

# SAMB for “D4h1”

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- Group: No. 123  $D_{4h}^1$   $P4/mmm$  [ tetragonal ]
  - Associated point group: No. 15  $D_{4h}$   $4/mmm$  [ tetragonal ]
  - Generation condition
    - model type: **tight\_binding**
    - time-reversal type: **electric**
    - irrep: [A1g]
    - spinful
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- Unit cell:  
 $a = 1.0$ ,  $b = 1.0$ ,  $c = 1.5$ ,  $\alpha = 90.0$ ,  $\beta = 90.0$ ,  $\gamma = 90.0$
- Lattice vectors:  
 $\mathbf{a}_1 = (1.0 \ 0 \ 0)$   
 $\mathbf{a}_2 = (0 \ 1.0 \ 0)$   
 $\mathbf{a}_3 = (0 \ 0 \ 1.5)$

Table 1: High-symmetry line:  $\Gamma$ -X.

	symbol	position		symbol	position
	$\Gamma$	$\begin{pmatrix} 0 & 0 & 0 \end{pmatrix}$		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 <sub>1</sub> [1a: 4/mmm]	A <sub>1</sub>	$\begin{pmatrix} 0 & 0 & 0 \end{pmatrix}$	[1,2,3,4,5,6,7,8,9,10,11,12,13,14,15,16]

- Bonds in (primitive) unit cell:

Table 4: Bond-clusters.

	bond	tail	head	$n$	#	$\mathbf{b@c}$	mapping
B <sub>1</sub> [2f: mmm.]	b <sub>1</sub>	A <sub>1</sub>	A <sub>1</sub>	1	1	$\begin{pmatrix} 0 & 1 & 0 \end{pmatrix} @ \begin{pmatrix} 0 & \frac{1}{2} & 0 \end{pmatrix}$	[1,-2,-3,4,-9,10,11,-12]
	b <sub>2</sub>	A <sub>1</sub>	A <sub>1</sub>	1	1	$\begin{pmatrix} 1 & 0 & 0 \end{pmatrix} @ \begin{pmatrix} \frac{1}{2} & 0 & 0 \end{pmatrix}$	[5,-6,-7,8,-13,14,15,-16]
B <sub>2</sub> [1c: 4/mmm]	b <sub>3</sub>	A <sub>1</sub>	A <sub>1</sub>	2	1	$\begin{pmatrix} 1 & 1 & 0 \end{pmatrix} @ \begin{pmatrix} \frac{1}{2} & \frac{1}{2} & 0 \end{pmatrix}$	[1,-2,5,-6,-9,10,-13,14]
	b <sub>4</sub>	A <sub>1</sub>	A <sub>1</sub>	2	1	$\begin{pmatrix} 1 & -1 & 0 \end{pmatrix} @ \begin{pmatrix} \frac{1}{2} & \frac{1}{2} & 0 \end{pmatrix}$	[3,-4,-7,8,-11,12,15,-16]
B <sub>3</sub> [1b: 4/mmm]	b <sub>5</sub>	A <sub>1</sub>	A <sub>1</sub>	3	1	$\begin{pmatrix} 0 & 0 & 1 \end{pmatrix} @ \begin{pmatrix} 0 & 0 & \frac{1}{2} \end{pmatrix}$	[1,2,-3,-4,-5,-6,7,8,-9,-10,11,12,13,14,-15,-16]
B <sub>4</sub> [2e: mmm.]	b <sub>6</sub>	A <sub>1</sub>	A <sub>1</sub>	4	1	$\begin{pmatrix} 0 & 1 & 1 \end{pmatrix} @ \begin{pmatrix} 0 & \frac{1}{2} & \frac{1}{2} \end{pmatrix}$	[1,-3,-9,11]
	b <sub>7</sub>	A <sub>1</sub>	A <sub>1</sub>	4	1	$\begin{pmatrix} 0 & 1 & -1 \end{pmatrix} @ \begin{pmatrix} 0 & \frac{1}{2} & \frac{1}{2} \end{pmatrix}$	[-2,4,10,-12]
	b <sub>8</sub>	A <sub>1</sub>	A <sub>1</sub>	4	1	$\begin{pmatrix} 1 & 0 & -1 \end{pmatrix} @ \begin{pmatrix} \frac{1}{2} & 0 & \frac{1}{2} \end{pmatrix}$	[5,-7,-13,15]
	b <sub>9</sub>	A <sub>1</sub>	A <sub>1</sub>	4	1	$\begin{pmatrix} 1 & 0 & 1 \end{pmatrix} @ \begin{pmatrix} \frac{1}{2} & 0 & \frac{1}{2} \end{pmatrix}$	[-6,8,14,-16]

- SAMB:

