SAMB for "C3h"

Generated on 2023-06-18 16:51 by MultiPie 1.1.10

- Group: No. 22 C_{3h} -6 [hexagonal]

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

- Kets: dimension = 32

Table 1: Hilbert space for full matrix.

No.	ket	No.	ket	No.	ket	No.	ket	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	$(p_y,\uparrow)$@O$_1$	8	$(p_y,\downarrow)$@O$_1$	9	$(p_z,\uparrow)$@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	$(p_z,\uparrow)$@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	$(s,\uparrow)$@H2_2	30	$(s,\downarrow)$@H2_2
31	$(s,\uparrow)$@H2_3	32	$(s,\downarrow)$@H2_3						

- Sites in (primitive) unit cell:

Table 2: Site-clusters.

	site	position	mapping
S_1 [1o: -6]	$H1_1$	$\begin{pmatrix} 0 & 0 & 0 \end{pmatrix}$	[1,2,3,4,5,6]
S_2 [3b: m..]	O_1	$\begin{pmatrix} \frac{1}{3} & 0 & 0 \end{pmatrix}$	[1,4]
	O_2	$\begin{pmatrix} 0 & \frac{1}{3} & 0 \end{pmatrix}$	[2,6]
	O_3	$\begin{pmatrix} -\frac{1}{3} & -\frac{1}{3} & 0 \end{pmatrix}$	[3,5]
S_3 [3b: m..]	$H2_1$	$\begin{pmatrix} \frac{1}{2} & \frac{1}{6} & 0 \end{pmatrix}$	[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	#	$\boldsymbol{b}$@$\boldsymbol{c}$	mapping
B_1 [3b: m..]	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	$\begin{pmatrix} 0 & \frac{1}{3} & 0 \end{pmatrix}$ @ $\begin{pmatrix} 0 & \frac{1}{6} & 0 \end{pmatrix}$	[2,6]
	b_3	O_3	$H1_1$	1	1	$\begin{pmatrix} -\frac{1}{3} & -\frac{1}{3} & 0 \end{pmatrix}$ @ $\begin{pmatrix} -\frac{1}{6} & -\frac{1}{6} & 0 \end{pmatrix}$	[3,5]
B_2 [3b: m..]	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	$\begin{pmatrix} 0 & -\frac{1}{6} & 0 \end{pmatrix}$ @ $\begin{pmatrix} -\frac{1}{3} & -\frac{5}{12} & 0 \end{pmatrix}$	[3,5]

- SAMB:

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

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

$\boxed{\text{No. 2}}$ $\hat{\mathbb{Q}}_0^{(A')}$ $[\mathrm{M}_1, \mathrm{S}_2]$

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

$\boxed{\text{No. 3}}$ $\hat{\mathbb{Q}}_0^{(A')}$ $[\mathrm{M}_2, \mathrm{S}_2]$

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

$\boxed{\text{No. 4}}$ $\hat{\mathbb{G}}_1^{(A')}$ $[\mathrm{M}_2, \mathrm{S}_2]$

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

$\boxed{\text{No. 5}}$ $\hat{\mathbb{Q}}_0^{(A')}(1,0)$ $[\mathrm{M}_2, \mathrm{S}_2]$

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

$\boxed{\text{No. 6}}$ $\hat{\mathbb{G}}_1^{(A')}(1,0)$ $[\mathrm{M}_2, \mathrm{S}_2]$

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

$\boxed{\text{No. 7}}$ $\hat{\mathbb{G}}_1^{(A')}(1,-1)$ $[\mathrm{M}_2, \mathrm{S}_2]$

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

$\boxed{\text{No. 8}}$ $\hat{\mathbb{Q}}_2^{(A')}(1,-1)$ $[\mathrm{M}_2, \mathrm{S}_2]$

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

$\boxed{\text{No. 9}}$ $\hat{\mathbb{Q}}_0^{(A')}$ $[\mathrm{M}_3, \mathrm{S}_2]$

