SAMB for "C3h"

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• Generation condition

model type: tight_bindingtime-reversal type: electric

irrep: [A']spinful

• Kets: dimension = 32

Table 1: Hilbert space for full matrix.

No.	ket								
1	(s,\uparrow) @H1 ₁	2	(s,\downarrow) @H1 ₁	3	(s,\uparrow) @O ₁	4	(s,\downarrow) @O ₁	5	(p_x,\uparrow) @O ₁
6	(p_x,\downarrow) @O ₁	7	(p_y,\uparrow) @ \mathcal{O}_1	8	(p_y,\downarrow) @O ₁	9	(p_z,\uparrow) @ \mathcal{O}_1	10	(p_z,\downarrow) @O ₁
11	(s,\uparrow) @ O_2	12	(s,\downarrow) @O ₂	13	(p_x,\uparrow) @ O_2	14	(p_x,\downarrow) @ O_2	15	(p_y,\uparrow) @ O_2
16	(p_y,\downarrow) @O ₂	17	(p_z,\uparrow) @ \mathcal{O}_2	18	(p_z,\downarrow) @ O_2	19	(s,\uparrow) @O ₃	20	(s,\downarrow) @O ₃
21	(p_x,\uparrow) @O ₃	22	(p_x,\downarrow) @O ₃	23	(p_y,\uparrow) @O ₃	24	(p_y,\downarrow) @O ₃	25	(p_z,\uparrow) @O ₃
26	(p_z,\downarrow) @O ₃	27	(s,\uparrow) @H2 ₁	28	(s,\downarrow) @H2 ₁	29	(s,\uparrow) @ $\mathrm{H2}_2$	30	(s,\downarrow) @H2 ₂
31	(s,\uparrow) @H2 ₃	32	(s,\downarrow) @H2 ₃						

 $\bullet~$ Sites in (primitive) unit cell:

Table 2: Site-clusters.

	site	position	mapping
S_1	$H1_1$	$\begin{pmatrix} 0 & 0 & 0 \end{pmatrix}$	[1,2,3,4,5,6]
S_2	O_1	$\begin{pmatrix} \frac{1}{3} & 0 & 0 \end{pmatrix}$	[1,4]
	O_2	$\left(0 \frac{1}{3} 0\right)$	[2,6]
	O_3	$\left(-\frac{1}{3} -\frac{1}{3} 0 \right)$	[3,5]
S_3	$H2_1$	$\begin{pmatrix} \frac{1}{2} & \frac{1}{6} & 0 \end{pmatrix}$	[1,4]
	$H2_2$	$\begin{pmatrix} -\frac{1}{6} & \frac{1}{3} & 0 \end{pmatrix}$	[2,6]
	$H2_3$	$\begin{pmatrix} -\frac{1}{3} & -\frac{1}{2} & 0 \end{pmatrix}$	[3,5]

• Bonds in (primitive) unit cell:

Table 3: Bond-clusters.

	bond	tail	head	n	#	b@c	mapping
B_1	b_1	O_1	$H1_1$	1	1	$\begin{pmatrix} \frac{1}{3} & 0 & 0 \end{pmatrix} @ \begin{pmatrix} \frac{1}{6} & 0 & 0 \end{pmatrix}$	[1,4]
	b_2	O_2	$H1_1$	1	1	$\left(0 \frac{1}{3} 0\right) @ \left(0 \frac{1}{6} 0\right)$	[2,6]
	b_3	O_3	$H1_1$	1	1	$\left(-\frac{1}{3} -\frac{1}{3} 0 \right) @ \left(-\frac{1}{6} -\frac{1}{6} 0 \right)$	[3,5]
B_2	b_4	H2 ₁	O_1	1	1	$\begin{pmatrix} \frac{1}{6} & \frac{1}{6} & 0 \end{pmatrix} @ \begin{pmatrix} \frac{5}{12} & \frac{1}{12} & 0 \end{pmatrix}$	[1,4]
	b_5	$H2_2$	O_2	1	1	$\begin{pmatrix} -\frac{1}{6} & 0 & 0 \end{pmatrix} @ \begin{pmatrix} -\frac{1}{12} & \frac{1}{3} & 0 \end{pmatrix}$	[2,6]
	b_6	$H2_3$	O_3	1	1	$\left(0 -\frac{1}{6} 0\right) @ \left(-\frac{1}{3} -\frac{5}{12} 0\right)$	[3,5]

• SAMB:

$$\begin{split} & \boxed{ \text{No. 1} } \quad \hat{\mathbb{Q}}_0^{(A')} \ [M_1, S_1] \\ \\ \hat{\mathbb{Z}}_1 &= \mathbb{X}_1[\mathbb{Q}_0^{(a,A')}] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A')}] \end{split}$$

No. 2
$$\hat{\mathbb{Q}}_0^{(A')}$$
 [M₁, S₂]

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

No. 3
$$\hat{\mathbb{Q}}_0^{(A')}$$
 [M₂, S₂]

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

No. 4
$$\hat{\mathbb{G}}_1^{(A')}$$
 [M₂, S₂]