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

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

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

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

$$\boxed{\text{No. 3}} \quad \hat{\mathbb{Q}}_2^{(A_{1g})} [\text{M}_3, \text{S}_1]$$

$$\hat{\mathbb{Z}}_3 = \mathbb{X}_{12}[\mathbb{Q}_2^{(a, A_{1g})}] \otimes \mathbb{Y}_1[\mathbb{Q}_0^{(s, A_{1g})}]$$

$$\boxed{\text{No. 4}} \quad \hat{\mathbb{Q}}_0^{(A_{1g})} (1, 1) [\text{M}_3, \text{S}_1]$$

$$\hat{\mathbb{Z}}_4 = \mathbb{X}_{13}[\mathbb{Q}_0^{(a, A_{1g})} (1, 1)] \otimes \mathbb{Y}_1[\mathbb{Q}_0^{(s, A_{1g})}]$$

$$\boxed{\text{No. 5}} \quad \hat{\mathbb{Q}}_2^{(A_{1g})} (1, -1) [\text{M}_3, \text{S}_1]$$

$$\hat{\mathbb{Z}}_5 = \mathbb{X}_{14}[\mathbb{Q}_2^{(a, A_{1g})} (1, -1)] \otimes \mathbb{Y}_1[\mathbb{Q}_0^{(s, A_{1g})}]$$

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

$$\hat{\mathbb{Z}}_6 = \mathbb{X}_1[\mathbb{Q}_0^{(a, A_{1g})}] \otimes \mathbb{Y}_2[\mathbb{Q}_0^{(b, A_{1g})}]$$

$$\boxed{\text{No. 7}} \quad \hat{\mathbb{Q}}_2^{(A_{1g})} (1, -1) [\text{M}_2, \text{B}_1]$$

$$\hat{\mathbb{Z}}_7 = -\frac{\sqrt{2}\mathbb{X}_3[\mathbb{M}_{2,0}^{(a, Eu)} (1, -1)] \otimes \mathbb{Y}_4[\mathbb{T}_{1,0}^{(b, Eu)}]}{2} + \frac{\sqrt{2}\mathbb{X}_4[\mathbb{M}_{2,1}^{(a, Eu)} (1, -1)] \otimes \mathbb{Y}_5[\mathbb{T}_{1,1}^{(b, Eu)}]}{2}$$

$$\boxed{\text{No. 8}} \quad \hat{\mathbb{Q}}_0^{(A_{1g})} (1, 0) [\text{M}_2, \text{B}_1]$$

$$\hat{\mathbb{Z}}_8 = \frac{\sqrt{2}\mathbb{X}_5[\mathbb{T}_{1,0}^{(a, Eu)} (1, 0)] \otimes \mathbb{Y}_4[\mathbb{T}_{1,0}^{(b, Eu)}]}{2} + \frac{\sqrt{2}\mathbb{X}_6[\mathbb{T}_{1,1}^{(a, Eu)} (1, 0)] \otimes \mathbb{Y}_5[\mathbb{T}_{1,1}^{(b, Eu)}]}{2}$$

$$\boxed{\text{No. 9}} \quad \hat{\mathbb{Q}}_0^{(A_{1g})} [\text{M}_2, \text{B}_1]$$

$$\hat{\mathbb{Z}}_9 = \frac{\sqrt{2}\mathbb{X}_8[\mathbb{T}_{1,0}^{(a, Eu)}] \otimes \mathbb{Y}_4[\mathbb{T}_{1,0}^{(b, Eu)}]}{2} + \frac{\sqrt{2}\mathbb{X}_9[\mathbb{T}_{1,1}^{(a, Eu)}] \otimes \mathbb{Y}_5[\mathbb{T}_{1,1}^{(b, Eu)}]}{2}$$

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

$$\hat{\mathbb{Z}}_{10} = \mathbb{X}_{11}[\mathbb{Q}_0^{(a, A_{1g})}] \otimes \mathbb{Y}_2[\mathbb{Q}_0^{(b, A_{1g})}]$$

$$\boxed{\text{No. 11}} \quad \hat{\mathbb{Q}}_2^{(A_{1g})} [\text{M}_3, \text{B}_1]$$

$$\hat{\mathbb{Z}}_{11} = \mathbb{X}_{12}[\mathbb{Q}_2^{(a, A_{1g})}] \otimes \mathbb{Y}_2[\mathbb{Q}_0^{(b, A_{1g})}]$$

$$\boxed{\text{No. 12}} \quad \hat{\mathbb{Q}}_0^{(A_{1g})} [\text{M}_3, \text{B}_1]$$

$$\hat{\mathbb{Z}}_{12} = \mathbb{X}_{15}[\mathbb{Q}_2^{(a, B_{1g})}] \otimes \mathbb{Y}_3[\mathbb{Q}_2^{(b, B_{1g})}]$$

$$\boxed{\text{No. 13}} \quad \hat{\mathbb{Q}}_0^{(A_{1g})} (1, 1) [\text{M}_3, \text{B}_1]$$

$$\hat{\mathbb{Z}}_{13} = \mathbb{X}_{13}[\mathbb{Q}_0^{(a, A_{1g})} (1, 1)] \otimes \mathbb{Y}_2[\mathbb{Q}_0^{(b, A_{1g})}]$$

$$\boxed{\text{No. 14}} \quad \hat{\mathbb{Q}}_2^{(A_{1g})} (1, -1) [\text{M}_3, \text{B}_1]$$

