

# 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 <sub>1</sub>	H1 <sub>1</sub>	$\begin{pmatrix} 0 & 0 & 0 \end{pmatrix}$	[1,2,3,4,5,6]
S <sub>2</sub>	O <sub>1</sub>	$\begin{pmatrix} \frac{1}{3} & 0 & 0 \end{pmatrix}$	[1,4]
	O <sub>2</sub>	$\begin{pmatrix} 0 & \frac{1}{3} & 0 \end{pmatrix}$	[2,6]
	O <sub>3</sub>	$\begin{pmatrix} -\frac{1}{3} & -\frac{1}{3} & 0 \end{pmatrix}$	[3,5]
S <sub>3</sub>	H2 <sub>1</sub>	$\begin{pmatrix} \frac{1}{2} & \frac{1}{6} & 0 \end{pmatrix}$	[1,4]
	H2 <sub>2</sub>	$\begin{pmatrix} -\frac{1}{6} & \frac{1}{3} & 0 \end{pmatrix}$	[2,6]
	H2 <sub>3</sub>	$\begin{pmatrix} -\frac{1}{3} & -\frac{1}{2} & 0 \end{pmatrix}$	[3,5]

- Bonds in (primitive) unit cell:

Table 3: Bond-clusters.

bond		tail	head	$n$	#	$\mathbf{b@c}$	mapping
B <sub>1</sub>	b <sub>1</sub>	O <sub>1</sub>	H1 <sub>1</sub>	1	1	$\begin{pmatrix} \frac{1}{3} & 0 & 0 \end{pmatrix} @ \begin{pmatrix} \frac{1}{6} & 0 & 0 \end{pmatrix}$	[1,4]
	b <sub>2</sub>	O <sub>2</sub>	H1 <sub>1</sub>	1	1	$\begin{pmatrix} 0 & \frac{1}{3} & 0 \end{pmatrix} @ \begin{pmatrix} 0 & \frac{1}{6} & 0 \end{pmatrix}$	[2,6]
	b <sub>3</sub>	O <sub>3</sub>	H1 <sub>1</sub>	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 <sub>2</sub>	b <sub>4</sub>	H2 <sub>1</sub>	O <sub>1</sub>	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 <sub>5</sub>	H2 <sub>2</sub>	O <sub>2</sub>	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 <sub>6</sub>	H2 <sub>3</sub>	O <sub>3</sub>	1	1	$\begin{pmatrix} 0 & -\frac{1}{6} & 0 \end{pmatrix} @ \begin{pmatrix} -\frac{1}{3} & -\frac{5}{12} & 0 \end{pmatrix}$	[3,5]

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- 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 <sub>1</sub>	(s, ↑), (s, ↓)	(s, ↑), (s, ↓)
M <sub>2</sub>	(s, ↑), (s, ↓)	(p <sub>x</sub> , ↑), (p <sub>x</sub> , ↓), (p <sub>y</sub> , ↑), (p <sub>y</sub> , ↓), (p <sub>z</sub> , ↑), (p <sub>z</sub> , ↓)
M <sub>3</sub>	(p <sub>x</sub> , ↑), (p <sub>x</sub> , ↓), (p <sub>y</sub> , ↑), (p <sub>y</sub> , ↓), (p <sub>z</sub> , ↑), (p <sub>z</sub> , ↓)	(p <sub>x</sub> , ↑), (p <sub>x</sub> , ↓), (p <sub>y</sub> , ↑), (p <sub>y</sub> , ↓), (p <sub>z</sub> , ↑), (p <sub>z</sub> , ↓)
M <sub>4</sub>	(p <sub>x</sub> , ↑), (p <sub>x</sub> , ↓), (p <sub>y</sub> , ↑), (p <sub>y</sub> , ↓), (p <sub>z</sub> , ↑), (p <sub>z</sub> , ↓)	(s, ↑), (s, ↓)

Table 5: Atomic SAMB.

symbol	type	group	form
X <sub>1</sub>	$\mathbb{Q}_0^{(a,A')}$	M <sub>1</sub>	$\begin{pmatrix} \frac{\sqrt{2}}{2} & 0 \\ 0 & \frac{\sqrt{2}}{2} \end{pmatrix}$
X <sub>2</sub>	$\mathbb{M}_1^{(a,A')}(1, -1)$	M <sub>1</sub>	$\begin{pmatrix} \frac{\sqrt{2}}{2} & 0 \\ 0 & -\frac{\sqrt{2}}{2} \end{pmatrix}$
X <sub>3</sub>	$\mathbb{Q}_{1,0}^{(a,E')}$	M <sub>2</sub>	$\begin{pmatrix} \frac{\sqrt{2}}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{2}}{2} & 0 & 0 & 0 & 0 \end{pmatrix}$
X <sub>4</sub>	$\mathbb{Q}_{1,1}^{(a,E')}$	M <sub>2</sub>	$\begin{pmatrix} 0 & 0 & \frac{\sqrt{2}}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{2}}{2} & 0 & 0 \end{pmatrix}$
X <sub>5</sub>	$\mathbb{Q}_{1,0}^{(a,E')}(1, 0)$	M <sub>2</sub>	$\begin{pmatrix} 0 & 0 & -\frac{i}{2} & 0 & 0 & \frac{1}{2} \\ 0 & 0 & 0 & \frac{i}{2} & -\frac{1}{2} & 0 \end{pmatrix}$
X <sub>6</sub>	$\mathbb{Q}_{1,1}^{(a,E')}(1, 0)$	M <sub>2</sub>	$\begin{pmatrix} \frac{i}{2} & 0 & 0 & 0 & 0 & -\frac{i}{2} \\ 0 & -\frac{i}{2} & 0 & 0 & -\frac{i}{2} & 0 \end{pmatrix}$
X <sub>7</sub>	$\mathbb{G}_{2,0}^{(a,E')}(1, -1)$	M <sub>2</sub>	$\begin{pmatrix} \frac{i}{2} & 0 & 0 & 0 & 0 & \frac{i}{2} \\ 0 & -\frac{i}{2} & 0 & 0 & \frac{i}{2} & 0 \end{pmatrix}$
X <sub>8</sub>	$\mathbb{G}_{2,1}^{(a,E')}(1, -1)$	M <sub>2</sub>	$\begin{pmatrix} 0 & 0 & \frac{i}{2} & 0 & 0 & \frac{1}{2} \\ 0 & 0 & 0 & -\frac{i}{2} & -\frac{1}{2} & 0 \end{pmatrix}$

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

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