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

No. 5
$$\hat{\mathbb{Q}}_0^{(A')}(1,0) [M_2, S_2]$$

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

No. 6
$$\hat{\mathbb{G}}_1^{(A')}(1,0)$$
 [M₂, S₂]

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

No. 7
$$\hat{\mathbb{G}}_1^{(A')}(1,-1)$$
 [M₂, S₂]

$$\hat{\mathbb{Z}}_7 = \frac{\sqrt{2}\mathbb{X}_7[\mathbb{G}_{2,0}^{(a,E')}(1,-1)] \otimes \mathbb{U}_3[\mathbb{Q}_{1,0}^{(s,E')}]}{2} + \frac{\sqrt{2}\mathbb{X}_8[\mathbb{G}_{2,1}^{(a,E')}(1,-1)] \otimes \mathbb{U}_4[\mathbb{Q}_{1,1}^{(s,E')}]}{2}$$

No. 8
$$\hat{\mathbb{Q}}_2^{(A')}(1,-1)$$
 [M₂, S₂]

$$\hat{\mathbb{Z}}_8 = \frac{\sqrt{2}\mathbb{X}_7[\mathbb{G}_{2,0}^{(a,E')}(1,-1)] \otimes \mathbb{U}_4[\mathbb{Q}_{1,1}^{(s,E')}]}{2} - \frac{\sqrt{2}\mathbb{X}_8[\mathbb{G}_{2,1}^{(a,E')}(1,-1)] \otimes \mathbb{U}_3[\mathbb{Q}_{1,0}^{(s,E')}]}{2}$$

No. 9
$$\hat{\mathbb{Q}}_0^{(A')}$$
 [M₃, S₂]

$$\hat{\mathbb{Z}}_9 = \mathbb{X}_9[\mathbb{Q}_0^{(a,A')}] \otimes \mathbb{U}_2[\mathbb{Q}_0^{(s,A')}]$$

No. 10
$$\hat{\mathbb{Q}}_{2}^{(A')}$$
 [M₃, S₂]

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

No. 11
$$\hat{\mathbb{Q}}_3^{(A',1)}$$
 [M₃, S₂]

$$\hat{\mathbb{Z}}_{11} = \frac{\sqrt{2}\mathbb{X}_{14}[\mathbb{Q}_{2,0}^{(a,E')}] \otimes \mathbb{U}_{4}[\mathbb{Q}_{1,1}^{(s,E')}]}{2} - \frac{\sqrt{2}\mathbb{X}_{15}[\mathbb{Q}_{2,1}^{(a,E')}] \otimes \mathbb{U}_{3}[\mathbb{Q}_{1,0}^{(s,E')}]}{2}$$

No. 12
$$\hat{\mathbb{Q}}_3^{(A',2)}$$
 [M₃, S₂]

$$\hat{\mathbb{Z}}_{12} = \frac{\sqrt{2}\mathbb{X}_{14}[\mathbb{Q}_{2,0}^{(a,E')}] \otimes \mathbb{U}_{3}[\mathbb{Q}_{1,0}^{(s,E')}]}{2} + \frac{\sqrt{2}\mathbb{X}_{15}[\mathbb{Q}_{2,1}^{(a,E')}] \otimes \mathbb{U}_{4}[\mathbb{Q}_{1,1}^{(s,E')}]}{2}$$

No. 13
$$\hat{\mathbb{Q}}_0^{(A')}(1,1)$$
 [M₃, S₂]

$$\hat{\mathbb{Z}}_{13} = \mathbb{X}_{11}[\mathbb{Q}_0^{(a,A')}(1,1)] \otimes \mathbb{U}_2[\mathbb{Q}_0^{(s,A')}]$$

No. 14
$$\hat{\mathbb{Q}}_2^{(A')}(1,-1)$$
 [M₃, S₂]

$$\hat{\mathbb{Z}}_{14} = \mathbb{X}_{12}[\mathbb{Q}_2^{(a,A')}(1,-1)] \otimes \mathbb{U}_2[\mathbb{Q}_0^{(s,A')}]$$

No. 15
$$\hat{\mathbb{Q}}_3^{(A',1)}(1,-1)$$
 [M₃, S₂]

$$\hat{\mathbb{Z}}_{15} = \frac{\sqrt{2}\mathbb{X}_{16}[\mathbb{Q}_{2,0}^{(a,E')}(1,-1)] \otimes \mathbb{U}_{4}[\mathbb{Q}_{1,1}^{(s,E')}]}{2} - \frac{\sqrt{2}\mathbb{X}_{17}[\mathbb{Q}_{2,1}^{(a,E')}(1,-1)] \otimes \mathbb{U}_{3}[\mathbb{Q}_{1,0}^{(s,E')}]}{2}$$

No. 16
$$\hat{\mathbb{Q}}_3^{(A',2)}(1,-1)$$
 [M₃, S₂]

$$\hat{\mathbb{Z}}_{16} = \frac{\sqrt{2}\mathbb{X}_{16}[\mathbb{Q}_{2,0}^{(a,E')}(1,-1)]\otimes \mathbb{U}_{3}[\mathbb{Q}_{1,0}^{(s,E')}]}{2} + \frac{\sqrt{2}\mathbb{X}_{17}[\mathbb{Q}_{2,1}^{(a,E')}(1,-1)]\otimes \mathbb{U}_{4}[\mathbb{Q}_{1,1}^{(s,E')}]}{2}$$