$$\hat{\mathbb{Z}}_{14} = \mathbb{X}_{14}[\mathbb{Q}_2^{(a, A_{1g})} (1, -1)] \otimes \mathbb{Y}_2[\mathbb{Q}_0^{(b, A_{1g})}]$$

$$\boxed{\text{No. 15}} \quad \hat{\mathbb{Q}}_0^{(A_{1g})} (1, -1) [\text{M}_3, \text{B}_1]$$

$$\hat{\mathbb{Z}}_{15} = \mathbb{X}_{19}[\mathbb{Q}_2^{(a, B_{1g})} (1, -1)] \otimes \mathbb{Y}_3[\mathbb{Q}_2^{(b, B_{1g})}]$$

$$\boxed{\text{No. 16}} \quad \hat{\mathbb{Q}}_0^{(A_{1g})} [\text{M}_1, \text{B}_2]$$

$$\hat{\mathbb{Z}}_{16} = \mathbb{X}_1[\mathbb{Q}_0^{(a, A_{1g})}] \otimes \mathbb{Y}_6[\mathbb{Q}_0^{(b, A_{1g})}]$$

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

$$\hat{\mathbb{Z}}_{17} = -\frac{\sqrt{2}\mathbb{X}_3[\mathbb{M}_{2,0}^{(a, Eu)} (1, -1)] \otimes \mathbb{Y}_8[\mathbb{T}_{1,0}^{(b, Eu)}]}{2} + \frac{\sqrt{2}\mathbb{X}_4[\mathbb{M}_{2,1}^{(a, Eu)} (1, -1)] \otimes \mathbb{Y}_9[\mathbb{T}_{1,1}^{(b, Eu)}]}{2}$$

$$\boxed{\text{No. 18}} \quad \hat{\mathbb{Q}}_0^{(A_{1g})}(1, 0) \text{ [M}_2, \text{B}_2]$$

$$\hat{\mathbb{Z}}_{18} = \frac{\sqrt{2}\mathbb{X}_5[\mathbb{T}_{1,0}^{(a,E_u)}(1, 0)] \otimes \mathbb{Y}_8[\mathbb{T}_{1,0}^{(b,E_u)}]}{2} + \frac{\sqrt{2}\mathbb{X}_6[\mathbb{T}_{1,1}^{(a,E_u)}(1, 0)] \otimes \mathbb{Y}_9[\mathbb{T}_{1,1}^{(b,E_u)}]}{2}$$

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

$$\hat{\mathbb{Z}}_{19} = \frac{\sqrt{2}\mathbb{X}_8[\mathbb{T}_{1,0}^{(a,E_u)}] \otimes \mathbb{Y}_8[\mathbb{T}_{1,0}^{(b,E_u)}]}{2} + \frac{\sqrt{2}\mathbb{X}_9[\mathbb{T}_{1,1}^{(a,E_u)}] \otimes \mathbb{Y}_9[\mathbb{T}_{1,1}^{(b,E_u)}]}{2}$$

$$\boxed{\text{No. 20}} \quad \hat{\mathbb{Q}}_0^{(A_{1g})} \text{ [M}_3, \text{B}_2]$$

$$\hat{\mathbb{Z}}_{20} = \mathbb{X}_{11}[\mathbb{Q}_0^{(a,A_{1g})}] \otimes \mathbb{Y}_6[\mathbb{Q}_0^{(b,A_{1g})}]$$

$$\boxed{\text{No. 21}} \quad \hat{\mathbb{Q}}_2^{(A_{1g})} \text{ [M}_3, \text{B}_2]$$

$$\hat{\mathbb{Z}}_{21} = \mathbb{X}_{12}[\mathbb{Q}_2^{(a,A_{1g})}] \otimes \mathbb{Y}_6[\mathbb{Q}_0^{(b,A_{1g})}]$$

$$\boxed{\text{No. 22}} \quad \hat{\mathbb{Q}}_0^{(A_{1g})} \text{ [M}_3, \text{B}_2]$$

$$\hat{\mathbb{Z}}_{22} = \mathbb{X}_{16}[\mathbb{Q}_2^{(a,B_{2g})}] \otimes \mathbb{Y}_7[\mathbb{Q}_2^{(b,B_{2g})}]$$

$$\boxed{\text{No. 23}} \quad \hat{\mathbb{Q}}_0^{(A_{1g})}(1, 1) \text{ [M}_3, \text{B}_2]$$

$$\hat{\mathbb{Z}}_{23} = \mathbb{X}_{13}[\mathbb{Q}_0^{(a,A_{1g})}(1, 1)] \otimes \mathbb{Y}_6[\mathbb{Q}_0^{(b,A_{1g})}]$$

$$\boxed{\text{No. 24}} \quad \hat{\mathbb{Q}}_2^{(A_{1g})}(1, -1) \text{ [M}_3, \text{B}_2]$$

$$\hat{\mathbb{Z}}_{24} = \mathbb{X}_{14}[\mathbb{Q}_2^{(a,A_{1g})}(1, -1)] \otimes \mathbb{Y}_6[\mathbb{Q}_0^{(b,A_{1g})}]$$

$$\boxed{\text{No. 25}} \quad \hat{\mathbb{Q}}_0^{(A_{1g})}(1, -1) \text{ [M}_3, \text{B}_2]$$

