

SAMB for “0h1”

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- Group: No. 221 O_h^1 $Pm-3m$ [cubic]
 - Associated point group: No. 32 O_h $m-3m$ [cubic]
 - Generation condition
 - model type: **tight_binding**
 - time-reversal type: **electric**
 - irrep: [A1g]
 - spinful
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- Unit cell:
 - $a = 1.0$, $b = 1.0$, $c = 1.0$, $\alpha = 90.0$, $\beta = 90.0$, $\gamma = 90.0$
- Lattice vectors:
 - $\mathbf{a}_1 = (1.0 \ 0 \ 0)$
 - $\mathbf{a}_2 = (0 \ 1.0 \ 0)$
 - $\mathbf{a}_3 = (0 \ 0 \ 1.0)$

Table 1: High-symmetry line: Γ -X.

	symbol	position		symbol	position
	Γ	$\begin{pmatrix} 0 & 0 & 0 \end{pmatrix}$		X	$\begin{pmatrix} \frac{1}{2} & 0 & 0 \end{pmatrix}$

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- Kets: dimension = 8

Table 2: Hilbert space for full matrix.

No.	ket	No.	ket	No.	ket	No.	ket	No.	ket
1	$(s, \uparrow)@A_1$	2	$(s, \downarrow)@A_1$	3	$(p_x, \uparrow)@A_1$	4	$(p_x, \downarrow)@A_1$	5	$(p_y, \uparrow)@A_1$
6	$(p_y, \downarrow)@A_1$	7	$(p_z, \uparrow)@A_1$	8	$(p_z, \downarrow)@A_1$				

- Sites in (primitive) unit cell:

Table 3: Site-clusters.

site	position	mapping
S ₁ [1a: m-3m]	A ₁	$\begin{pmatrix} 0 & 0 & 0 \end{pmatrix}$ [1,2,3,4,5,6,7,8,9,10,11,12,13,14,15,16,17,18,19,20,21,22,23,24,25,26,27,28,29,30,31,32,33,34,35,36,37,38,39,40,41,42,43,44,45,46,47,48]

- Bonds in (primitive) unit cell:

Table 4: Bond-clusters.

	bond	tail	head	n	#	$\mathbf{b@c}$	mapping
B ₁ [3d: 4/mm.m]	b ₁	A ₁	A ₁	1	1	$\begin{pmatrix} 0 & 0 & 1 \end{pmatrix} @ \begin{pmatrix} 0 & 0 & \frac{1}{2} \end{pmatrix}$	[1,2,-3,-4,-5,-8,19,22,-25,-26,27,28,29,32,-43,-46]
	b ₂	A ₁	A ₁	1	1	$\begin{pmatrix} 1 & 0 & 0 \end{pmatrix} @ \begin{pmatrix} \frac{1}{2} & 0 & 0 \end{pmatrix}$	[6,-9,11,-12,13,-14,21,-24,-30,33,-35,36,-37,38,-45,48]
	b ₃	A ₁	A ₁	1	1	$\begin{pmatrix} 0 & 1 & 0 \end{pmatrix} @ \begin{pmatrix} 0 & \frac{1}{2} & 0 \end{pmatrix}$	[7,-10,15,16,-17,-18,-20,23,-31,34,-39,-40,41,42,44,-47]
B ₂ [3c: 4/mm.m]	b ₄	A ₁	A ₁	2	1	$\begin{pmatrix} 0 & 1 & 1 \end{pmatrix} @ \begin{pmatrix} 0 & \frac{1}{2} & \frac{1}{2} \end{pmatrix}$	[1,-3,7,-10,-25,27,-31,34]
	b ₅	A ₁	A ₁	2	1	$\begin{pmatrix} 0 & 1 & -1 \end{pmatrix} @ \begin{pmatrix} 0 & \frac{1}{2} & \frac{1}{2} \end{pmatrix}$	[-2,4,-20,23,26,-28,44,-47]
	b ₆	A ₁	A ₁	2	1	$\begin{pmatrix} 1 & 0 & -1 \end{pmatrix} @ \begin{pmatrix} \frac{1}{2} & 0 & \frac{1}{2} \end{pmatrix}$	[5,-12,13,-19,-29,36,-37,43]
	b ₇	A ₁	A ₁	2	1	$\begin{pmatrix} 1 & -1 & 0 \end{pmatrix} @ \begin{pmatrix} \frac{1}{2} & \frac{1}{2} & 0 \end{pmatrix}$	[6,-16,18,-24,-30,40,-42,48]
	b ₈	A ₁	A ₁	2	1	$\begin{pmatrix} 1 & 0 & 1 \end{pmatrix} @ \begin{pmatrix} \frac{1}{2} & 0 & \frac{1}{2} \end{pmatrix}$	[-8,11,-14,22,32,-35,38,-46]
	b ₉	A ₁	A ₁	2	1	$\begin{pmatrix} 1 & 1 & 0 \end{pmatrix} @ \begin{pmatrix} \frac{1}{2} & \frac{1}{2} & 0 \end{pmatrix}$	[-9,15,-17,21,33,-39,41,-45]

- SAMB:

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

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

$$\boxed{\text{No. 2}} \quad \hat{\mathbb{Q}}_0^{(A_{1g})} [\text{M}_3, \text{S}_1]$$

$$\hat{\mathbb{Z}}_2 = \mathbb{X}_{11}[\mathbb{Q}_0^{(a, A_{1g})}] \otimes \mathbb{Y}_1[\mathbb{Q}_0^{(s, A_{1g})}]$$

$$\boxed{\text{No. 3}} \quad \hat{\mathbb{Q}}_0^{(A_{1g})}(1, 1) [\text{M}_3, \text{S}_1]$$

$$\hat{\mathbb{Z}}_3 = \mathbb{X}_{12}[\mathbb{Q}_0^{(a, A_{1g})}(1, 1)] \otimes \mathbb{Y}_1[\mathbb{Q}_0^{(s, A_{1g})}]$$

$$\boxed{\text{No. 4}} \quad \hat{\mathbb{Q}}_0^{(A_{1g})} [\text{M}_1, \text{B}_1]$$

$$\hat{\mathbb{Z}}_4 = \mathbb{X}_1[\mathbb{Q}_0^{(a, A_{1g})}] \otimes \mathbb{Y}_2[\mathbb{Q}_0^{(b, A_{1g})}]$$