No. 17
$$\hat{\mathbb{G}}_{1}^{(A')}(1,0)$$
 [M₃, S₂]

$$\hat{\mathbb{Z}}_{17} = \mathbb{X}_{13}[\mathbb{Q}_1^{(a,A')}(1,0)] \otimes \mathbb{U}_2[\mathbb{Q}_0^{(s,A')}]$$

No. 18
$$\hat{\mathbb{Q}}_0^{(A')}$$
 [M₁, S₃]

$$\hat{\mathbb{Z}}_{18} = \mathbb{X}_1[\mathbb{Q}_0^{(a,A')}] \otimes \mathbb{U}_5[\mathbb{Q}_0^{(s,A')}]$$

No. 19
$$\hat{\mathbb{Q}}_0^{(A')}$$
 [M₁, B₁]

$$\hat{\mathbb{Z}}_{19} = \mathbb{X}_1[\mathbb{Q}_0^{(a,A')}] \otimes \mathbb{U}_6[\mathbb{Q}_0^{(u,A')}]$$

No. 20
$$\hat{\mathbb{G}}_1^{(A')}(1,-1)$$
 [M₁, B₁]

$$\hat{\mathbb{Z}}_{20} = \mathbb{X}_2[\mathbb{M}_1^{(a,A')}(1,-1)] \otimes \mathbb{U}_9[\mathbb{T}_0^{(u,A')}]$$

No. 21
$$\hat{\mathbb{Q}}_0^{(A')}$$
 [M₄, B₁]

$$\hat{\mathbb{Z}}_{21} = \frac{\sqrt{2}\mathbb{X}_{18}[\mathbb{Q}_{1,0}^{(a,E')}] \otimes \mathbb{U}_{7}[\mathbb{Q}_{1,0}^{(u,E')}]}{2} + \frac{\sqrt{2}\mathbb{X}_{19}[\mathbb{Q}_{1,1}^{(a,E')}] \otimes \mathbb{U}_{8}[\mathbb{Q}_{1,1}^{(u,E')}]}{2}$$

No. 22
$$\hat{\mathbb{G}}_{1}^{(A')}$$
 [M₄, B₁]

$$\hat{\mathbb{Z}}_{22} = \frac{\sqrt{2}\mathbb{X}_{18}[\mathbb{Q}_{1,0}^{(a,E')}] \otimes \mathbb{U}_{8}[\mathbb{Q}_{1,1}^{(u,E')}]}{2} - \frac{\sqrt{2}\mathbb{X}_{19}[\mathbb{Q}_{1,1}^{(a,E')}] \otimes \mathbb{U}_{7}[\mathbb{Q}_{1,0}^{(u,E')}]}{2}$$

No. 23
$$\hat{\mathbb{Q}}_0^{(A')}(1,0)$$
 [M₄, B₁]

$$\hat{\mathbb{Z}}_{23} = \frac{\sqrt{2}\mathbb{X}_{20}[\mathbb{Q}_{1,0}^{(a,E')}(1,0)] \otimes \mathbb{U}_{7}[\mathbb{Q}_{1,0}^{(u,E')}]}{2} + \frac{\sqrt{2}\mathbb{X}_{21}[\mathbb{Q}_{1,1}^{(a,E')}(1,0)] \otimes \mathbb{U}_{8}[\mathbb{Q}_{1,1}^{(u,E')}]}{2}$$

No. 24
$$\hat{\mathbb{G}}_{1}^{(A')}(1,0)$$
 [M₄, B₁]

$$\hat{\mathbb{Z}}_{24} = \frac{\sqrt{2}\mathbb{X}_{20}[\mathbb{Q}_{1,0}^{(a,E')}(1,0)] \otimes \mathbb{U}_{8}[\mathbb{Q}_{1,1}^{(u,E')}]}{2} - \frac{\sqrt{2}\mathbb{X}_{21}[\mathbb{Q}_{1,1}^{(a,E')}(1,0)] \otimes \mathbb{U}_{7}[\mathbb{Q}_{1,0}^{(u,E')}]}{2}$$

No. 25
$$\hat{\mathbb{G}}_1^{(A')}(1,-1)$$
 [M₄, B₁]

$$\hat{\mathbb{Z}}_{25} = \frac{\sqrt{2}\mathbb{X}_{22}[\mathbb{G}_{2,0}^{(a,E')}(1,-1)] \otimes \mathbb{U}_{7}[\mathbb{Q}_{1,0}^{(u,E')}]}{2} + \frac{\sqrt{2}\mathbb{X}_{23}[\mathbb{G}_{2,1}^{(a,E')}(1,-1)] \otimes \mathbb{U}_{8}[\mathbb{Q}_{1,1}^{(u,E')}]}{2}$$