$$\hat{\mathbb{Z}}_{25} = \mathbb{X}_{20}[\mathbb{Q}_2^{(a,B_{2g})}(1, -1)] \otimes \mathbb{Y}_7[\mathbb{Q}_2^{(b,B_{2g})}]$$

$$\boxed{\text{No. 26}} \quad \hat{\mathbb{Q}}_0^{(A_{1g})} \text{ [M}_1, \text{B}_3]$$

$$\hat{\mathbb{Z}}_{26} = \mathbb{X}_1[\mathbb{Q}_0^{(a,A_{1g})}] \otimes \mathbb{Y}_{10}[\mathbb{Q}_0^{(b,A_{1g})}]$$

$$\boxed{\text{No. 27}} \quad \hat{\mathbb{Q}}_0^{(A_{1g})}(1, 0) \text{ [M}_2, \text{B}_3]$$

$$\hat{\mathbb{Z}}_{27} = \mathbb{X}_{10}[\mathbb{T}_1^{(a, A_{2u})}(1, 0)] \otimes \mathbb{Y}_{11}[\mathbb{T}_1^{(b, A_{2u})}]$$

$$\boxed{\text{No. 28}} \quad \hat{\mathbb{Q}}_0^{(A_{1g})} \text{ [M}_2, \text{B}_3]$$

$$\hat{\mathbb{Z}}_{28} = \mathbb{X}_7[\mathbb{T}_1^{(a, A_{2u})}] \otimes \mathbb{Y}_{11}[\mathbb{T}_1^{(b, A_{2u})}]$$

$$\boxed{\text{No. 29}} \quad \hat{\mathbb{Q}}_0^{(A_{1g})} \text{ [M}_3, \text{B}_3]$$

$$\hat{\mathbb{Z}}_{29} = \mathbb{X}_{11}[\mathbb{Q}_0^{(a, A_{1g})}] \otimes \mathbb{Y}_{10}[\mathbb{Q}_0^{(b, A_{1g})}]$$

$$\boxed{\text{No. 30}} \quad \hat{\mathbb{Q}}_2^{(A_{1g})} \text{ [M}_3, \text{B}_3]$$

$$\hat{\mathbb{Z}}_{30} = \mathbb{X}_{12}[\mathbb{Q}_2^{(a, A_{1g})}] \otimes \mathbb{Y}_{10}[\mathbb{Q}_0^{(b, A_{1g})}]$$

$$\boxed{\text{No. 31}} \quad \hat{\mathbb{Q}}_0^{(A_{1g})}(1, 1) \text{ [M}_3, \text{B}_3]$$

$$\hat{\mathbb{Z}}_{31} = \mathbb{X}_{13}[\mathbb{Q}_0^{(a, A_{1g})}(1, 1)] \otimes \mathbb{Y}_{10}[\mathbb{Q}_0^{(b, A_{1g})}]$$

$$\boxed{\text{No. 32}} \quad \hat{\mathbb{Q}}_2^{(A_{1g})}(1, -1) \text{ [M}_3, \text{B}_3]$$

$$\hat{\mathbb{Z}}_{32} = \mathbb{X}_{14}[\mathbb{Q}_2^{(a, A_{1g})}(1, -1)] \otimes \mathbb{Y}_{10}[\mathbb{Q}_0^{(b, A_{1g})}]$$

$$\boxed{\text{No. 33}} \quad \hat{\mathbb{Q}}_0^{(A_{1g})} \text{ [M}_1, \text{B}_4]$$

$$\hat{\mathbb{Z}}_{33} = \mathbb{X}_1[\mathbb{Q}_0^{(a, A_{1g})}] \otimes \mathbb{Y}_{12}[\mathbb{Q}_0^{(b, A_{1g})}]$$

$$\boxed{\text{No. 34}} \quad \hat{\mathbb{Q}}_2^{(A_{1g})}(1, -1) \text{ [M}_2, \text{B}_4]$$

$$\hat{\mathbb{Z}}_{34} = -\frac{\sqrt{2}\mathbb{X}_3[\mathbb{M}_{2,0}^{(a, E_u)}(1, -1)] \otimes \mathbb{Y}_{17}[\mathbb{T}_{1,0}^{(b, E_u)}]}{2} + \frac{\sqrt{2}\mathbb{X}_4[\mathbb{M}_{2,1}^{(a, E_u)}(1, -1)] \otimes \mathbb{Y}_{18}[\mathbb{T}_{1,1}^{(b, E_u)}]}{2}$$

$$\boxed{\text{No. 35}} \quad \hat{\mathbb{Q}}_2^{(A_{1g})}(1, -1) \text{ [M}_2, \text{B}_4]$$

$$\hat{\mathbb{Z}}_{35} = -\mathbb{X}_2[\mathbb{M}_2^{(a, B_{2u})}(1, -1)] \otimes \mathbb{Y}_{19}[\mathbb{T}_3^{(b, B_{2u})}]$$

$$\boxed{\text{No. 36}} \quad \hat{\mathbb{Q}}_0^{(A_{1g})}(1, 0) \text{ [M}_2, \text{B}_4]$$