$$\boxed{\text{No. 5}} \quad \hat{\mathbb{Q}}_0^{(A_{1g})} [\text{M}_2, \text{B}_1]$$

$$\hat{\mathbb{Z}}_5 = \frac{\sqrt{3}\mathbb{X}_5[\mathbb{T}_{1,0}^{(a, T_{1u})}] \otimes \mathbb{Y}_5[\mathbb{T}_{1,0}^{(b, T_{1u})}]}{3} + \frac{\sqrt{3}\mathbb{X}_6[\mathbb{T}_{1,1}^{(a, T_{1u})}] \otimes \mathbb{Y}_6[\mathbb{T}_{1,1}^{(b, T_{1u})}]}{3} + \frac{\sqrt{3}\mathbb{X}_7[\mathbb{T}_{1,2}^{(a, T_{1u})}] \otimes \mathbb{Y}_7[\mathbb{T}_{1,2}^{(b, T_{1u})}]}{3}$$

$$\boxed{\text{No. 6}} \quad \hat{\mathbb{Q}}_0^{(A_{1g})}(1, 0) [\text{M}_2, \text{B}_1]$$

$$\hat{\mathbb{Z}}_6 = \frac{\sqrt{3}\mathbb{X}_{10}[\mathbb{T}_{1,2}^{(a, T_{1u})}(1, 0)] \otimes \mathbb{Y}_7[\mathbb{T}_{1,2}^{(b, T_{1u})}]}{3} + \frac{\sqrt{3}\mathbb{X}_8[\mathbb{T}_{1,0}^{(a, T_{1u})}(1, 0)] \otimes \mathbb{Y}_5[\mathbb{T}_{1,0}^{(b, T_{1u})}]}{3} + \frac{\sqrt{3}\mathbb{X}_9[\mathbb{T}_{1,1}^{(a, T_{1u})}(1, 0)] \otimes \mathbb{Y}_6[\mathbb{T}_{1,1}^{(b, T_{1u})}]}{3}$$

$$\boxed{\text{No. 7}} \quad \hat{\mathbb{Q}}_0^{(A_{1g})} [\text{M}_3, \text{B}_1]$$

$$\hat{\mathbb{Z}}_7 = \mathbb{X}_{11}[\mathbb{Q}_0^{(a, A_{1g})}] \otimes \mathbb{Y}_2[\mathbb{Q}_0^{(b, A_{1g})}]$$

$$\boxed{\text{No. 8}} \quad \hat{\mathbb{Q}}_0^{(A_{1g})}(1, 1) [\text{M}_3, \text{B}_1]$$

$$\hat{\mathbb{Z}}_8 = \mathbb{X}_{12}[\mathbb{Q}_0^{(a, A_{1g})}(1, 1)] \otimes \mathbb{Y}_2[\mathbb{Q}_0^{(b, A_{1g})}]$$

$$\boxed{\text{No. 9}} \quad \hat{\mathbb{Q}}_0^{(A_{1g})} [\text{M}_3, \text{B}_1]$$

$$\hat{\mathbb{Z}}_9 = \frac{\sqrt{2}\mathbb{X}_{13}[\mathbb{Q}_{2,0}^{(a,E_g)}] \otimes \mathbb{Y}_3[\mathbb{Q}_{2,0}^{(b,E_g)}]}{2} + \frac{\sqrt{2}\mathbb{X}_{14}[\mathbb{Q}_{2,1}^{(a,E_g)}] \otimes \mathbb{Y}_4[\mathbb{Q}_{2,1}^{(b,E_g)}]}{2}$$

$$\boxed{\text{No. 10}} \quad \hat{\mathbb{Q}}_0^{(A_{1g})}(1, -1) [\text{M}_3, \text{B}_1]$$

$$\hat{\mathbb{Z}}_{10} = \frac{\sqrt{2}\mathbb{X}_{18}[\mathbb{Q}_{2,0}^{(a,E_g)}(1, -1)] \otimes \mathbb{Y}_3[\mathbb{Q}_{2,0}^{(b,E_g)}]}{2} + \frac{\sqrt{2}\mathbb{X}_{19}[\mathbb{Q}_{2,1}^{(a,E_g)}(1, -1)] \otimes \mathbb{Y}_4[\mathbb{Q}_{2,1}^{(b,E_g)}]}{2}$$

$$\boxed{\text{No. 11}} \quad \hat{\mathbb{Q}}_0^{(A_{1g})} [\text{M}_1, \text{B}_2]$$

$$\hat{\mathbb{Z}}_{11} = \mathbb{X}_1[\mathbb{Q}_0^{(a,A_{1g})}] \otimes \mathbb{Y}_8[\mathbb{Q}_0^{(b,A_{1g})}]$$

$$\boxed{\text{No. 12}} \quad \hat{\mathbb{Q}}_4^{(A_{1g})}(1, -1) [\text{M}_2, \text{B}_2]$$

$$\hat{\mathbb{Z}}_{12} = \frac{\sqrt{3}\mathbb{X}_2[\mathbb{M}_{2,0}^{(a,T_{2u})}(1, -1)] \otimes \mathbb{Y}_{17}[\mathbb{T}_{3,0}^{(b,T_{2u})}]}{3} + \frac{\sqrt{3}\mathbb{X}_3[\mathbb{M}_{2,1}^{(a,T_{2u})}(1, -1)] \otimes \mathbb{Y}_{18}[\mathbb{T}_{3,1}^{(b,T_{2u})}]}{3} + \frac{\sqrt{3}\mathbb{X}_4[\mathbb{M}_{2,2}^{(a,T_{2u})}(1, -1)] \otimes \mathbb{Y}_{19}[\mathbb{T}_{3,2}^{(b,T_{2u})}]}{3}$$

$$\boxed{\text{No. 13}} \quad \hat{\mathbb{Q}}_0^{(A_{1g})} [\text{M}_2, \text{B}_2]$$