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

$\boxed{\text{No. 10}}$ $\hat{\mathbb{Q}}_2^{(A')}$ $[\mathrm{M}_3, \mathrm{S}_2]$

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

$\boxed{\text{No. 11}}$ $\hat{\mathbb{Q}}_3^{(A',1)}$ $[\mathrm{M}_3, \mathrm{S}_2]$

$$\hat{\mathbb{Z}}_{11} = \frac{\sqrt{2}\mathbb{X}_{14}[\mathbb{Q}_{2,0}^{(a,E')}] \otimes \mathbb{U}_4[\mathbb{Q}_{1,1}^{(s,E')}]}{2} - \frac{\sqrt{2}\mathbb{X}_{15}[\mathbb{Q}_{2,1}^{(a,E')}] \otimes \mathbb{U}_3[\mathbb{Q}_{1,0}^{(s,E')}]}{2}$$

$\boxed{\text{No. 12}}$ $\hat{\mathbb{Q}}_3^{(A',2)}$ $[\mathrm{M}_3, \mathrm{S}_2]$

$$\hat{\mathbb{Z}}_{12} = \frac{\sqrt{2}\mathbb{X}_{14}[\mathbb{Q}_{2,0}^{(a,E')}] \otimes \mathbb{U}_3[\mathbb{Q}_{1,0}^{(s,E')}]}{2} + \frac{\sqrt{2}\mathbb{X}_{15}[\mathbb{Q}_{2,1}^{(a,E')}] \otimes \mathbb{U}_4[\mathbb{Q}_{1,1}^{(s,E')}]}{2}$$

$\boxed{\text{No. 13}}$ $\hat{\mathbb{Q}}_0^{(A')}(1,1)$ $[\mathrm{M}_3, \mathrm{S}_2]$

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

$\boxed{\text{No. 14}}$ $\hat{\mathbb{Q}}_2^{(A')}(1,-1)$ $[\mathrm{M}_3, \mathrm{S}_2]$

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

$\boxed{\text{No. 15}}$ $\hat{\mathbb{Q}}_3^{(A',1)}(1,-1)$ $[\mathrm{M}_3, \mathrm{S}_2]$

$$\hat{\mathbb{Z}}_{15} = \frac{\sqrt{2}\mathbb{X}_{16}[\mathbb{Q}_{2,0}^{(a,E')}(1,-1)] \otimes \mathbb{U}_4[\mathbb{Q}_{1,1}^{(s,E')}]}{2} - \frac{\sqrt{2}\mathbb{X}_{17}[\mathbb{Q}_{2,1}^{(a,E')}(1,-1)] \otimes \mathbb{U}_3[\mathbb{Q}_{1,0}^{(s,E')}]}{2}$$

$\boxed{\text{No. 16}}$ $\hat{\mathbb{Q}}_3^{(A',2)}(1,-1)$ $[\mathrm{M}_3, \mathrm{S}_2]$

$$\hat{\mathbb{Z}}_{16} = \frac{\sqrt{2}\mathbb{X}_{16}[\mathbb{Q}_{2,0}^{(a,E')}(1,-1)] \otimes \mathbb{U}_3[\mathbb{Q}_{1,0}^{(s,E')}]}{2} + \frac{\sqrt{2}\mathbb{X}_{17}[\mathbb{Q}_{2,1}^{(a,E')}(1,-1)] \otimes \mathbb{U}_4[\mathbb{Q}_{1,1}^{(s,E')}]}{2}$$

$\boxed{\text{No. 17}}$ $\hat{\mathbb{G}}_1^{(A')}(1,0)$ $[\mathrm{M}_3, \mathrm{S}_2]$

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

$\boxed{\text{No. 18}}$ $\hat{\mathbb{Q}}_0^{(A')}$ $[\mathrm{M}_1, \mathrm{S}_3]$

