & \frac{3\sqrt{19}}{38} \\ -\frac{\sqrt{19}i}{19} & 0 & \frac{3\sqrt{19}}{38} & 0 \\ 0 & \frac{3\sqrt{19}}{38} & 0 & -\frac{2\sqrt{19}i}{19} \\ \frac{3\sqrt{19}}{38} & 0 & \frac{2\sqrt{19}i}{19} & 0 \end{pmatrix}$
$\mathbb{X}_8$	$\mathbb{M}_1^{(a,A')}(1,-1)$	M_1	$\begin{pmatrix} 0 & -\frac{7\sqrt{38}i}{76} & 0 & -\frac{\sqrt{38}}{76} \\ \frac{7\sqrt{38}i}{76} & 0 & -\frac{\sqrt{38}}{76} & 0 \\ 0 & -\frac{\sqrt{38}}{76} & 0 & -\frac{5\sqrt{38}i}{76} \\ -\frac{\sqrt{38}}{76} & 0 & \frac{5\sqrt{38}i}{76} & 0 \end{pmatrix}$

continued ...

Table 6

symbol	type	group	form
$\mathbb{X}_9$	$\mathbb{M}_3^{(a,A',1)}(1,-1)$	M_1	$\begin{pmatrix} 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & -\frac{1}{2} \\ \frac{1}{2} & 0 & 0 & 0 \\ 0 & -\frac{1}{2} & 0 & 0 \end{pmatrix}$
$\mathbb{X}_{10}$	$\mathbb{M}_3^{(a,A',2)}(1,-1)$	M_1	$\begin{pmatrix} 0 & \frac{\sqrt{2}i}{4} & 0 & -\frac{\sqrt{2}}{4} \\ -\frac{\sqrt{2}i}{4} & 0 & -\frac{\sqrt{2}}{4} & 0 \\ 0 & -\frac{\sqrt{2}}{4} & 0 & -\frac{\sqrt{2}i}{4} \\ -\frac{\sqrt{2}}{4} & 0 & \frac{\sqrt{2}i}{4} & 0 \end{pmatrix}$
$\mathbb{X}_{11}$	$\mathbb{M}_1^{(a,A'',1)}(1,1)$	M_1	$\begin{pmatrix} 0 & \frac{2\sqrt{19}}{19} & 0 & -\frac{3\sqrt{19}i}{38} \\ \frac{2\sqrt{19}}{19} & 0 & \frac{3\sqrt{19}i}{38} & 0 \\ 0 & -\frac{3\sqrt{19}i}{38} & 0 & -\frac{\sqrt{19}}{19} \\ \frac{3\sqrt{19}i}{38} & 0 & -\frac{\sqrt{19}}{19} & 0 \end{pmatrix}$
$\mathbb{X}_{12}$	$\mathbb{M}_1^{(a,A'',2)}(1,1)$	M_1	$\begin{pmatrix} -\frac{1}{2} & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 \\ 0 & 0 & -\frac{1}{2} & 0 \\ 0 & 0 & 0 & \frac{1}{2} \end{pmatrix}$
$\mathbb{X}_{13}$	$\mathbb{M}_1^{(a,A'',1)}(1,-1)$	M_1	$\begin{pmatrix} 0 & \frac{5\sqrt{38}}{76} & 0 & \frac{\sqrt{38}i}{76} \\ \frac{5\sqrt{38}}{76} & 0 & -\frac{\sqrt{38}i}{76} & 0 \\ 0 & \frac{\sqrt{38}i}{76} & 0 & \frac{7\sqrt{38}}{76} \\ -\frac{\sqrt{38}i}{76} & 0 & \frac{7\sqrt{38}}{76} & 0 \end{pmatrix}$
$\mathbb{X}_{14}$	$\mathbb{M}_3^{(a,A'',1)}(1,-1)$	M_1	$\begin{pmatrix} 0 & \frac{\sqrt{2}}{4} & 0 & \frac{\sqrt{2}i}{4} \\ \frac{\sqrt{2}}{4} & 0 & -\frac{\sqrt{2}i}{4} & 0 \\ 0 & \frac{\sqrt{2}i}{4} & 0 & -\frac{\sqrt{2}}{4} \\ -\frac{\sqrt{2}i}{4} & 0 & -\frac{\sqrt{2}}{4} & 0 \end{pmatrix}$
$\mathbb{X}_{15}$	$\mathbb{M}_3^{(a,A'',4)}(1,-1)$	M_1	$\begin{pmatrix} \frac{1}{2} & 0 & 0 & 0 \\ 0 & -\frac{1}{2} & 0 & 0 \\ 0 & 0 & -\frac{1}{2} & 0 \\ 0 & 0 & 0 & \frac{1}{2} \end{pmatrix}$
$\mathbb{X}_{16}$	$\mathbb{M}_1^{(a,A'',2)}$	M_1	$\begin{pmatrix} 0 & 0 & -\frac{i}{2} & 0 \\ 0 & 0 & 0 & -\frac{i}{2} \\ \frac{i}{2} & 0 & 0 & 0 \\ 0 & \frac{i}{2} & 0 & 0 \end{pmatrix}$