$$\hat{\mathbb{Z}}_{13} = \frac{\sqrt{3}\mathbb{X}_5[\mathbb{T}_{1,0}^{(a,T_{1u})}] \otimes \mathbb{Y}_{14}[\mathbb{T}_{1,0}^{(b,T_{1u})}]}{3} + \frac{\sqrt{3}\mathbb{X}_6[\mathbb{T}_{1,1}^{(a,T_{1u})}] \otimes \mathbb{Y}_{15}[\mathbb{T}_{1,1}^{(b,T_{1u})}]}{3} + \frac{\sqrt{3}\mathbb{X}_7[\mathbb{T}_{1,2}^{(a,T_{1u})}] \otimes \mathbb{Y}_{16}[\mathbb{T}_{1,2}^{(b,T_{1u})}]}{3}$$

$$\boxed{\text{No. 14}} \quad \hat{\mathbb{Q}}_0^{(A_{1g})}(1, 0) [\text{M}_2, \text{B}_2]$$

$$\hat{\mathbb{Z}}_{14} = \frac{\sqrt{3}\mathbb{X}_{10}[\mathbb{T}_{1,2}^{(a,T_{1u})}(1, 0)] \otimes \mathbb{Y}_{16}[\mathbb{T}_{1,2}^{(b,T_{1u})}]}{3} + \frac{\sqrt{3}\mathbb{X}_8[\mathbb{T}_{1,0}^{(a,T_{1u})}(1, 0)] \otimes \mathbb{Y}_{14}[\mathbb{T}_{1,0}^{(b,T_{1u})}]}{3} + \frac{\sqrt{3}\mathbb{X}_9[\mathbb{T}_{1,1}^{(a,T_{1u})}(1, 0)] \otimes \mathbb{Y}_{15}[\mathbb{T}_{1,1}^{(b,T_{1u})}]}{3}$$

$$\boxed{\text{No. 15}} \quad \hat{\mathbb{Q}}_0^{(A_{1g})} [\text{M}_3, \text{B}_2]$$

$$\hat{\mathbb{Z}}_{15} = \mathbb{X}_{11}[\mathbb{Q}_0^{(a,A_{1g})}] \otimes \mathbb{Y}_8[\mathbb{Q}_0^{(b,A_{1g})}]$$

$$\boxed{\text{No. 16}} \quad \hat{\mathbb{Q}}_0^{(A_{1g})}(1, 1) [\text{M}_3, \text{B}_2]$$

$$\hat{\mathbb{Z}}_{16} = \mathbb{X}_{12}[\mathbb{Q}_0^{(a,A_{1g})}(1, 1)] \otimes \mathbb{Y}_8[\mathbb{Q}_0^{(b,A_{1g})}]$$

$$\boxed{\text{No. 17}} \quad \hat{\mathbb{Q}}_0^{(A_{1g})} [\text{M}_3, \text{B}_2]$$

$$\begin{aligned} \hat{\mathbb{Z}}_{17} = & \frac{\sqrt{5}\mathbb{X}_{13}[\mathbb{Q}_{2,0}^{(a,E_g)}] \otimes \mathbb{Y}_9[\mathbb{Q}_{2,0}^{(b,E_g)}]}{5} + \frac{\sqrt{5}\mathbb{X}_{14}[\mathbb{Q}_{2,1}^{(a,E_g)}] \otimes \mathbb{Y}_{10}[\mathbb{Q}_{2,1}^{(b,E_g)}]}{5} + \frac{\sqrt{5}\mathbb{X}_{15}[\mathbb{Q}_{2,0}^{(a,T_{2g})}] \otimes \mathbb{Y}_{11}[\mathbb{Q}_{2,0}^{(b,T_{2g})}]}{5} \\ & + \frac{\sqrt{5}\mathbb{X}_{16}[\mathbb{Q}_{2,1}^{(a,T_{2g})}] \otimes \mathbb{Y}_{12}[\mathbb{Q}_{2,1}^{(b,T_{2g})}]}{5} + \frac{\sqrt{5}\mathbb{X}_{17}[\mathbb{Q}_{2,2}^{(a,T_{2g})}] \otimes \mathbb{Y}_{13}[\mathbb{Q}_{2,2}^{(b,T_{2g})}]}{5} \end{aligned}$$

$$\boxed{\text{No. 18}} \quad \hat{\mathbb{Q}}_4^{(A_{1g})} [\text{M}_3, \text{B}_2]$$

$$\begin{aligned} \hat{\mathbb{Z}}_{18} = & \frac{\sqrt{30}\mathbb{X}_{13}[\mathbb{Q}_{2,0}^{(a,E_g)}] \otimes \mathbb{Y}_9[\mathbb{Q}_{2,0}^{(b,E_g)}]}{10} + \frac{\sqrt{30}\mathbb{X}_{14}[\mathbb{Q}_{2,1}^{(a,E_g)}] \otimes \mathbb{Y}_{10}[\mathbb{Q}_{2,1}^{(b,E_g)}]}{10} - \frac{\sqrt{30}\mathbb{X}_{15}[\mathbb{Q}_{2,0}^{(a,T_{2g})}] \otimes \mathbb{Y}_{11}[\mathbb{Q}_{2,0}^{(b,T_{2g})}]}{15} \\ & - \frac{\sqrt{30}\mathbb{X}_{16}[\mathbb{Q}_{2,1}^{(a,T_{2g})}] \otimes \mathbb{Y}_{12}[\mathbb{Q}_{2,1}^{(b,T_{2g})}]}{15} - \frac{\sqrt{30}\mathbb{X}_{17}[\mathbb{Q}_{2,2}^{(a,T_{2g})}] \otimes \mathbb{Y}_{13}[\mathbb{Q}_{2,2}^{(b,T_{2g})}]}{15} \end{aligned}$$

$$\boxed{\text{No. 19}} \quad \hat{\mathbb{Q}}_0^{(A_{1g})}(1, -1) [\text{M}_3, \text{B}_2]$$

$$\begin{aligned} \hat{\mathbb{Z}}_{19} = & \frac{\sqrt{5}\mathbb{X}_{18}[\mathbb{Q}_{2,0}^{(a,E_g)}(1, -1)] \otimes \mathbb{Y}_9[\mathbb{Q}_{2,0}^{(b,E_g)}]}{5} + \frac{\sqrt{5}\mathbb{X}_{19}[\mathbb{Q}_{2,1}^{(a,E_g)}(1, -1)] \otimes \mathbb{Y}_{10}[\mathbb{Q}_{2,1}^{(b,E_g)}]}{5} + \frac{\sqrt{5}\mathbb{X}_{20}[\mathbb{Q}_{2,0}^{(a,T_{2g})}(1, -1)] \otimes \mathbb{Y}_{11}[\mathbb{Q}_{2,0}^{(b,T_{2g})}]}{5} \\ & + \frac{\sqrt{5}\mathbb{X}_{21}[\mathbb{Q}_{2,1}^{(a,T_{2g})}(1, -1)] \otimes \mathbb{Y}_{12}[\mathbb{Q}_{2,1}^{(b,T_{2g})}]}{5} + \frac{\sqrt{5}\mathbb{X}_{22}[\mathbb{Q}_{2,2}^{(a,T_{2g})}(1, -1)] \otimes \mathbb{Y}_{13}[\mathbb{Q}_{2,2}^{(b,T_{2g})}]}{5} \end{aligned}$$