No. 26
$$\hat{\mathbb{Q}}_2^{(A')}(1,-1)$$
 [M₄, B₁]

$$\hat{\mathbb{Z}}_{26} = \frac{\sqrt{2}\mathbb{X}_{22}[\mathbb{G}_{2,0}^{(a,E')}(1,-1)] \otimes \mathbb{U}_{8}[\mathbb{Q}_{1,1}^{(u,E')}]}{2} - \frac{\sqrt{2}\mathbb{X}_{23}[\mathbb{G}_{2,1}^{(a,E')}(1,-1)] \otimes \mathbb{U}_{7}[\mathbb{Q}_{1,0}^{(u,E')}]}{2}$$

No. 27
$$\hat{\mathbb{Q}}_0^{(A')}$$
 [M₁, B₂]

$$\hat{\mathbb{Z}}_{27} = \mathbb{X}_1[\mathbb{Q}_0^{(a,A')}] \otimes \mathbb{U}_{10}[\mathbb{Q}_0^{(u,A')}]$$

No. 28
$$\hat{\mathbb{G}}_1^{(A')}(1,-1)$$
 [M₁, B₂]

$$\hat{\mathbb{Z}}_{28} = \mathbb{X}_2[\mathbb{M}_1^{(a,A')}(1,-1)] \otimes \mathbb{U}_{13}[\mathbb{T}_0^{(u,A')}]$$

No. 29
$$\hat{\mathbb{Q}}_0^{(A')}$$
 [M₂, B₂]

$$\hat{\mathbb{Z}}_{29} = \frac{\sqrt{2}\mathbb{X}_{3}[\mathbb{Q}_{1,0}^{(a,E')}] \otimes \mathbb{U}_{11}[\mathbb{Q}_{1,0}^{(u,E')}]}{2} + \frac{\sqrt{2}\mathbb{X}_{4}[\mathbb{Q}_{1,1}^{(a,E')}] \otimes \mathbb{U}_{12}[\mathbb{Q}_{1,1}^{(u,E')}]}{2}$$

No. 30
$$\hat{\mathbb{G}}_{1}^{(A')}$$
 [M₂, B₂]

$$\hat{\mathbb{Z}}_{30} = \frac{\sqrt{2}\mathbb{X}_3[\mathbb{Q}_{1,0}^{(a,E')}] \otimes \mathbb{U}_{12}[\mathbb{Q}_{1,1}^{(u,E')}]}{2} - \frac{\sqrt{2}\mathbb{X}_4[\mathbb{Q}_{1,1}^{(a,E')}] \otimes \mathbb{U}_{11}[\mathbb{Q}_{1,0}^{(u,E')}]}{2}$$

No. 31
$$\hat{\mathbb{Q}}_0^{(A')}(1,0)$$
 [M₂, B₂]

$$\hat{\mathbb{Z}}_{31} = \frac{\sqrt{2}\mathbb{X}_{5}[\mathbb{Q}_{1,0}^{(a,E')}(1,0)] \otimes \mathbb{U}_{11}[\mathbb{Q}_{1,0}^{(u,E')}]}{2} + \frac{\sqrt{2}\mathbb{X}_{6}[\mathbb{Q}_{1,1}^{(a,E')}(1,0)] \otimes \mathbb{U}_{12}[\mathbb{Q}_{1,1}^{(u,E')}]}{2}$$

No. 32
$$\hat{\mathbb{G}}_{1}^{(A')}(1,0)$$
 [M₂, B₂]

$$\hat{\mathbb{Z}}_{32} = \frac{\sqrt{2}\mathbb{X}_{5}[\mathbb{Q}_{1,0}^{(a,E')}(1,0)] \otimes \mathbb{U}_{12}[\mathbb{Q}_{1,1}^{(u,E')}]}{2} - \frac{\sqrt{2}\mathbb{X}_{6}[\mathbb{Q}_{1,1}^{(a,E')}(1,0)] \otimes \mathbb{U}_{11}[\mathbb{Q}_{1,0}^{(u,E')}]}{2}$$

No. 33
$$\hat{\mathbb{G}}_{1}^{(A')}(1,-1)$$
 [M₂, B₂]

$$\hat{\mathbb{Z}}_{33} = \frac{\sqrt{2}\mathbb{X}_{7}[\mathbb{G}_{2,0}^{(a,E')}(1,-1)] \otimes \mathbb{U}_{11}[\mathbb{Q}_{1,0}^{(u,E')}]}{2} + \frac{\sqrt{2}\mathbb{X}_{8}[\mathbb{G}_{2,1}^{(a,E')}(1,-1)] \otimes \mathbb{U}_{12}[\mathbb{Q}_{1,1}^{(u,E')}]}{2}$$

$$\begin{split} & \boxed{\text{No. } 34} \quad \hat{\mathbb{Q}}_{2}^{(A')}(1,-1) \ [M_{2},B_{2}] \\ & \hat{\mathbb{Z}}_{34} = \frac{\sqrt{2}\mathbb{X}_{7}[\mathbb{G}_{2,0}^{(a,E')}(1,-1)] \otimes \mathbb{U}_{12}[\mathbb{Q}_{1,1}^{(u,E')}]}{2} - \frac{\sqrt{2}\mathbb{X}_{8}[\mathbb{G}_{2,1}^{(a,E')}(1,-1)] \otimes \mathbb{U}_{11}[\mathbb{Q}_{1,0}^{(u,E')}]}{2} \end{split}$$

