

SAMB for “C3h”

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- 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	#	$\mathbf{b@c}$	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:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

$$\hat{\mathbb{Z}}_{34} = \frac{\sqrt{2}\mathbb{X}_7[\mathbb{G}_{2,0}^{(a,E')}(1, -1)] \otimes \mathbb{U}_{12}[\mathbb{Q}_{1,1}^{(u,E')}] }{2} - \frac{\sqrt{2}\mathbb{X}_8[\mathbb{G}_{2,1}^{(a,E')}(1, -1)] \otimes \mathbb{U}_{11}[\mathbb{Q}_{1,0}^{(u,E')}] }{2}$$

Table 4: Atomic SAMB group.

group	bra	ket
M ₁	(s, ↑), (s, ↓)	(s, ↑), (s, ↓)
M ₂	(s, ↑), (s, ↓)	(p _x , ↑), (p _x , ↓), (p _y , ↑), (p _y , ↓), (p _z , ↑), (p _z , ↓)
M ₃	(p _x , ↑), (p _x , ↓), (p _y , ↑), (p _y , ↓), (p _z , ↑), (p _z , ↓)	(p _x , ↑), (p _x , ↓), (p _y , ↑), (p _y , ↓), (p _z , ↑), (p _z , ↓)
M ₄	(p _x , ↑), (p _x , ↓), (p _y , ↑), (p _y , ↓), (p _z , ↑), (p _z , ↓)	(s, ↑), (s, ↓)

Table 5: Atomic SAMB.

symbol	type	group	form
X ₁	$\mathbb{Q}_0^{(a,A')}$	M ₁	$\begin{pmatrix} \frac{\sqrt{2}}{2} & 0 \\ 0 & \frac{\sqrt{2}}{2} \end{pmatrix}$
X ₂	$\mathbb{M}_1^{(a,A')}(1, -1)$	M ₁	$\begin{pmatrix} \frac{\sqrt{2}}{2} & 0 \\ 0 & -\frac{\sqrt{2}}{2} \end{pmatrix}$
X ₃	$\mathbb{Q}_{1,0}^{(a,E')}$	M ₂	$\begin{pmatrix} \frac{\sqrt{2}}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{2}}{2} & 0 & 0 & 0 & 0 \end{pmatrix}$
X ₄	$\mathbb{Q}_{1,1}^{(a,E')}$	M ₂	$\begin{pmatrix} 0 & 0 & \frac{\sqrt{2}}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{2}}{2} & 0 & 0 \end{pmatrix}$
X ₅	$\mathbb{Q}_{1,0}^{(a,E')}(1, 0)$	M ₂	$\begin{pmatrix} 0 & 0 & -\frac{i}{2} & 0 & 0 & \frac{1}{2} \\ 0 & 0 & 0 & \frac{i}{2} & -\frac{1}{2} & 0 \end{pmatrix}$
X ₆	$\mathbb{Q}_{1,1}^{(a,E')}(1, 0)$	M ₂	$\begin{pmatrix} \frac{i}{2} & 0 & 0 & 0 & 0 & -\frac{i}{2} \\ 0 & -\frac{i}{2} & 0 & 0 & -\frac{i}{2} & 0 \end{pmatrix}$
X ₇	$\mathbb{G}_{2,0}^{(a,E')}(1, -1)$	M ₂	$\begin{pmatrix} \frac{i}{2} & 0 & 0 & 0 & 0 & \frac{i}{2} \\ 0 & -\frac{i}{2} & 0 & 0 & \frac{i}{2} & 0 \end{pmatrix}$
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	$\begin{pmatrix} \frac{\sqrt{2}}{2} & 0 \\ 0 & \frac{\sqrt{2}}{2} \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix}$

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	$\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{6}i}{6} & 0 \\ 0 & \frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 \end{pmatrix}$

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
$Q_0^{(A')}$	$\frac{\sqrt{6}}{6}$	$\frac{\sqrt{6}}{6}$	$\frac{\sqrt{6}}{6}$	$\frac{\sqrt{6}}{6}$	$\frac{\sqrt{6}}{6}$	$\frac{\sqrt{6}}{6}$
$Q_1^{(A'')}$	$\frac{\sqrt{6}}{6}$	$\frac{\sqrt{6}}{6}$	$\frac{\sqrt{6}}{6}$	$-\frac{\sqrt{6}}{6}$	$-\frac{\sqrt{6}}{6}$	$-\frac{\sqrt{6}}{6}$
$Q_{1,0}^{(E')}$	$-\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{3}$	$-\frac{\sqrt{3}}{6}$	$-\frac{\sqrt{3}}{6}$	$-\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{3}$
$Q_{1,1}^{(E')}$	$-\frac{1}{2}$	0	$\frac{1}{2}$	$-\frac{1}{2}$	$\frac{1}{2}$	0
$Q_{2,0}^{(E'')}$	$-\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{3}$	$-\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$	$-\frac{\sqrt{3}}{3}$
$Q_{2,1}^{(E'')}$	$-\frac{1}{2}$	0	$\frac{1}{2}$	$\frac{1}{2}$	$-\frac{1}{2}$	0