Table 7: Cluster SAMB.

symbol	type	cluster	form
$\mathbb{Y}_1$	$\mathbb{Q}_0^{(s,A')}$	S_1	$\begin{pmatrix}1\end{pmatrix}$
$\mathbb{Y}_2$	$\mathbb{Q}_0^{(b,A')}$	B_1	$\begin{pmatrix}1\end{pmatrix}$
$\mathbb{Y}_3$	$\mathbb{T}_1^{(b,A'')}$	B_1	$\begin{pmatrix}i\end{pmatrix}$
$\mathbb{Y}_4$	$\mathbb{Q}_0^{(b,A')}$	B_2	$\begin{pmatrix}1\end{pmatrix}$
$\mathbb{Y}_5$	$\mathbb{T}_0^{(b,A')}$	B_2	$\begin{pmatrix}i\end{pmatrix}$
$\mathbb{Y}_6$	$\mathbb{Q}_0^{(b,A')}$	B_3	$\begin{pmatrix}1\end{pmatrix}$
$\mathbb{Y}_7$	$\mathbb{T}_0^{(b,A')}$	B_3	$\begin{pmatrix}i\end{pmatrix}$
$\mathbb{Y}_8$	$\mathbb{Q}_0^{(b,A')}$	B_4	$\begin{pmatrix}1\end{pmatrix}$
$\mathbb{Y}_9$	$\mathbb{T}_0^{(b,A')}$	B_4	$\begin{pmatrix}i\end{pmatrix}$
$\mathbb{Y}_{10}$	$\mathbb{Q}_0^{(b,A')}$	B_5	$\begin{pmatrix}\frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2}\end{pmatrix}$
$\mathbb{Y}_{11}$	$\mathbb{Q}_1^{(b,A'')}$	B_5	$\begin{pmatrix}\frac{\sqrt{2}}{2} & -\frac{\sqrt{2}}{2}\end{pmatrix}$
$\mathbb{Y}_{12}$	$\mathbb{T}_0^{(b,A')}$	B_5	$\begin{pmatrix}\frac{\sqrt{2}i}{2} & \frac{\sqrt{2}i}{2}\end{pmatrix}$
$\mathbb{Y}_{13}$	$\mathbb{T}_1^{(b,A'')}$	B_5	$\begin{pmatrix}\frac{\sqrt{2}i}{2} & -\frac{\sqrt{2}i}{2}\end{pmatrix}$
$\mathbb{Y}_{14}$	$\mathbb{Q}_0^{(b,A')}$	B_6	$\begin{pmatrix}\frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2}\end{pmatrix}$
$\mathbb{Y}_{15}$	$\mathbb{Q}_1^{(b,A'')}$	B_6	$\begin{pmatrix}\frac{\sqrt{2}}{2} & -\frac{\sqrt{2}}{2}\end{pmatrix}$
$\mathbb{Y}_{16}$	$\mathbb{T}_0^{(b,A')}$	B_6	$\begin{pmatrix}\frac{\sqrt{2}i}{2} & \frac{\sqrt{2}i}{2}\end{pmatrix}$
$\mathbb{Y}_{17}$	$\mathbb{T}_1^{(b,A'')}$	B_6	$\begin{pmatrix}\frac{\sqrt{2}i}{2} & -\frac{\sqrt{2}i}{2}\end{pmatrix}$
$\mathbb{Y}_{18}$	$\mathbb{Q}_0^{(b,A')}$	B_7	$\begin{pmatrix}1\end{pmatrix}$
$\mathbb{Y}_{19}$	$\mathbb{T}_0^{(b,A')}$	B_7	$\begin{pmatrix}i\end{pmatrix}$