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

$\boxed{\text{No. 19}}$ $\hat{\mathbb{Q}}_0^{(A')}$ $[\mathrm{M}_1, \mathrm{B}_1]$

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

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

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

$\boxed{\text{No. 21}}$ $\hat{\mathbb{Q}}_0^{(A')}$ $[\mathrm{M}_4, \mathrm{B}_1]$

$$\hat{\mathbb{Z}}_{21} = \frac{\sqrt{2}\mathbb{X}_{18}[\mathbb{Q}_{1,0}^{(a,E')}] \otimes \mathbb{U}_7[\mathbb{Q}_{1,0}^{(u,E')}]}{2} + \frac{\sqrt{2}\mathbb{X}_{19}[\mathbb{Q}_{1,1}^{(a,E')}] \otimes \mathbb{U}_8[\mathbb{Q}_{1,1}^{(u,E')}]}{2}$$

$\boxed{\text{No. 22}}$ $\hat{\mathbb{G}}_1^{(A')}$ $[\mathrm{M}_4, \mathrm{B}_1]$

$$\hat{\mathbb{Z}}_{22} = \frac{\sqrt{2}\mathbb{X}_{18}[\mathbb{Q}_{1,0}^{(a,E')}] \otimes \mathbb{U}_8[\mathbb{Q}_{1,1}^{(u,E')}]}{2} - \frac{\sqrt{2}\mathbb{X}_{19}[\mathbb{Q}_{1,1}^{(a,E')}] \otimes \mathbb{U}_7[\mathbb{Q}_{1,0}^{(u,E')}]}{2}$$

$\boxed{\text{No. 23}}$ $\hat{\mathbb{Q}}_0^{(A')}(1,0)$ $[\mathrm{M}_4, \mathrm{B}_1]$

$$\hat{\mathbb{Z}}_{23} = \frac{\sqrt{2}\mathbb{X}_{20}[\mathbb{Q}_{1,0}^{(a,E')}(1,0)] \otimes \mathbb{U}_7[\mathbb{Q}_{1,0}^{(u,E')}]}{2} + \frac{\sqrt{2}\mathbb{X}_{21}[\mathbb{Q}_{1,1}^{(a,E')}(1,0)] \otimes \mathbb{U}_8[\mathbb{Q}_{1,1}^{(u,E')}]}{2}$$

$\boxed{\text{No. 24}}$ $\hat{\mathbb{G}}_1^{(A')}(1,0)$ $[\mathrm{M}_4, \mathrm{B}_1]$

$$\hat{\mathbb{Z}}_{24} = \frac{\sqrt{2}\mathbb{X}_{20}[\mathbb{Q}_{1,0}^{(a,E')}(1,0)] \otimes \mathbb{U}_8[\mathbb{Q}_{1,1}^{(u,E')}]}{2} - \frac{\sqrt{2}\mathbb{X}_{21}[\mathbb{Q}_{1,1}^{(a,E')}(1,0)] \otimes \mathbb{U}_7[\mathbb{Q}_{1,0}^{(u,E')}]}{2}$$

$\boxed{\text{No. 25}}$ $\hat{\mathbb{G}}_1^{(A')}(1,-1)$ $[\mathrm{M}_4, \mathrm{B}_1]$

$$\hat{\mathbb{Z}}_{25} = \frac{\sqrt{2}\mathbb{X}_{22}[\mathbb{G}_{2,0}^{(a,E')}(1,-1)] \otimes \mathbb{U}_7[\mathbb{Q}_{1,0}^{(u,E')}]}{2} + \frac{\sqrt{2}\mathbb{X}_{23}[\mathbb{G}_{2,1}^{(a,E')}(1,-1)] \otimes \mathbb{U}_8[\mathbb{Q}_{1,1}^{(u,E')}]}{2}$$