$$\hat{\mathbb{Z}}_{36} = \frac{\sqrt{3}\mathbb{X}_{10}[\mathbb{T}_1^{(a, A_{2u})}(1, 0)] \otimes \mathbb{Y}_{16}[\mathbb{T}_1^{(b, A_{2u})}]}{3} + \frac{\sqrt{3}\mathbb{X}_5[\mathbb{T}_{1,0}^{(a, Eu)}(1, 0)] \otimes \mathbb{Y}_{17}[\mathbb{T}_{1,0}^{(b, Eu)}]}{3} + \frac{\sqrt{3}\mathbb{X}_6[\mathbb{T}_{1,1}^{(a, Eu)}(1, 0)] \otimes \mathbb{Y}_{18}[\mathbb{T}_{1,1}^{(b, Eu)}]}{3}$$

$$\boxed{\text{No. 37}} \quad \hat{\mathbb{Q}}_2^{(A_{1g})}(1, 0) \text{ [M}_2, \text{B}_4]$$

$$\hat{\mathbb{Z}}_{37} = \frac{\sqrt{6}\mathbb{X}_{10}[\mathbb{T}_1^{(a, A_{2u})}(1, 0)] \otimes \mathbb{Y}_{16}[\mathbb{T}_1^{(b, A_{2u})}]}{3} - \frac{\sqrt{6}\mathbb{X}_5[\mathbb{T}_{1,0}^{(a, Eu)}(1, 0)] \otimes \mathbb{Y}_{17}[\mathbb{T}_{1,0}^{(b, Eu)}]}{6} - \frac{\sqrt{6}\mathbb{X}_6[\mathbb{T}_{1,1}^{(a, Eu)}(1, 0)] \otimes \mathbb{Y}_{18}[\mathbb{T}_{1,1}^{(b, Eu)}]}{6}$$

$$\boxed{\text{No. 38}} \quad \hat{\mathbb{Q}}_0^{(A_{1g})} \text{ [M}_2, \text{B}_4]$$

$$\hat{\mathbb{Z}}_{38} = \frac{\sqrt{3}\mathbb{X}_7[\mathbb{T}_1^{(a, A_{2u})}] \otimes \mathbb{Y}_{16}[\mathbb{T}_1^{(b, A_{2u})}]}{3} + \frac{\sqrt{3}\mathbb{X}_8[\mathbb{T}_{1,0}^{(a, Eu)}] \otimes \mathbb{Y}_{17}[\mathbb{T}_{1,0}^{(b, Eu)}]}{3} + \frac{\sqrt{3}\mathbb{X}_9[\mathbb{T}_{1,1}^{(a, Eu)}] \otimes \mathbb{Y}_{18}[\mathbb{T}_{1,1}^{(b, Eu)}]}{3}$$

$$\boxed{\text{No. 39}} \quad \hat{\mathbb{Q}}_2^{(A_{1g})} \text{ [M}_2, \text{B}_4]$$

$$\hat{\mathbb{Z}}_{39} = \frac{\sqrt{6}\mathbb{X}_7[\mathbb{T}_1^{(a, A_{2u})}] \otimes \mathbb{Y}_{16}[\mathbb{T}_1^{(b, A_{2u})}]}{3} - \frac{\sqrt{6}\mathbb{X}_8[\mathbb{T}_{1,0}^{(a, Eu)}] \otimes \mathbb{Y}_{17}[\mathbb{T}_{1,0}^{(b, Eu)}]}{6} - \frac{\sqrt{6}\mathbb{X}_9[\mathbb{T}_{1,1}^{(a, Eu)}] \otimes \mathbb{Y}_{18}[\mathbb{T}_{1,1}^{(b, Eu)}]}{6}$$

$$\boxed{\text{No. 40}} \quad \hat{\mathbb{Q}}_0^{(A_{1g})} \text{ [M}_3, \text{B}_4]$$

$$\hat{\mathbb{Z}}_{40} = \mathbb{X}_{11}[\mathbb{Q}_0^{(a, A_{1g})}] \otimes \mathbb{Y}_{12}[\mathbb{Q}_0^{(b, A_{1g})}]$$

$$\boxed{\text{No. 41}} \quad \hat{\mathbb{Q}}_2^{(A_{1g})} \text{ [M}_3, \text{B}_4]$$

$$\hat{\mathbb{Z}}_{41} = \mathbb{X}_{12}[\mathbb{Q}_2^{(a, A_{1g})}] \otimes \mathbb{Y}_{12}[\mathbb{Q}_0^{(b, A_{1g})}]$$

$$\boxed{\text{No. 42}} \quad \hat{\mathbb{Q}}_0^{(A_{1g})} \text{ [M}_3, \text{B}_4]$$

$$\hat{\mathbb{Z}}_{42} = \frac{\sqrt{3}\mathbb{X}_{15}[\mathbb{Q}_2^{(a, B_{1g})}] \otimes \mathbb{Y}_{13}[\mathbb{Q}_2^{(b, B_{1g})}]}{3} + \frac{\sqrt{3}\mathbb{X}_{17}[\mathbb{Q}_{2,0}^{(a, E_g)}] \otimes \mathbb{Y}_{14}[\mathbb{Q}_{2,0}^{(b, E_g)}]}{3} + \frac{\sqrt{3}\mathbb{X}_{18}[\mathbb{Q}_{2,1}^{(a, E_g)}] \otimes \mathbb{Y}_{15}[\mathbb{Q}_{2,1}^{(b, E_g)}]}{3}$$