$$\boxed{\text{No. 20}} \quad \hat{\mathbb{Q}}_4^{(A_{1g})}(1, -1) [\text{M}_3, \text{B}_2]$$

$$\begin{aligned} \hat{\mathbb{Z}}_{20} = & \frac{\sqrt{30}\mathbb{X}_{18}[\mathbb{Q}_{2,0}^{(a,E_g)}(1, -1)] \otimes \mathbb{Y}_9[\mathbb{Q}_{2,0}^{(b,E_g)}]}{10} + \frac{\sqrt{30}\mathbb{X}_{19}[\mathbb{Q}_{2,1}^{(a,E_g)}(1, -1)] \otimes \mathbb{Y}_{10}[\mathbb{Q}_{2,1}^{(b,E_g)}]}{10} - \frac{\sqrt{30}\mathbb{X}_{20}[\mathbb{Q}_{2,0}^{(a,T_{2g})}(1, -1)] \otimes \mathbb{Y}_{11}[\mathbb{Q}_{2,0}^{(b,T_{2g})}]}{15} \\ & - \frac{\sqrt{30}\mathbb{X}_{21}[\mathbb{Q}_{2,1}^{(a,T_{2g})}(1, -1)] \otimes \mathbb{Y}_{12}[\mathbb{Q}_{2,1}^{(b,T_{2g})}]}{15} - \frac{\sqrt{30}\mathbb{X}_{22}[\mathbb{Q}_{2,2}^{(a,T_{2g})}(1, -1)] \otimes \mathbb{Y}_{13}[\mathbb{Q}_{2,2}^{(b,T_{2g})}]}{15} \end{aligned}$$

Table 5: 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	$(p_x, \uparrow), (p_x, \downarrow), (p_y, \uparrow), (p_y, \downarrow), (p_z, \uparrow), (p_z, \downarrow)$	$(p_x, \uparrow), (p_x, \downarrow), (p_y, \uparrow), (p_y, \downarrow), (p_z, \uparrow), (p_z, \downarrow)$

Table 6: Atomic SAMB.

symbol	type	group	form
\mathbb{X}_1	$\mathbb{Q}_0^{(a, A_{1g})}$	M_1	$\begin{pmatrix} \frac{\sqrt{2}}{2} & 0 \\ 0 & \frac{\sqrt{2}}{2} \end{pmatrix}$
\mathbb{X}_2	$\mathbb{M}_{2,0}^{(a, T_{2u})}(1, -1)$	M_2	$\begin{pmatrix} 0 & 0 & \frac{1}{2} & 0 & 0 & -\frac{i}{2} \\ 0 & 0 & 0 & -\frac{1}{2} & \frac{i}{2} & 0 \end{pmatrix}$
\mathbb{X}_3	$\mathbb{M}_{2,1}^{(a, T_{2u})}(1, -1)$	M_2	$\begin{pmatrix} \frac{1}{2} & 0 & 0 & 0 & 0 & \frac{1}{2} \\ 0 & -\frac{1}{2} & 0 & 0 & \frac{1}{2} & 0 \end{pmatrix}$
\mathbb{X}_4	$\mathbb{M}_{2,2}^{(a, T_{2u})}(1, -1)$	M_2	$\begin{pmatrix} 0 & -\frac{i}{2} & 0 & \frac{1}{2} & 0 & 0 \\ \frac{i}{2} & 0 & \frac{1}{2} & 0 & 0 & 0 \end{pmatrix}$
\mathbb{X}_5	$\mathbb{T}_{1,0}^{(a, T_{1u})}$	M_2	$\begin{pmatrix} \frac{\sqrt{2}i}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{2}i}{2} & 0 & 0 & 0 & 0 \end{pmatrix}$
\mathbb{X}_6	$\mathbb{T}_{1,1}^{(a, T_{1u})}$	M_2	$\begin{pmatrix} 0 & 0 & \frac{\sqrt{2}i}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{2}i}{2} & 0 & 0 \end{pmatrix}$
\mathbb{X}_7	$\mathbb{T}_{1,2}^{(a, T_{1u})}$	M_2	$\begin{pmatrix} 0 & 0 & 0 & 0 & \frac{\sqrt{2}i}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{2}i}{2} \end{pmatrix}$
\mathbb{X}_8	$\mathbb{T}_{1,0}^{(a, T_{1u})}(1, 0)$	M_2	$\begin{pmatrix} 0 & 0 & -\frac{1}{2} & 0 & 0 & -\frac{i}{2} \\ 0 & 0 & 0 & \frac{1}{2} & \frac{i}{2} & 0 \end{pmatrix}$
\mathbb{X}_9	$\mathbb{T}_{1,1}^{(a, T_{1u})}(1, 0)$	M_2	$\begin{pmatrix} \frac{1}{2} & 0 & 0 & 0 & 0 & -\frac{1}{2} \\ 0 & -\frac{1}{2} & 0 & 0 & -\frac{1}{2} & 0 \end{pmatrix}$
\mathbb{X}_{10}	$\mathbb{T}_{1,2}^{(a, T_{1u})}(1, 0)$	M_2	$\begin{pmatrix} 0 & \frac{i}{2} & 0 & \frac{1}{2} & 0 & 0 \\ -\frac{i}{2} & 0 & \frac{1}{2} & 0 & 0 & 0 \end{pmatrix}$
\mathbb{X}_{11}	$\mathbb{Q}_0^{(a, A_{1g})}$	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}_{12}	$\mathbb{Q}_0^{(a, A_{1g})}(1, 1)$	M_3	$\begin{pmatrix} 0 & 0 & -\frac{\sqrt{3}i}{6} & 0 & 0 & \frac{\sqrt{3}}{6} \\ 0 & 0 & 0 & \frac{\sqrt{3}i}{6} & -\frac{\sqrt{3}}{6} & 0 \\ \frac{\sqrt{3}i}{6} & 0 & 0 & 0 & 0 & -\frac{\sqrt{3}i}{6} \\ 0 & -\frac{\sqrt{3}i}{6} & 0 & 0 & -\frac{\sqrt{3}i}{6} & 0 \\ 0 & -\frac{\sqrt{3}}{6} & 0 & \frac{\sqrt{3}i}{6} & 0 & 0 \\ \frac{\sqrt{3}}{6} & 0 & \frac{\sqrt{3}i}{6} & 0 & 0 & 0 \end{pmatrix}$

continued ...