$\boxed{\text{No. 26}}$ $\hat{\mathbb{Q}}_2^{(A')}(1,-1)$ $[\mathrm{M}_4, \mathrm{B}_1]$

$$\hat{\mathbb{Z}}_{26} = \frac{\sqrt{2}\mathbb{X}_{22}[\mathbb{G}_{2,0}^{(a,E')}(1,-1)] \otimes \mathbb{U}_8[\mathbb{Q}_{1,1}^{(u,E')}]}{2} - \frac{\sqrt{2}\mathbb{X}_{23}[\mathbb{G}_{2,1}^{(a,E')}(1,-1)] \otimes \mathbb{U}_7[\mathbb{Q}_{1,0}^{(u,E')}]}{2}$$

$\boxed{\text{No. 27}}$ $\hat{\mathbb{Q}}_0^{(A')}$ $[\mathrm{M}_1, \mathrm{B}_2]$

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

$\boxed{\text{No. 28}}$ $\hat{\mathbb{G}}_1^{(A')}(1,-1)$ $[\mathrm{M}_1, \mathrm{B}_2]$

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

$\boxed{\text{No. 29}}$ $\hat{\mathbb{Q}}_0^{(A')}$ $[\mathrm{M}_2, \mathrm{B}_2]$

$$\hat{\mathbb{Z}}_{29} = \frac{\sqrt{2}\mathbb{X}_3[\mathbb{Q}_{1,0}^{(a,E')}] \otimes \mathbb{U}_{11}[\mathbb{Q}_{1,0}^{(u,E')}]}{2} + \frac{\sqrt{2}\mathbb{X}_4[\mathbb{Q}_{1,1}^{(a,E')}] \otimes \mathbb{U}_{12}[\mathbb{Q}_{1,1}^{(u,E')}]}{2}$$

$\boxed{\text{No. 30}}$ $\hat{\mathbb{G}}_1^{(A')}$ $[\mathrm{M}_2, \mathrm{B}_2]$

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

$\boxed{\text{No. 31}}$ $\hat{\mathbb{Q}}_0^{(A')}(1,0)$ $[\mathrm{M}_2, \mathrm{B}_2]$

$$\hat{\mathbb{Z}}_{31} = \frac{\sqrt{2}\mathbb{X}_5[\mathbb{Q}_{1,0}^{(a,E')}(1,0)] \otimes \mathbb{U}_{11}[\mathbb{Q}_{1,0}^{(u,E')}]}{2} + \frac{\sqrt{2}\mathbb{X}_6[\mathbb{Q}_{1,1}^{(a,E')}(1,0)] \otimes \mathbb{U}_{12}[\mathbb{Q}_{1,1}^{(u,E')}]}{2}$$

$\boxed{\text{No. 32}}$ $\hat{\mathbb{G}}_1^{(A')}(1,0)$ $[\mathrm{M}_2, \mathrm{B}_2]$

$$\hat{\mathbb{Z}}_{32} = \frac{\sqrt{2}\mathbb{X}_5[\mathbb{Q}_{1,0}^{(a,E')}(1,0)] \otimes \mathbb{U}_{12}[\mathbb{Q}_{1,1}^{(u,E')}]}{2} - \frac{\sqrt{2}\mathbb{X}_6[\mathbb{Q}_{1,1}^{(a,E')}(1,0)] \otimes \mathbb{U}_{11}[\mathbb{Q}_{1,0}^{(u,E')}]}{2}$$

$\boxed{\text{No. 33}}$ $\hat{\mathbb{G}}_1^{(A')}(1,-1)$ $[\mathrm{M}_2, \mathrm{B}_2]$

$$\hat{\mathbb{Z}}_{33} = \frac{\sqrt{2}\mathbb{X}_7[\mathbb{G}_{2,0}^{(a,E')}(1,-1)] \otimes \mathbb{U}_{11}[\mathbb{Q}_{1,0}^{(u,E')}]}{2} + \frac{\sqrt{2}\mathbb{X}_8[\mathbb{G}_{2,1}^{(a,E')}(1,-1)] \otimes \mathbb{U}_{12}[\mathbb{Q}_{1,1}^{(u,E')}]}{2}$$