$$\boxed{\text{No. 43}} \quad \hat{\mathbb{Q}}_2^{(A_{1g})} \text{ [M}_3, \text{B}_4]$$

$$\hat{\mathbb{Z}}_{43} = -\frac{\sqrt{6}\mathbb{X}_{15}[\mathbb{Q}_2^{(a, B_{1g})}] \otimes \mathbb{Y}_{13}[\mathbb{Q}_2^{(b, B_{1g})}]}{3} + \frac{\sqrt{6}\mathbb{X}_{17}[\mathbb{Q}_{2,0}^{(a, E_g)}] \otimes \mathbb{Y}_{14}[\mathbb{Q}_{2,0}^{(b, E_g)}]}{6} + \frac{\sqrt{6}\mathbb{X}_{18}[\mathbb{Q}_{2,1}^{(a, E_g)}] \otimes \mathbb{Y}_{15}[\mathbb{Q}_{2,1}^{(b, E_g)}]}{6}$$

$$\boxed{\text{No. 44}} \quad \hat{\mathbb{Q}}_0^{(A_{1g})}(1, 1) \text{ [M}_3, \text{B}_4]$$

$$\hat{\mathbb{Z}}_{44} = \mathbb{X}_{13}[\mathbb{Q}_0^{(a, A_{1g})}(1, 1)] \otimes \mathbb{Y}_{12}[\mathbb{Q}_0^{(b, A_{1g})}]$$

$$\boxed{\text{No. 45}} \quad \hat{\mathbb{Q}}_2^{(A_{1g})}(1, -1) \text{ [M}_3, \text{B}_4]$$

$$\hat{\mathbb{Z}}_{45} = \mathbb{X}_{14}[\mathbb{Q}_2^{(a, A_{1g})}(1, -1)] \otimes \mathbb{Y}_{12}[\mathbb{Q}_0^{(b, A_{1g})}]$$

$$\boxed{\text{No. 46}} \quad \hat{\mathbb{Q}}_0^{(A_{1g})}(1, -1) \text{ [M}_3, \text{B}_4]$$

$$\hat{\mathbb{Z}}_{46} = \frac{\sqrt{3}\mathbb{X}_{19}[\mathbb{Q}_2^{(a, B_{1g})}(1, -1)] \otimes \mathbb{Y}_{13}[\mathbb{Q}_2^{(b, B_{1g})}]}{3} + \frac{\sqrt{3}\mathbb{X}_{21}[\mathbb{Q}_{2,0}^{(a, E_g)}(1, -1)] \otimes \mathbb{Y}_{14}[\mathbb{Q}_{2,0}^{(b, E_g)}]}{3} + \frac{\sqrt{3}\mathbb{X}_{22}[\mathbb{Q}_{2,1}^{(a, E_g)}(1, -1)] \otimes \mathbb{Y}_{15}[\mathbb{Q}_{2,1}^{(b, E_g)}]}{3}$$

$$\boxed{\text{No. 47}} \quad \hat{\mathbb{Q}}_2^{(A_{1g})}(1, -1) \text{ [M}_3, \text{B}_4]$$

$$\hat{\mathbb{Z}}_{47} = -\frac{\sqrt{6}\mathbb{X}_{19}[\mathbb{Q}_2^{(a, B_{1g})}(1, -1)] \otimes \mathbb{Y}_{13}[\mathbb{Q}_2^{(b, B_{1g})}]}{3} + \frac{\sqrt{6}\mathbb{X}_{21}[\mathbb{Q}_{2,0}^{(a, E_g)}(1, -1)] \otimes \mathbb{Y}_{14}[\mathbb{Q}_{2,0}^{(b, E_g)}]}{6} + \frac{\sqrt{6}\mathbb{X}_{22}[\mathbb{Q}_{2,1}^{(a, E_g)}(1, -1)] \otimes \mathbb{Y}_{15}[\mathbb{Q}_{2,1}^{(b, E_g)}]}{6}$$

$$\boxed{\text{No. 48}} \quad \hat{\mathbb{Q}}_2^{(A_{1g})}(1, 0) \text{ [M}_3, \text{B}_4]$$

$$\hat{\mathbb{Z}}_{48} = \frac{\sqrt{2}\mathbb{X}_{23}[\mathbb{G}_{1,0}^{(a, E_g)}(1, 0)] \otimes \mathbb{Y}_{14}[\mathbb{Q}_{2,0}^{(b, E_g)}]}{2} - \frac{\sqrt{2}\mathbb{X}_{24}[\mathbb{G}_{1,1}^{(a, E_g)}(1, 0)] \otimes \mathbb{Y}_{15}[\mathbb{Q}_{2,1}^{(b, E_g)}]}{2}$$

Table 5: Atomic SAMB group.