Table 6

symbol	type	group	form
\mathbb{X}_{13}	$\mathbb{Q}_{2,0}^{(a,E_g)}$	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}_{14}	$\mathbb{Q}_{2,1}^{(a,E_g)}$	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}	$\mathbb{Q}_{2,0}^{(a,T_{2g})}$	M_3	$\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{2} \\ 0 & 0 & \frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2} & 0 & 0 \end{pmatrix}$
\mathbb{X}_{16}	$\mathbb{Q}_{2,1}^{(a,T_{2g})}$	M_3	$\begin{pmatrix} 0 & 0 & 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{2} \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{1}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 & 0 & 0 \end{pmatrix}$
\mathbb{X}_{17}	$\mathbb{Q}_{2,2}^{(a,T_{2g})}$	M_3	$\begin{pmatrix} 0 & 0 & \frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2} & 0 & 0 \\ \frac{1}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$

continued ...

Table 6

symbol	type	group	form
\mathbb{X}_{18}	$\mathbb{Q}_{2,0}^{(a,E_g)}(1,-1)$	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}_{19}	$\mathbb{Q}_{2,1}^{(a,E_g)}(1,-1)$	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}_{20}	$\mathbb{Q}_{2,0}^{(a,T_{2g})}(1,-1)$	M_3	$\begin{pmatrix} 0 & 0 & 0 & -\frac{\sqrt{2}}{4} & \frac{\sqrt{2}i}{4} & 0 \\ 0 & 0 & \frac{\sqrt{2}}{4} & 0 & 0 & -\frac{\sqrt{2}i}{4} \\ 0 & \frac{\sqrt{2}}{4} & 0 & 0 & 0 & 0 \\ -\frac{\sqrt{2}}{4} & 0 & 0 & 0 & 0 & 0 \\ -\frac{\sqrt{2}i}{4} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{2}i}{4} & 0 & 0 & 0 & 0 \end{pmatrix}$
\mathbb{X}_{21}	$\mathbb{Q}_{2,1}^{(a,T_{2g})}(1,-1)$	M_3	$\begin{pmatrix} 0 & 0 & 0 & -\frac{\sqrt{2}i}{4} & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{2}i}{4} & 0 & 0 & 0 \\ 0 & \frac{\sqrt{2}i}{4} & 0 & 0 & -\frac{\sqrt{2}i}{4} & 0 \\ \frac{\sqrt{2}i}{4} & 0 & 0 & 0 & 0 & \frac{\sqrt{2}i}{4} \\ 0 & 0 & \frac{\sqrt{2}i}{4} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{2}i}{4} & 0 & 0 \end{pmatrix}$
\mathbb{X}_{22}	$\mathbb{Q}_{2,2}^{(a,T_{2g})}(1,-1)$	M_3	$\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{2}i}{4} \\ 0 & 0 & 0 & 0 & \frac{\sqrt{2}i}{4} & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{2}}{4} \\ 0 & 0 & 0 & 0 & \frac{\sqrt{2}}{4} & 0 \\ 0 & -\frac{\sqrt{2}i}{4} & 0 & \frac{\sqrt{2}}{4} & 0 & 0 \\ -\frac{\sqrt{2}i}{4} & 0 & -\frac{\sqrt{2}}{4} & 0 & 0 & 0 \end{pmatrix}$

Table 7: Cluster SAMB.