Table 4: Atomic SAMB group.

group	bra	ket
M_1	$(s,\uparrow),(s,\downarrow)$	$(s,\uparrow),(s,\downarrow)$
M_2	$(s,\uparrow),(s,\downarrow)$	$(p_x,\uparrow),(p_x,\downarrow),(p_y,\uparrow),(p_y,\downarrow),(p_z,\uparrow),(p_z,\downarrow)$
M_3	$(p_x,\uparrow),(p_x,\downarrow),(p_y,\uparrow),(p_y,\downarrow),(p_z,\uparrow),(p_z,\downarrow)$	$(p_x,\uparrow),(p_x,\downarrow),(p_y,\uparrow),(p_y,\downarrow),(p_z,\uparrow),(p_z,\downarrow)$
M_4	$(p_x,\uparrow),(p_x,\downarrow),(p_y,\uparrow),(p_y,\downarrow),(p_z,\uparrow),(p_z,\downarrow)$	$(s,\uparrow),(s,\downarrow)$

Table 5: Atomic SAMB.

symbol	type	group	form
\mathbb{X}_1	$\mathbb{Q}_0^{(a,A')}$	M_1	$\begin{pmatrix} \frac{\sqrt{2}}{2} & 0 \\ 0 & \frac{\sqrt{2}}{2} \end{pmatrix}$
\mathbb{X}_2	$\mathbb{M}_1^{(a,A')}(1,-1)$	M_1	$\begin{pmatrix} \frac{\sqrt{2}}{2} & 0\\ 0 & -\frac{\sqrt{2}}{2} \end{pmatrix}$
\mathbb{X}_3	$\mathbb{Q}_{1,0}^{(a,E')}$	M_2	$\begin{pmatrix} \frac{\sqrt{2}}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & \sqrt{2} & 0 & 0 & 0 & 0 \end{pmatrix}$
\mathbb{X}_4	$\mathbb{Q}_{1,1}^{(a,E')}$	M_2	$\begin{pmatrix} 0 & 0 & \frac{\sqrt{2}}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{2}}{2} & 0 & 0 \end{pmatrix}$
\mathbb{X}_5	$\mathbb{Q}_{1,0}^{(a,E')}(1,0)$	M_2	$\begin{pmatrix} 0 & 0 & -\frac{\imath}{2} & 0 & 0 & \frac{1}{2} \\ 0 & 0 & 0 & \frac{\imath}{2} & -\frac{1}{2} & 0 \end{pmatrix}$
\mathbb{X}_6	$\mathbb{Q}_{1,1}^{(a,E')}(1,0)$	M_2	$\begin{pmatrix} \frac{i}{2} & 0 & 0 & 0 & 0 & -\frac{i}{2} \\ 0 & -\frac{i}{2} & 0 & 0 & -\frac{i}{2} & 0 \end{pmatrix}$
\mathbb{X}_7	$\mathbb{G}_{2,0}^{(a,E')}(1,-1)$	M_2	$\begin{pmatrix} \frac{i}{2} & 0 & 0 & 0 & 0 & \frac{i}{2} \\ 0 & -\frac{i}{2} & 0 & 0 & \frac{i}{2} & 0 \end{pmatrix} \begin{pmatrix} 0 & 0 & \frac{i}{2} & 0 & 0 & \frac{1}{2} \\ 0 & 0 & 0 & -\frac{i}{2} & -\frac{1}{2} & 0 \end{pmatrix}$
X ₈	$\mathbb{G}_{2,1}^{(a,E')}(1,-1)$	M_2	$\begin{pmatrix} 0 & 0 & \frac{i}{2} & 0 & 0 & \frac{1}{2} \\ 0 & 0 & 0 & -\frac{i}{2} & -\frac{1}{2} & 0 \end{pmatrix}$