group	bra	ket
M <sub>1</sub>	$(s, \uparrow), (s, \downarrow)$	$(s, \uparrow), (s, \downarrow)$
M <sub>2</sub>	$(s, \uparrow), (s, \downarrow)$	$(p_x, \uparrow), (p_x, \downarrow), (p_y, \uparrow), (p_y, \downarrow), (p_z, \uparrow), (p_z, \downarrow)$
M <sub>3</sub>	$(p_x, \uparrow), (p_x, \downarrow), (p_y, \uparrow), (p_y, \downarrow), (p_z, \uparrow), (p_z, \downarrow)$	$(p_x, \uparrow), (p_x, \downarrow), (p_y, \uparrow), (p_y, \downarrow), (p_z, \uparrow), (p_z, \downarrow)$



Table 6: Atomic SAMB.

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

continued ...

Table 6

symbol	type	group	form
$\mathbb{X}_{13}$	$\mathbb{Q}_0^{(a,A_{1g})}(1,1)$	$M_3$	$\begin{pmatrix} 0 & 0 & -\frac{\sqrt{3}i}{6} & 0 & 0 & \frac{\sqrt{3}}{6} \\ 0 & 0 & 0 & \frac{\sqrt{3}i}{6} & -\frac{\sqrt{3}}{6} & 0 \\ \frac{\sqrt{3}i}{6} & 0 & 0 & 0 & 0 & -\frac{\sqrt{3}i}{6} \\ 0 & -\frac{\sqrt{3}i}{6} & 0 & 0 & -\frac{\sqrt{3}}{6} & 0 \\ 0 & -\frac{\sqrt{3}}{6} & 0 & \frac{\sqrt{3}i}{6} & 0 & 0 \\ \frac{\sqrt{3}}{6} & 0 & \frac{\sqrt{3}i}{6} & 0 & 0 & 0 \end{pmatrix}$
$\mathbb{X}_{14}$	$\mathbb{Q}_2^{(a,A_{1g})}(1,-1)$	$M_3$	$\begin{pmatrix} 0 & 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 & -\frac{\sqrt{6}}{12} \\ 0 & 0 & 0 & \frac{\sqrt{6}i}{6} & \frac{\sqrt{6}}{12} & 0 \\ \frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 & \frac{\sqrt{6}}{12} \\ 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 & \frac{\sqrt{6}i}{12} & 0 \\ 0 & \frac{\sqrt{6}}{12} & 0 & -\frac{\sqrt{6}i}{12} & 0 & 0 \\ -\frac{\sqrt{6}}{12} & 0 & -\frac{\sqrt{6}i}{12} & 0 & 0 & 0 \end{pmatrix}$
$\mathbb{X}_{15}$	$\mathbb{Q}_2^{(a,B_{1g})}$	$M_3$	$\begin{pmatrix} \frac{1}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{1}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$
$\mathbb{X}_{16}$	$\mathbb{Q}_2^{(a,B_{2g})}$	$M_3$	$\begin{pmatrix} 0 & 0 & \frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2} & 0 & 0 \\ \frac{1}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$
$\mathbb{X}_{17}$	$\mathbb{Q}_{2,0}^{(a,E_g)}$	$M_3$	$\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{2} \\ 0 & 0 & \frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2} & 0 & 0 \end{pmatrix}$

continued ...

Table 6

symbol	type	group	form
$\mathbb{X}_{18}$	$\mathbb{Q}_{2,1}^{(a,E_g)}$	$M_3$	$\begin{pmatrix} 0 & 0 & 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{2} \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{1}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 & 0 & 0 \end{pmatrix}$
$\mathbb{X}_{19}$	$\mathbb{Q}_2^{(a,B_{1g})}(1,-1)$	$M_3$	$\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{2}}{4} \\ 0 & 0 & 0 & 0 & \frac{\sqrt{2}}{4} & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{2}i}{4} \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{2}i}{4} & 0 \\ 0 & \frac{\sqrt{2}}{4} & 0 & \frac{\sqrt{2}i}{4} & 0 & 0 \\ -\frac{\sqrt{2}}{4} & 0 & \frac{\sqrt{2}i}{4} & 0 & 0 & 0 \end{pmatrix}$
$\mathbb{X}_{20}$	$\mathbb{Q}_2^{(a,B_{2g})}(1,-1)$	$M_3$	$\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{2}i}{4} \\ 0 & 0 & 0 & 0 & \frac{\sqrt{2}i}{4} & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{2}}{4} \\ 0 & 0 & 0 & 0 & \frac{\sqrt{2}}{4} & 0 \\ 0 & -\frac{\sqrt{2}i}{4} & 0 & \frac{\sqrt{2}}{4} & 0 & 0 \\ -\frac{\sqrt{2}i}{4} & 0 & -\frac{\sqrt{2}}{4} & 0 & 0 & 0 \end{pmatrix}$
$\mathbb{X}_{21}$	$\mathbb{Q}_{2,0}^{(a,E_g)}(1,-1)$	$M_3$	$\begin{pmatrix} 0 & 0 & 0 & -\frac{\sqrt{2}}{4} & \frac{\sqrt{2}i}{4} & 0 \\ 0 & 0 & \frac{\sqrt{2}}{4} & 0 & 0 & -\frac{\sqrt{2}i}{4} \\ 0 & \frac{\sqrt{2}}{4} & 0 & 0 & 0 & 0 \\ -\frac{\sqrt{2}}{4} & 0 & 0 & 0 & 0 & 0 \\ -\frac{\sqrt{2}i}{4} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{2}i}{4} & 0 & 0 & 0 & 0 \end{pmatrix}$
$\mathbb{X}_{22}$	$\mathbb{Q}_{2,1}^{(a,E_g)}(1,-1)$	$M_3$	$\begin{pmatrix} 0 & 0 & 0 & -\frac{\sqrt{2}i}{4} & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{2}i}{4} & 0 & 0 & 0 \\ 0 & \frac{\sqrt{2}i}{4} & 0 & 0 & -\frac{\sqrt{2}i}{4} & 0 \\ \frac{\sqrt{2}i}{4} & 0 & 0 & 0 & 0 & \frac{\sqrt{2}i}{4} \\ 0 & 0 & \frac{\sqrt{2}i}{4} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{2}i}{4} & 0 & 0 \end{pmatrix}$