symbol	type	cluster	form
\mathbb{Y}_1	$\mathbb{Q}_0^{(s, A_{1g})}$	S_1	$\begin{pmatrix} 1 \end{pmatrix}$
\mathbb{Y}_2	$\mathbb{Q}_0^{(b, A_{1g})}$	B_1	$\begin{pmatrix} \frac{\sqrt{3}}{3} & \frac{\sqrt{3}}{3} & \frac{\sqrt{3}}{3} \end{pmatrix}$
\mathbb{Y}_3	$\mathbb{Q}_{2,0}^{(b, E_g)}$	B_1	$\begin{pmatrix} -\frac{\sqrt{6}}{3} & \frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} \end{pmatrix}$
\mathbb{Y}_4	$\mathbb{Q}_{2,1}^{(b, E_g)}$	B_1	$\begin{pmatrix} 0 & -\frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2} \end{pmatrix}$
\mathbb{Y}_5	$\mathbb{T}_{1,0}^{(b, T_{1u})}$	B_1	$\begin{pmatrix} 0 & i & 0 \end{pmatrix}$
\mathbb{Y}_6	$\mathbb{T}_{1,1}^{(b, T_{1u})}$	B_1	$\begin{pmatrix} 0 & 0 & i \end{pmatrix}$
\mathbb{Y}_7	$\mathbb{T}_{1,2}^{(b, T_{1u})}$	B_1	$\begin{pmatrix} i & 0 & 0 \end{pmatrix}$
\mathbb{Y}_8	$\mathbb{Q}_0^{(b, A_{1g})}$	B_2	$\begin{pmatrix} \frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} \end{pmatrix}$
\mathbb{Y}_9	$\mathbb{Q}_{2,0}^{(b, E_g)}$	B_2	$\begin{pmatrix} -\frac{\sqrt{3}}{6} & -\frac{\sqrt{3}}{6} & -\frac{\sqrt{3}}{6} & \frac{\sqrt{3}}{3} & -\frac{\sqrt{3}}{6} & \frac{\sqrt{3}}{3} \end{pmatrix}$
\mathbb{Y}_{10}	$\mathbb{Q}_{2,1}^{(b, E_g)}$	B_2	$\begin{pmatrix} \frac{1}{2} & \frac{1}{2} & -\frac{1}{2} & 0 & -\frac{1}{2} & 0 \end{pmatrix}$
\mathbb{Y}_{11}	$\mathbb{Q}_{2,0}^{(b, T_{2g})}$	B_2	$\begin{pmatrix} \frac{\sqrt{2}}{2} & -\frac{\sqrt{2}}{2} & 0 & 0 & 0 & 0 \end{pmatrix}$
\mathbb{Y}_{12}	$\mathbb{Q}_{2,1}^{(b, T_{2g})}$	B_2	$\begin{pmatrix} 0 & 0 & -\frac{\sqrt{2}}{2} & 0 & \frac{\sqrt{2}}{2} & 0 \end{pmatrix}$
\mathbb{Y}_{13}	$\mathbb{Q}_{2,2}^{(b, T_{2g})}$	B_2	$\begin{pmatrix} 0 & 0 & 0 & -\frac{\sqrt{2}}{2} & 0 & \frac{\sqrt{2}}{2} \end{pmatrix}$
\mathbb{Y}_{14}	$\mathbb{T}_{1,0}^{(b, T_{1u})}$	B_2	$\begin{pmatrix} 0 & 0 & \frac{i}{2} & \frac{i}{2} & \frac{i}{2} & \frac{i}{2} \end{pmatrix}$
\mathbb{Y}_{15}	$\mathbb{T}_{1,1}^{(b, T_{1u})}$	B_2	$\begin{pmatrix} \frac{i}{2} & \frac{i}{2} & 0 & -\frac{i}{2} & 0 & \frac{i}{2} \end{pmatrix}$
\mathbb{Y}_{16}	$\mathbb{T}_{1,2}^{(b, T_{1u})}$	B_2	$\begin{pmatrix} \frac{i}{2} & -\frac{i}{2} & -\frac{i}{2} & 0 & \frac{i}{2} & 0 \end{pmatrix}$
\mathbb{Y}_{17}	$\mathbb{T}_{3,0}^{(b, T_{2u})}$	B_2	$\begin{pmatrix} 0 & 0 & \frac{i}{2} & -\frac{i}{2} & \frac{i}{2} & -\frac{i}{2} \end{pmatrix}$
\mathbb{Y}_{18}	$\mathbb{T}_{3,1}^{(b, T_{2u})}$	B_2	$\begin{pmatrix} -\frac{i}{2} & -\frac{i}{2} & 0 & -\frac{i}{2} & 0 & \frac{i}{2} \end{pmatrix}$
\mathbb{Y}_{19}	$\mathbb{T}_{3,2}^{(b, T_{2u})}$	B_2	$\begin{pmatrix} \frac{i}{2} & -\frac{i}{2} & \frac{i}{2} & 0 & -\frac{i}{2} & 0 \end{pmatrix}$

Table 8: Polar harmonics.

No.	symbol	rank	irrep.	mul.	comp.	form
1	$\mathbb{Q}_0^{(A_{1g})}$	0	A_{1g}	—	—	1

continued ...

Table 8

No.	symbol	rank	irrep.	mul.	comp.	form
2	$\mathbb{Q}_{1,0}^{(T_{1u})}$	1	T_{1u}	—	0	x
3	$\mathbb{Q}_{1,1}^{(T_{1u})}$	1	T_{1u}	—	1	y
4	$\mathbb{Q}_{1,2}^{(T_{1u})}$	1	T_{1u}	—	2	z
5	$\mathbb{Q}_{2,0}^{(E_g)}$	2	E_g	—	0	$-\frac{x^2}{2} - \frac{y^2}{2} + z^2$
6	$\mathbb{Q}_{2,1}^{(E_g)}$	2	E_g	—	1	$\frac{\sqrt{3}(x-y)(x+y)}{2}$
7	$\mathbb{Q}_{2,0}^{(T_{2g})}$	2	T_{2g}	—	0	$\sqrt{3}yz$
8	$\mathbb{Q}_{2,1}^{(T_{2g})}$	2	T_{2g}	—	1	$\sqrt{3}xz$
9	$\mathbb{Q}_{2,2}^{(T_{2g})}$	2	T_{2g}	—	2	$\sqrt{3}xy$
10	$\mathbb{Q}_{3,0}^{(T_{2u})}$	3	T_{2u}	—	0	$\frac{\sqrt{15}x(y-z)(y+z)}{2}$
11	$\mathbb{Q}_{3,1}^{(T_{2u})}$	3	T_{2u}	—	1	$-\frac{\sqrt{15}y(x-z)(x+z)}{2}$
12	$\mathbb{Q}_{3,2}^{(T_{2u})}$	3	T_{2u}	—	2	$\frac{\sqrt{15}z(x-y)(x+y)}{2}$

Table 9: Axial harmonics.

No.	symbol	rank	irrep.	mul.	comp.	form
1	$\mathbb{G}_{2,0}^{(T_{2u})}$	2	T_{2u}	—	0	$\sqrt{3}YZ$
2	$\mathbb{G}_{2,1}^{(T_{2u})}$	2	T_{2u}	—	1	$\sqrt{3}XZ$
3	$\mathbb{G}_{2,2}^{(T_{2u})}$	2	T_{2u}	—	2	$\sqrt{3}XY$

-
- Group info.: Generator = $\{2_{001}|0\}$, $\{2_{010}|0\}$, $\{3_{111}^+|0\}$, $\{2_{110}|0\}$, $\{-1|0\}$