Table 5

symbol	type	group	form
\mathbb{X}_9	$\mathbb{Q}_0^{(a,A')}$	$ m M_3$	$\begin{pmatrix} \frac{\sqrt{6}}{6} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{6}}{6} & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{6}}{6} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{6}}{6} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{6}}{6} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{6}}{6} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{6}}{6} & 0 \end{pmatrix}$
\mathbb{X}_{10}	$\mathbb{Q}_2^{(a,A')}$	$ m M_3$	$ \begin{bmatrix} -\frac{\sqrt{3}}{6} & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{3}}{6} & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{3}}{6} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{3}}{6} & 0 & 0 \end{bmatrix} $
\mathbb{X}_{11}	$\mathbb{Q}_0^{(a,A')}(1,1)$	$ m M_3$	$\begin{bmatrix} 0 & 0 & 0 & 0 & \frac{\sqrt{3}}{3} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{3}}{3} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{3}}{3} & 0 \\ 0 & 0 & -\frac{\sqrt{3}i}{6} & 0 & 0 & \frac{\sqrt{3}}{6} \\ 0 & 0 & 0 & \frac{\sqrt{3}i}{6} & -\frac{\sqrt{3}}{6} & 0 \\ \frac{\sqrt{3}i}{6} & 0 & 0 & 0 & 0 & -\frac{\sqrt{3}i}{6} \\ 0 & -\frac{\sqrt{3}i}{6} & 0 & 0 & 0 & -\frac{\sqrt{3}i}{6} & 0 \\ 0 & -\frac{\sqrt{3}}{6} & 0 & 0 & \frac{\sqrt{3}i}{6} & 0 & 0 \\ \frac{\sqrt{3}}{6} & 0 & \frac{\sqrt{3}i}{6} & 0 & 0 & 0 \\ \frac{\sqrt{3}}{6} & 0 & \frac{\sqrt{3}i}{6} & 0 & 0 & -\frac{\sqrt{6}}{12} \\ 0 & 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 & -\frac{\sqrt{6}}{12} & 0 \\ \frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 & 0 & \sqrt{6}i \end{bmatrix}$
\mathbb{X}_{12}	$\mathbb{Q}_2^{(a,A')}(1,-1)$	$ m M_3$	$\begin{bmatrix} 0 & 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 & -\frac{\sqrt{0}}{12} \\ 0 & 0 & 0 & \frac{\sqrt{6}i}{6} & \frac{\sqrt{6}}{12} & 0 \\ \frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 & \frac{\sqrt{6}i}{12} \\ 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 & \frac{\sqrt{6}i}{12} & 0 \\ 0 & \frac{\sqrt{6}}{12} & 0 & -\frac{\sqrt{6}i}{12} & 0 & 0 \\ -\frac{\sqrt{6}}{12} & 0 & -\frac{\sqrt{6}i}{12} & 0 & 0 & 0 \end{bmatrix}$
\mathbb{X}_{13}	$\mathbb{G}_{1}^{(a,A')}(1,0)$	$ m M_3$	$ \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{2}i}{4} \\ 0 & 0 & 0 & 0 & \frac{\sqrt{2}i}{4} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{2}}{4} \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{2}}{4} & 0 \\ 0 & -\frac{\sqrt{2}i}{4} & 0 & -\frac{\sqrt{2}}{4} & 0 & 0 \\ -\frac{\sqrt{2}i}{4} & 0 & \frac{\sqrt{2}}{4} & 0 & 0 & 0 \end{pmatrix} $

symbol	type	group	form
\mathbb{X}_{14}	$\mathbb{Q}_{2,0}^{(a,E')}$	$ m M_3$	$\begin{pmatrix} \frac{1}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{1}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 &$
\mathbb{X}_{15}	$\mathbb{Q}_{2,1}^{(a,E')}$	$ m M_3$	$\begin{pmatrix} 0 & 0 & -\frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{1}{2} & 0 & 0 \\ -\frac{1}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{1}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0$
\mathbb{X}_{16}	$\mathbb{Q}_{2,0}^{(a,E')}(1,-1)$	$ m M_3$	$ \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{2}}{4} \\ 0 & 0 & 0 & 0 & \frac{\sqrt{2}}{4} & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{2}i}{4} \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{2}i}{4} & 0 \\ 0 & \frac{\sqrt{2}}{4} & 0 & \frac{\sqrt{2}i}{4} & 0 & 0 \\ -\frac{\sqrt{2}}{4} & 0 & \frac{\sqrt{2}i}{4} & 0 & 0 & 0 \end{pmatrix} $
\mathbb{X}_{17}	$\mathbb{Q}_{2,1}^{(a,E')}(1,-1)$	$ m M_3$	$ \left(\begin{array}{cccccccccccccccccccccccccccccccccccc$
\mathbb{X}_{18}	$\mathbb{Q}_{1,0}^{(a,E')}$	$ m M_4$	$\begin{pmatrix} \frac{\sqrt{2}}{2} & 0\\ 0 & \frac{\sqrt{2}}{2}\\ 0 & 0\\ 0 & 0\\ 0 & 0\\ 0 & 0 \end{pmatrix}$

Table 5

Table 5			
symbol	type	group	form
\mathbb{X}_{19}	$\mathbb{Q}_{1,1}^{(a,E')}$	$ m M_4$	$\begin{pmatrix} 0 & 0 \\ 0 & 0 \\ \frac{\sqrt{2}}{2} & 0 \\ 0 & \frac{\sqrt{2}}{2} \\ 0 & 0 \\ 0 & 0 \end{pmatrix}$
\mathbb{X}_{20}	$\mathbb{Q}_{1,0}^{(a,E')}(1,0)$	$ m M_4$	$\begin{pmatrix} 0 & 0 \\ 0 & 0 \\ \frac{i}{2} & 0 \\ 0 & -\frac{i}{2} \\ 0 & -\frac{1}{2} \\ \frac{1}{2} & 0 \end{pmatrix}$
\mathbb{X}_{21}	$\mathbb{Q}_{1,1}^{(a,E')}(1,0)$	$ m M_4$	$\begin{pmatrix} -\frac{i}{2} & 0 \\ 0 & \frac{i}{2} \\ 0 & 0 \\ 0 & 0 \\ 0 & \frac{i}{2} \\ \frac{i}{2} & 0 \end{pmatrix}$ $\begin{pmatrix} -\frac{i}{2} & 0 \\ 0 & \frac{i}{2} \\ 0 & 0 \\ 0 & 0 \end{pmatrix}$
\mathbb{X}_{22}	$\mathbb{G}_{2,0}^{(a,E')}(1,-1)$	M4	$\begin{pmatrix} 0 & -\frac{i}{2} \\ -\frac{i}{2} & 0 \end{pmatrix}$
\mathbb{X}_{23}	$\mathbb{G}_{2,1}^{(a,E')}(1,-1)$	$ m M_4$	$\begin{pmatrix} 0 & 0 \\ 0 & 0 \\ -\frac{i}{2} & 0 \\ 0 & \frac{i}{2} \\ 0 & -\frac{1}{2} \\ \frac{1}{2} & 0 \end{pmatrix}$