$\boxed{\text{No. 34}}$ $\hat{\mathbb{Q}}_{2}^{(A')}(1,-1)$ $[\mathrm{M}_2, \mathrm{B}_2]$

$$\hat{\mathbb{Z}}_{34} = \frac{\sqrt{2}\mathbb{X}_{7}[\mathbb{G}_{2,0}^{(a,E')}(1,-1)] \otimes \mathbb{U}_{12}[\mathbb{Q}_{1,1}^{(u,E')}]}{2} - \frac{\sqrt{2}\mathbb{X}_{8}[\mathbb{G}_{2,1}^{(a,E')}(1,-1)] \otimes \mathbb{U}_{11}[\mathbb{Q}_{1,0}^{(u,E')}]}{2}$$

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	$\begin{pmatrix} \frac{\sqrt{2}}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{2}}{2} & 0 & 0 & 0 & 0 \end{pmatrix}$
$\mathbb{X}_4$	$\mathbb{Q}_{1,1}^{(a,E')}$	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	$\begin{pmatrix} 0 & 0 & -\frac{i}{2} & 0 & 0 & \frac{1}{2} \\ 0 & 0 & 0 & \frac{i}{2} & -\frac{1}{2} & 0 \end{pmatrix}$
$\mathbb{X}_6$	$\mathbb{Q}_{1,1}^{(a,E')}(1,0)$	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	$\begin{pmatrix} \frac{i}{2} & 0 & 0 & 0 & 0 & \frac{i}{2} \\ 0 & -\frac{i}{2} & 0 & 0 & \frac{i}{2} & 0 \end{pmatrix}$
$\mathbb{X}_8$	$\mathbb{G}_{2,1}^{(a,E')}(1,-1)$	M_2	$\begin{pmatrix} 0 & 0 & \frac{i}{2} & 0 & 0 & \frac{1}{2} \\ 0 & 0 & 0 & -\frac{i}{2} & -\frac{1}{2} & 0 \end{pmatrix}$

continued ...

Table 5

symbol	type	group	form
$\mathbb{X}_9$	$\mathbb{Q}_0^{(a,A')}$	M_3	$\begin{pmatrix} \frac{\sqrt{6}}{6} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{6}}{6} & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{6}}{6} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{6}}{6} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{6}}{6} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{6}}{6} \end{pmatrix}$
$\mathbb{X}_{10}$	$\mathbb{Q}_2^{(a,A')}$	M_3	$\begin{pmatrix} -\frac{\sqrt{3}}{6} & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{3}}{6} & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{3}}{6} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{3}}{6} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{3}}{3} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{3}}{3} \end{pmatrix}$
$\mathbb{X}_{11}$	$\mathbb{Q}_0^{(a,A')}(1,1)$	M_3	$\begin{pmatrix} 0 & 0 & -\frac{\sqrt{3}i}{6} & 0 & 0 & \frac{\sqrt{3}}{6} \\ 0 & 0 & 0 & \frac{\sqrt{3}i}{6} & -\frac{\sqrt{3}}{6} & 0 \\ \frac{\sqrt{3}i}{6} & 0 & 0 & 0 & 0 & -\frac{\sqrt{3}i}{6} \\ 0 & -\frac{\sqrt{3}i}{6} & 0 & 0 & -\frac{\sqrt{3}i}{6} & 0 \\ 0 & -\frac{\sqrt{3}}{6} & 0 & \frac{\sqrt{3}i}{6} & 0 & 0 \\ \frac{\sqrt{3}}{6} & 0 & \frac{\sqrt{3}i}{6} & 0 & 0 & 0 \end{pmatrix}$
$\mathbb{X}_{12}$	$\mathbb{Q}_2^{(a,A')}(1,-1)$	M_3	$\begin{pmatrix} 0 & 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 & -\frac{\sqrt{6}}{12} \\ 0 & 0 & 0 & \frac{\sqrt{6}i}{6} & \frac{\sqrt{6}}{12} & 0 \\ \frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 & \frac{\sqrt{6}i}{12} \\ 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 & \frac{\sqrt{6}i}{12} & 0 \\ 0 & \frac{\sqrt{6}}{12} & 0 & -\frac{\sqrt{6}i}{12} & 0 & 0 \\ -\frac{\sqrt{6}}{12} & 0 & -\frac{\sqrt{6}i}{12} & 0 & 0 & 0 \end{pmatrix}$
$\mathbb{X}_{13}$	$\mathbb{G}_1^{(a,A')}(1,0)$	M_3	$\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{2}i}{4} \\ 0 & 0 & 0 & 0 & \frac{\sqrt{2}i}{4} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{2}}{4} \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{2}}{4} & 0 \\ 0 & -\frac{\sqrt{2}i}{4} & 0 & -\frac{\sqrt{2}}{4} & 0 & 0 \\ -\frac{\sqrt{2}i}{4} & 0 & \frac{\sqrt{2}}{4} & 0 & 0 & 0 \end{pmatrix}$