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

rep. SO	symmetry operations
$\{1 0\}$	$\{1 0\}$
$\{2_{001} 0\}$	$\{2_{001} 0\}, \{2_{100} 0\}, \{2_{010} 0\}$
$\{2_{110} 0\}$	$\{2_{110} 0\}, \{2_{101} 0\}, \{2_{011} 0\}, \{2_{1-10} 0\}, \{2_{-101} 0\}, \{2_{01-1} 0\}$
$\{3_{111}^+ 0\}$	$\{3_{111}^+ 0\}, \{3_{1-1-1}^+ 0\}, \{3_{-11-1}^+ 0\}, \{3_{-1-11}^+ 0\}, \{3_{-111}^- 0\}, \{3_{1-1-1}^- 0\}, \{3_{-11-1}^- 0\}, \{3_{-1-11}^- 0\}$
$\{4_{001}^+ 0\}$	$\{4_{001}^+ 0\}, \{4_{100}^+ 0\}, \{4_{010}^+ 0\}, \{4_{001}^- 0\}, \{4_{100}^- 0\}, \{4_{010}^- 0\}$
$\{-1 0\}$	$\{-1 0\}$
$\{m_{001} 0\}$	$\{m_{001} 0\}, \{m_{100} 0\}, \{m_{010} 0\}$
$\{m_{110} 0\}$	$\{m_{110} 0\}, \{m_{101} 0\}, \{m_{011} 0\}, \{m_{1-10} 0\}, \{m_{-101} 0\}, \{m_{01-1} 0\}$
$\{-3_{111}^+ 0\}$	$\{-3_{111}^+ 0\}, \{-3_{1-1-1}^+ 0\}, \{-3_{-11-1}^+ 0\}, \{-3_{-1-11}^+ 0\}, \{-3_{-111}^- 0\}, \{-3_{1-1-1}^- 0\}, \{-3_{-11-1}^- 0\}, \{-3_{-1-11}^- 0\}$
$\{-4_{001}^+ 0\}$	$\{-4_{001}^+ 0\}, \{-4_{100}^+ 0\}, \{-4_{010}^+ 0\}, \{-4_{001}^- 0\}, \{-4_{100}^- 0\}, \{-4_{010}^- 0\}$

Table 11: Symmetry operations.

No.	SO	No.	SO	No.	SO	No.	SO	No.	SO
1	$\{1 0\}$	2	$\{2_{001} 0\}$	3	$\{2_{100} 0\}$	4	$\{2_{010} 0\}$	5	$\{2_{110} 0\}$
6	$\{2_{101} 0\}$	7	$\{2_{011} 0\}$	8	$\{2_{1-10} 0\}$	9	$\{2_{-101} 0\}$	10	$\{2_{01-1} 0\}$
11	$\{3_{111}^+ 0\}$	12	$\{3_{1-1-1}^+ 0\}$	13	$\{3_{-11-1}^+ 0\}$	14	$\{3_{-1-11}^+ 0\}$	15	$\{3_{-111}^- 0\}$
16	$\{3_{1-1-1}^- 0\}$	17	$\{3_{-11-1}^- 0\}$	18	$\{3_{-1-11}^- 0\}$	19	$\{4_{001}^+ 0\}$	20	$\{4_{100}^+ 0\}$
21	$\{4_{010}^+ 0\}$	22	$\{4_{001}^- 0\}$	23	$\{4_{100}^- 0\}$	24	$\{4_{010}^- 0\}$	25	$\{-1 0\}$
26	$\{m_{001} 0\}$	27	$\{m_{100} 0\}$	28	$\{m_{010} 0\}$	29	$\{m_{110} 0\}$	30	$\{m_{101} 0\}$
31	$\{m_{011} 0\}$	32	$\{m_{1-10} 0\}$	33	$\{m_{-101} 0\}$	34	$\{m_{01-1} 0\}$	35	$\{-3_{111}^+ 0\}$
36	$\{-3_{1-1-1}^+ 0\}$	37	$\{-3_{-11-1}^+ 0\}$	38	$\{-3_{-1-11}^+ 0\}$	39	$\{-3_{-111}^- 0\}$	40	$\{-3_{1-1-1}^- 0\}$
41	$\{-3_{-11-1}^- 0\}$	42	$\{-3_{-1-11}^- 0\}$	43	$\{-4_{001}^+ 0\}$	44	$\{-4_{100}^+ 0\}$	45	$\{-4_{010}^+ 0\}$
46	$\{-4_{001}^- 0\}$	47	$\{-4_{100}^- 0\}$	48	$\{-4_{010}^- 0\}$				

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

	1	2 ₀₀₁	2 ₁₁₀	3 ⁺ ₁₁₁	4 ⁺ ₀₀₁	-1	m ₀₀₁	m ₁₁₀	-3 ⁺ ₁₁₁	-4 ⁺ ₀₀₁
A_{1g}	1	1	1	1	1	1	1	1	1	1
A_{2g}	1	1	-1	1	-1	1	1	-1	1	-1
E_g	2	2	0	-1	0	2	2	0	-1	0
T_{1g}	3	-1	-1	0	1	3	-1	-1	0	1
T_{2g}	3	-1	1	0	-1	3	-1	1	0	-1
A_{1u}	1	1	1	1	1	-1	-1	-1	-1	-1
A_{2u}	1	1	-1	1	-1	-1	-1	1	-1	1
E_u	2	2	0	-1	0	-2	-2	0	1	0
T_{1u}	3	-1	-1	0	1	-3	1	1	0	-1
T_{2u}	3	-1	1	0	-1	-3	1	-1	0	1

Table 13: Parity conversion.

\leftrightarrow	\leftrightarrow	\leftrightarrow	\leftrightarrow	\leftrightarrow
$A_{1g} (A_{1u})$	$A_{2g} (A_{2u})$	$E_g (E_u)$	$T_{1g} (T_{1u})$	$T_{2g} (T_{2u})$
$A_{1u} (A_{1g})$	$A_{2u} (A_{2g})$	$E_u (E_g)$	$T_{1u} (T_{1g})$	$T_{2u} (T_{2g})$

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

	A_{1g}	A_{2g}	E_g	T_{1g}	T_{2g}	A_{1u}	A_{2u}	E_u	T_{1u}	T_{2u}
A_{1g}	A_{1g}	A_{2g}	E_g	T_{1g}	T_{2g}	A_{1u}	A_{2u}	E_u	T_{1u}	T_{2u}
A_{2g}		A_{1g}	E_g	T_{2g}	T_{1g}	A_{2u}	A_{1u}	E_u	T_{2u}	T_{1u}
E_g			$A_{1g} + E_g$	$T_{1g} + T_{2g}$	$T_{1g} + T_{2g}$	E_u	E_u	$A_{1u} + A_{2u} + E_u$	$T_{1u} + T_{2u}$	$T_{1u} + T_{2u}$
T_{1g}				$A_{1g} + E_g + T_{2g}$	$A_{2g} + E_g + T_{1g} + T_{2g}$	T_{1u}	T_{2u}	$T_{1u} + T_{2u}$	$A_{1u} + E_u + T_{1u} + T_{2u}$	$A_{2u} + E_u + T_{1u} + T_{2u}$
T_{2g}					$A_{1g} + E_g + T_{2g}$	T_{2u}	T_{1u}	$T_{1u} + T_{2u}$	$A_{2u} + E_u + T_{1u} + T_{2u}$	$A_{1u} + E_u + T_{1u} + T_{2u}$
A_{1u}						A_{1g}	A_{2g}	E_g	T_{1g}	T_{2g}
A_{2u}							A_{1g}	E_g	T_{2g}	T_{1g}
E_u								$A_{1g} + E_g$	$T_{1g} + T_{2g}$	$T_{1g} + T_{2g}$
T_{1u}									$A_{1g} + E_g + T_{2g}$	$A_{2g} + E_g + T_{1g} + T_{2g}$
T_{2u}										$A_{1g} + E_g + T_{2g}$