Table 6: Uniform SAMB.

symbol	type	cluster	form
\mathbb{U}_1	$\mathbb{Q}_0^{(s,A')}$	S_1	$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0$
\mathbb{U}_2	$\mathbb{Q}_0^{(s,A')}$	S_2	$\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{3}}{3} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{3}}{3} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{3}}{3} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0$
\mathbb{U}_3	$\mathbb{Q}_{1,0}^{(s,E')}$	S_2	$\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{6}}{6} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{6}}{3} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{6}}{6} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0$
\mathbb{U}_4	$\mathbb{Q}_{1,1}^{(s,E')}$	S_2	$\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{2}}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0$

Table 6

symbol	type	cluster	form
\mathbb{U}_5	$\mathbb{Q}_0^{(s,A')}$	S_3	$\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 &$
\mathbb{U}_6	$\mathbb{Q}_0^{(u,A')}$	В1	$\begin{pmatrix} 0 & \frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} & 0 & 0 & 0 \\ \frac{\sqrt{6}}{6} & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{\sqrt{6}}{6} & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{\sqrt{6}}{6} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0$
\mathbb{U}_7	$\mathbb{Q}_{1,0}^{(u,E')}$	B_1	$\begin{pmatrix} 0 & -\frac{\sqrt{3}}{6} & \frac{\sqrt{3}}{3} & -\frac{\sqrt{3}}{6} & 0 & 0 & 0 \\ -\frac{\sqrt{3}}{6} & 0 & 0 & 0 & 0 & 0 & 0 \\ -\frac{\sqrt{3}}{6} & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{\sqrt{3}}{3} & 0 & 0 & 0 & 0 & 0 & 0 \\ -\frac{\sqrt{3}}{6} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0$
\mathbb{U}_8	$\mathbb{Q}_{1,1}^{(u,E')}$	B_1	$\begin{pmatrix} 0 & -\frac{1}{2} & 0 & \frac{1}{2} & 0 & 0 & 0 \\ -\frac{1}{2} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0$

Table 6

symbol	type	cluster	form
\mathbb{U}_9	$\mathbb{T}_0^{(u,A')}$	B_1	$ \begin{pmatrix} 0 & -\frac{\sqrt{6}i}{6} & -\frac{\sqrt{6}i}{6} & -\frac{\sqrt{6}i}{6} & 0 & 0 & 0 \\ \frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0$
\mathbb{U}_{10}	$\mathbb{Q}_0^{(u,A')}$	В2	$\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 &$
\mathbb{U}_{11}	$\mathbb{Q}_{1,0}^{(u,E')}$	B_2	$ \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 &$
\mathbb{U}_{12}	$\mathbb{Q}_{1,1}^{(u,E')}$	B_2	$\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 &$

Table 6

symbol	type	cluster				fc	rm		
			/ 0	0	0	0	0	0	0 \
			0	0	0	0	$-\frac{\sqrt{6}i}{6}$	0	0
			0	0	0	0	0	$-\frac{\sqrt{6}i}{6}$	0
\mathbb{U}_{13}	$\mathbb{T}_0^{(u,A')}$	B_2	0	0	0	0	0	0	$-\frac{\sqrt{6}i}{6}$
			0	$\frac{\sqrt{6}i}{6}$	0	0	0	0	0
			0	0	$\frac{\sqrt{6}i}{6}$	0	0	0	0
			0	0	0	$\frac{\sqrt{6}i}{6}$	0	0	0 /

Table 7: Polar harmonics.

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

Table 8: Axial harmonics.

No.	symbol	rank	irrep.	mul.	comp.	form
1	$\mathbb{G}_1^{(A')}$	1	A'	_	_	Z
2	$\mathbb{G}_{2,0}^{(E')}$	2	E'	_	0	$\sqrt{3}XZ$
3	$\mathbb{G}_{2,1}^{(E')}$	2	E'	_	1	$\sqrt{3}YZ$

 \bullet Group info.: Generator = $3^+_{\ 001},\ m_{001}$

Table 9: Conjugacy class.

rep. SO	symmetry operations
1	1
3 ⁺ ₀₀₁	3 ⁺ ₀₀₁
3-001	3_001
m_{001}	m ₀₀₁
-6^{+}_{001}	-6^{+}_{001}
-6^{-}_{001}	-6^{-}_{001}

Table 10: Symmetry operations.