continued …

Table 5

symbol	type	group	form
$\mathbb{X}_{14}$	$\mathbb{Q}_{2,0}^{(a,E')}$	M_3	$\begin{pmatrix} \frac{1}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{1}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$
$\mathbb{X}_{15}$	$\mathbb{Q}_{2,1}^{(a,E')}$	M_3	$\begin{pmatrix} 0 & 0 & -\frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{1}{2} & 0 & 0 \\ -\frac{1}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{1}{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$
$\mathbb{X}_{16}$	$\mathbb{Q}_{2,0}^{(a,E')}(1,-1)$	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_3	$\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{2}i}{4} \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{2}i}{4} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{2}}{4} \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{2}}{4} & 0 \\ 0 & \frac{\sqrt{2}i}{4} & 0 & -\frac{\sqrt{2}}{4} & 0 & 0 \\ \frac{\sqrt{2}i}{4} & 0 & \frac{\sqrt{2}}{4} & 0 & 0 & 0 \end{pmatrix}$
$\mathbb{X}_{18}$	$\mathbb{Q}_{1,0}^{(a,E')}$	M_4	$\begin{pmatrix} \frac{\sqrt{2}}{2} & 0 \\ 0 & \frac{\sqrt{2}}{2} \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix}$

continued ...

Table 5

symbol	type	group	form
$\mathbb{X}_{19}$	$\mathbb{Q}_{1,1}^{(a,E')}$	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_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_4	$\begin{pmatrix} -\frac{i}{2} & 0 \\ 0 & \frac{i}{2} \\ 0 & 0 \\ 0 & 0 \\ 0 & \frac{i}{2} \\ \frac{i}{2} & 0 \end{pmatrix}$
$\mathbb{X}_{22}$	$\mathbb{G}_{2,0}^{(a,E')}(1,-1)$	M_4	$\begin{pmatrix} -\frac{i}{2} & 0 \\ 0 & \frac{i}{2} \\ 0 & 0 \\ 0 & 0 \\ 0 & -\frac{i}{2} \\ -\frac{i}{2} & 0 \end{pmatrix}$
$\mathbb{X}_{23}$	$\mathbb{G}_{2,1}^{(a,E')}(1,-1)$	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	$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$
$\mathbb{U}_2$	$\mathbb{Q}_0^{(s,A')}$	S_2	$\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{3}}{3} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{3}}{3} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{3}}{3} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$
$\mathbb{U}_3$	$\mathbb{Q}_{1,0}^{(s,E')}$	S_2	$\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{6}}{6} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{6}}{3} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{6}}{6} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$
$\mathbb{U}_4$	$\mathbb{Q}_{1,1}^{(s,E')}$	S_2	$\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{2}}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{2}}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$

continued ...