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

A_{1g}	A_{2g}	E_g	T_{1g}	T_{2g}	A_{1u}	A_{2u}	E_u	T_{1u}	T_{2u}
—	—	A_{2g}	T_{1g}	T_{1g}	—	—	A_{2g}	T_{1g}	T_{1g}

Table 16: Virtual-cluster sites.

No.	position	No.	position	No.	position	No.	position
1	$\begin{pmatrix} 3 & 2 & 1 \end{pmatrix}$	2	$\begin{pmatrix} -3 & -2 & 1 \end{pmatrix}$	3	$\begin{pmatrix} 3 & -2 & -1 \end{pmatrix}$	4	$\begin{pmatrix} -3 & 2 & -1 \end{pmatrix}$
5	$\begin{pmatrix} 2 & 3 & -1 \end{pmatrix}$	6	$\begin{pmatrix} 1 & -2 & 3 \end{pmatrix}$	7	$\begin{pmatrix} -3 & 1 & 2 \end{pmatrix}$	8	$\begin{pmatrix} -2 & -3 & -1 \end{pmatrix}$
9	$\begin{pmatrix} -1 & -2 & -3 \end{pmatrix}$	10	$\begin{pmatrix} -3 & -1 & -2 \end{pmatrix}$	11	$\begin{pmatrix} 1 & 3 & 2 \end{pmatrix}$	12	$\begin{pmatrix} -1 & -3 & 2 \end{pmatrix}$
13	$\begin{pmatrix} 1 & -3 & -2 \end{pmatrix}$	14	$\begin{pmatrix} -1 & 3 & -2 \end{pmatrix}$	15	$\begin{pmatrix} 2 & 1 & 3 \end{pmatrix}$	16	$\begin{pmatrix} -2 & 1 & -3 \end{pmatrix}$
17	$\begin{pmatrix} -2 & -1 & 3 \end{pmatrix}$	18	$\begin{pmatrix} 2 & -1 & -3 \end{pmatrix}$	19	$\begin{pmatrix} -2 & 3 & 1 \end{pmatrix}$	20	$\begin{pmatrix} 3 & -1 & 2 \end{pmatrix}$
21	$\begin{pmatrix} 1 & 2 & -3 \end{pmatrix}$	22	$\begin{pmatrix} 2 & -3 & 1 \end{pmatrix}$	23	$\begin{pmatrix} 3 & 1 & -2 \end{pmatrix}$	24	$\begin{pmatrix} -1 & 2 & 3 \end{pmatrix}$
25	$\begin{pmatrix} -3 & -2 & -1 \end{pmatrix}$	26	$\begin{pmatrix} 3 & 2 & -1 \end{pmatrix}$	27	$\begin{pmatrix} -3 & 2 & 1 \end{pmatrix}$	28	$\begin{pmatrix} 3 & -2 & 1 \end{pmatrix}$
29	$\begin{pmatrix} -2 & -3 & 1 \end{pmatrix}$	30	$\begin{pmatrix} -1 & 2 & -3 \end{pmatrix}$	31	$\begin{pmatrix} 3 & -1 & -2 \end{pmatrix}$	32	$\begin{pmatrix} 2 & 3 & 1 \end{pmatrix}$
33	$\begin{pmatrix} 1 & 2 & 3 \end{pmatrix}$	34	$\begin{pmatrix} 3 & 1 & 2 \end{pmatrix}$	35	$\begin{pmatrix} -1 & -3 & -2 \end{pmatrix}$	36	$\begin{pmatrix} 1 & 3 & -2 \end{pmatrix}$
37	$\begin{pmatrix} -1 & 3 & 2 \end{pmatrix}$	38	$\begin{pmatrix} 1 & -3 & 2 \end{pmatrix}$	39	$\begin{pmatrix} -2 & -1 & -3 \end{pmatrix}$	40	$\begin{pmatrix} 2 & -1 & 3 \end{pmatrix}$
41	$\begin{pmatrix} 2 & 1 & -3 \end{pmatrix}$	42	$\begin{pmatrix} -2 & 1 & 3 \end{pmatrix}$	43	$\begin{pmatrix} 2 & -3 & -1 \end{pmatrix}$	44	$\begin{pmatrix} -3 & 1 & -2 \end{pmatrix}$
45	$\begin{pmatrix} -1 & -2 & 3 \end{pmatrix}$	46	$\begin{pmatrix} -2 & 3 & -1 \end{pmatrix}$	47	$\begin{pmatrix} -3 & -1 & 2 \end{pmatrix}$	48	$\begin{pmatrix} 1 & -2 & -3 \end{pmatrix}$

Table 17: Virtual-cluster basis.

symbol	1	2	3	4	5	6	7	8	9	10
$\mathbb{Q}_0^{(A_{1g})}$	$\frac{\sqrt{3}}{12}$	$\frac{\sqrt{3}}{12}$	$\frac{\sqrt{3}}{12}$	$\frac{\sqrt{3}}{12}$	$\frac{\sqrt{3}}{12}$	$\frac{\sqrt{3}}{12}$	$\frac{\sqrt{3}}{12}$	$\frac{\sqrt{3}}{12}$	$\frac{\sqrt{3}}{12}$	$\frac{\sqrt{3}}{12}$

continued ...

[illegible]

14

[illegible]

continued ...

Table 17

[illegible]

continued ...

Table 17

[illegible]

continued ...

Table 17

[illegible]

continued ...

Table 17

[illegible]

continued ...

Table 17

[illegible]

continued ...

Table 17

[illegible]