No.	SO	No.	SO	No.	SO	No.	SO	No.	SO
1	1	2	3 ⁺ ₀₀₁	3	3-001	4	m_{001}	5	-6^{+}_{001}
 6	-6^{-}_{001}								

Table 11: Character table.

	1	3 ⁺ ₀₀₁	3-001	m ₀₀₁	-6^{+}_{001}	-6^{-}_{001}
A'	1	1	1	1	1	1
$A^{\prime\prime}$	1	1	1	-1	-1	-1
$E'^{(a)}$	1	ω^*	ω	1	ω	ω^*
$E'^{(b)}$	1	ω	ω^*	1	ω^*	ω
$E^{\prime\prime(a)}$	1	ω^*	ω	-1	$-\omega$	$-\omega^*$
$E^{\prime\prime(b)}$	1	ω	ω^*	-1	$-\omega^*$	$-\omega$

Table 12: Parity conversion.

\leftrightarrow	\leftrightarrow	\leftrightarrow	\leftrightarrow	\leftrightarrow
$ \begin{array}{c} A' \left(A'' \right) \\ E'^{(b)} \left(E''^{(b)} \right) \end{array} $	$A^{\prime\prime}$ (A^{\prime})	$E^{\prime\prime(a)} (E^{\prime(a)})$	$E^{\prime\prime(b)} (E^{\prime(b)})$	$E^{\prime(a)} (E^{\prime\prime(a)})$

Table 13: Symmetric product, $[\Gamma \otimes \Gamma']_+$.

	A'	$A^{\prime\prime}$	$E'^{(a)}$	$E'^{(b)}$	$E^{\prime\prime(a)}$	$E^{\prime\prime(b)}$
A'	A'	$A^{\prime\prime}$	$E'^{(a)}$	$E'^{(b)}$	$E^{\prime\prime(a)}$	$E^{\prime\prime(b)}$
$A^{\prime\prime}$		A'	$E^{\prime\prime(a)}$	$E^{\prime\prime(b)}$	$E'^{(a)}$	$E'^{(b)}$
$E'^{(a)}$			$E'^{(b)}$	A'	$E^{\prime\prime(b)}$	$A^{\prime\prime}$
$E'^{(b)}$				$E'^{(a)}$	$A^{\prime\prime}$	$E^{\prime\prime(a)}$
$E^{\prime\prime(a)}$					$E'^{(b)}$	A'
$E^{\prime\prime(b)}$						$E'^{(a)}$

Table 14: Anti-symmetric product, $[\Gamma \otimes \Gamma]_-$.

_	A'	$A^{\prime\prime}$	$E'^{(a)}$	$E'^{(b)}$	$E^{\prime\prime(a)}$	$E^{\prime\prime(b)}$
	_	_	_	_	_	_

Table 15: Virtual-cluster sites.

No.	position	No.	position	No.	position	No.	position
1	$\begin{pmatrix} -1 & -1 & 1 \end{pmatrix}$	2	$\begin{pmatrix} 1 & 0 & 1 \end{pmatrix}$	3	$\begin{pmatrix} 0 & 1 & 1 \end{pmatrix}$	4	$\begin{pmatrix} -1 & -1 & -1 \end{pmatrix}$
5	$\begin{pmatrix} 0 & 1 & -1 \end{pmatrix}$	6	$\begin{pmatrix} 1 & 0 & -1 \end{pmatrix}$				

Table 16: Virtual-cluster basis.

symbol	1	2	3	4	5	6
$\mathbb{Q}_0^{(A')}$	$\frac{\sqrt{6}}{6}$	$\frac{\sqrt{6}}{6}$	$\frac{\sqrt{6}}{6}$	$\frac{\sqrt{6}}{6}$	$\frac{\sqrt{6}}{6}$	$\frac{\sqrt{6}}{6}$
$\mathbb{Q}_1^{(A^{\prime\prime})}$	$\frac{\sqrt{6}}{6}$	$\frac{\sqrt{6}}{6}$	$\frac{\sqrt{6}}{6}$	$-\frac{\sqrt{6}}{6}$	$-\frac{\sqrt{6}}{6}$	$-\frac{\sqrt{6}}{6}$
$\mathbb{Q}_{1,0}^{(E')}$	$-\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{3}$	$-\frac{\sqrt{3}}{6}$	$-\frac{\sqrt{3}}{6}$	$-\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{3}$
$\mathbb{Q}_{1,1}^{(E')}$	$-\frac{1}{2}$	0	$\frac{1}{2}$	$-\frac{1}{2}$	$\frac{1}{2}$	0
$\mathbb{Q}_{2,0}^{(E^{\prime\prime})}$	$-\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{3}$	$-\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$	$-\frac{\sqrt{3}}{3}$
$\mathbb{Q}_{2,1}^{(E^{\prime\prime})}$	$-\frac{1}{2}$	0	$\frac{1}{2}$	$\frac{1}{2}$	$-\frac{1}{2}$	0