Table 6

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

continued ...

Table 6

symbol	type	cluster	form
$\mathbb{U}_9$	$\mathbb{T}_0^{(u,A')}$	B_1	$\begin{pmatrix} 0 & -\frac{\sqrt{6}i}{6} & -\frac{\sqrt{6}i}{6} & -\frac{\sqrt{6}i}{6} & 0 & 0 & 0 \\ \frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$
$\mathbb{U}_{10}$	$\mathbb{Q}_0^{(u,A')}$	B_2	$\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{6}}{6} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{6}}{6} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{6}}{6} \\ 0 & \frac{\sqrt{6}}{6} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{6}}{6} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{6}}{6} & 0 & 0 & 0 \end{pmatrix}$
$\mathbb{U}_{11}$	$\mathbb{Q}_{1,0}^{(u,E')}$	B_2	$\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{3}}{6} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{3}}{3} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{3}}{6} \\ 0 & -\frac{\sqrt{3}}{6} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{3}}{3} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{3}}{6} & 0 & 0 & 0 \end{pmatrix}$
$\mathbb{U}_{12}$	$\mathbb{Q}_{1,1}^{(u,E')}$	B_2	$\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{1}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{2} \\ 0 & -\frac{1}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2} & 0 & 0 & 0 \end{pmatrix}$

continued ...

Table 6

symbol	type	cluster	form
$\mathbb{U}_{13}$	$\mathbb{T}_0^{(u,A')}$	B_2	$\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{6}i}{6} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{6}i}{6} \\ 0 & \frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{6}i}{6} & 0 & 0 & 0 \end{pmatrix}$

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	$\sqrt{3}YZ$

- 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''	1	1	1	-1	-1	-1
$E'^{(a)}$	1	ω^*	ω	1	ω	ω^*
$E'^{(b)}$	1	ω	ω^*	1	ω^*	ω
$E''^{(a)}$	1	ω^*	ω	-1	$-\omega$	$-\omega^*$
$E''^{(b)}$	1	ω	ω^*	-1	$-\omega^*$	$-\omega$

Table 12: Parity conversion.

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

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

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

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

A'	A''	$E'^{(a)}$	$E'^{(b)}$	$E''^{(a)}$	$E''^{(b)}$
$-$	$-$	$-$	$-$	$-$	$-$

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
$\mathbb{Q}_{0}^{(A')}$	$\frac{\sqrt{6}}{6}$	$\frac{\sqrt{6}}{6}$	$\frac{\sqrt{6}}{6}$	$\frac{\sqrt{6}}{6}$	$\frac{\sqrt{6}}{6}$	$\frac{\sqrt{6}}{6}$
$\mathbb{Q}_{1}^{(A'')}$	$\frac{\sqrt{6}}{6}$	$\frac{\sqrt{6}}{6}$	$\frac{\sqrt{6}}{6}$	$-\frac{\sqrt{6}}{6}$	$-\frac{\sqrt{6}}{6}$	$-\frac{\sqrt{6}}{6}$
$\mathbb{Q}_{1,0}^{(E')}$	$-\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{3}$	$-\frac{\sqrt{3}}{6}$	$-\frac{\sqrt{3}}{6}$	$-\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{3}$
$\mathbb{Q}_{1,1}^{(E')}$	$-\frac{1}{2}$	0	$\frac{1}{2}$	$-\frac{1}{2}$	$\frac{1}{2}$	0
$\mathbb{Q}_{2,0}^{(E'')}$	$-\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{3}$	$-\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$	$-\frac{\sqrt{3}}{3}$
$\mathbb{Q}_{2,1}^{(E'')}$	$-\frac{1}{2}$	0	$\frac{1}{2}$	$\frac{1}{2}$	$-\frac{1}{2}$	0