Table 8: Polar harmonics.

No.	symbol	rank	irrep.	mul.	comp.	form
1	$\mathbb{Q}_0^{(A')}$	0	A'	–	–	1
2	$\mathbb{Q}_1^{(A'')}$	1	A''	–	–	y
3	$\mathbb{Q}_2^{(A'',1)}$	2	A''	1	–	$\sqrt{3}yz$
4	$\mathbb{Q}_2^{(A'',2)}$	2	A''	2	–	$\sqrt{3}xy$
5	$\mathbb{Q}_2^{(A',2)}$	2	A'	2	–	$\frac{\sqrt{3}(x-y)(x+y)}{2}$
6	$\mathbb{Q}_2^{(A',3)}$	2	A'	3	–	$\sqrt{3}xz$

Table 9: Axial harmonics.

No.	symbol	rank	irrep.	mul.	comp.	form
1	$\mathbb{G}_1^{(A'',1)}$	1	A''	1	–	X
2	$\mathbb{G}_1^{(A'',2)}$	1	A''	2	–	Z
3	$\mathbb{G}_1^{(A')}$	1	A'	–	–	Y
4	$\mathbb{G}_3^{(A'',1)}$	3	A''	1	–	$\frac{X\left(2X^2-3Y^2-3Z^2\right)}{2}$
5	$\mathbb{G}_3^{(A'',4)}$	3	A''	4	–	$\frac{\sqrt{15}Z(X-Y)(X+Y)}{2}$
6	$\mathbb{G}_3^{(A',1)}$	3	A'	1	–	$\sqrt{15}XYZ$
7	$\mathbb{G}_3^{(A',2)}$	3	A'	2	–	$-\frac{Y\left(3X^2-2Y^2+3Z^2\right)}{2}$

- Group info.: Generator = $\{\mathrm{m}_{010}|0\}$

Table 10: Conjugacy class (point-group part).

rep. SO	symmetry operations
$\{1\|0\}$	$\{1\|0\}$
$\{\mathrm{m}_{010}\|0\}$	$\{\mathrm{m}_{010}\|0\}$

Table 11: Symmetry operations.

	No.	SO	No.	SO	No.	SO	No.	SO	No.	SO
	1	$\{1\|0\}$	2	$\{\mathrm{m}_{010}\|0\}$						

Table 12: Character table (point-group part).

		1	m_{010}
A'		1	1
A''		1	-1

Table 13: Parity conversion.

$\leftrightarrow$	$\leftrightarrow$
A' (A'')	A'' (A')

Table 14: Symmetric product, $[\Gamma \otimes \Gamma']_+$.

	A'	A''
A'	A'	A''
A''		A'

Table 15: Anti-symmetric product, $[\Gamma \otimes \Gamma]_-$.

	A'	A''
	$-$	$-$

Table 16: Virtual-cluster sites.

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

Table 17: Virtual-cluster basis.

symbol	1	2
$\mathbb{Q}_0^{(A')}$	$\frac{\sqrt{2}}{2}$	$\frac{\sqrt{2}}{2}$
$\mathbb{Q}_1^{(A'')}$	$\frac{\sqrt{2}}{2}$	$-\frac{\sqrt{2}}{2}$