continued ...

Table 6

symbol	type	group	form
$\mathbb{X}_{23}$	$\mathbb{G}_{1,0}^{(a,E_g)}(1,0)$	$M_3$	$\begin{pmatrix} 0 & 0 & 0 & -\frac{\sqrt{2}}{4} & -\frac{\sqrt{2}i}{4} & 0 \\ 0 & 0 & \frac{\sqrt{2}}{4} & 0 & 0 & \frac{\sqrt{2}i}{4} \\ 0 & \frac{\sqrt{2}}{4} & 0 & 0 & 0 & 0 \\ -\frac{\sqrt{2}}{4} & 0 & 0 & 0 & 0 & 0 \\ \frac{\sqrt{2}i}{4} & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{2}i}{4} & 0 & 0 & 0 & 0 \end{pmatrix}$
$\mathbb{X}_{24}$	$\mathbb{G}_{1,1}^{(a,E_g)}(1,0)$	$M_3$	$\begin{pmatrix} 0 & 0 & 0 & \frac{\sqrt{2}i}{4} & 0 & 0 \\ 0 & 0 & \frac{\sqrt{2}i}{4} & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{2}i}{4} & 0 & 0 & -\frac{\sqrt{2}i}{4} & 0 \\ -\frac{\sqrt{2}i}{4} & 0 & 0 & 0 & 0 & \frac{\sqrt{2}i}{4} \\ 0 & 0 & \frac{\sqrt{2}i}{4} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{2}i}{4} & 0 & 0 \end{pmatrix}$

Table 7: Cluster SAMB.

symbol	type	cluster	form
$\mathbb{Y}_1$	$\mathbb{Q}_0^{(s,A_{1g})}$	$S_1$	$\begin{pmatrix} 1 \end{pmatrix}$
$\mathbb{Y}_2$	$\mathbb{Q}_0^{(b,A_{1g})}$	$B_1$	$\begin{pmatrix} \frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2} \end{pmatrix}$
$\mathbb{Y}_3$	$\mathbb{Q}_2^{(b,B_{1g})}$	$B_1$	$\begin{pmatrix} \frac{\sqrt{2}}{2} & -\frac{\sqrt{2}}{2} \end{pmatrix}$
$\mathbb{Y}_4$	$\mathbb{T}_{1,0}^{(b,E_u)}$	$B_1$	$\begin{pmatrix} 0 & i \end{pmatrix}$
$\mathbb{Y}_5$	$\mathbb{T}_{1,1}^{(b,E_u)}$	$B_1$	$\begin{pmatrix} i & 0 \end{pmatrix}$
$\mathbb{Y}_6$	$\mathbb{Q}_0^{(b,A_{1g})}$	$B_2$	$\begin{pmatrix} \frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2} \end{pmatrix}$
$\mathbb{Y}_7$	$\mathbb{Q}_2^{(b,B_{2g})}$	$B_2$	$\begin{pmatrix} \frac{\sqrt{2}}{2} & -\frac{\sqrt{2}}{2} \end{pmatrix}$
$\mathbb{Y}_8$	$\mathbb{T}_{1,0}^{(b,E_u)}$	$B_2$	$\begin{pmatrix} \frac{\sqrt{2}i}{2} & \frac{\sqrt{2}i}{2} \end{pmatrix}$
$\mathbb{Y}_9$	$\mathbb{T}_{1,1}^{(b,E_u)}$	$B_2$	$\begin{pmatrix} \frac{\sqrt{2}i}{2} & -\frac{\sqrt{2}i}{2} \end{pmatrix}$
$\mathbb{Y}_{10}$	$\mathbb{Q}_0^{(b,A_{1g})}$	$B_3$	$\begin{pmatrix} 1 \end{pmatrix}$
$\mathbb{Y}_{11}$	$\mathbb{T}_1^{(b,A_{2u})}$	$B_3$	$\begin{pmatrix} i \end{pmatrix}$

continued ...

Table 7

symbol	type	cluster	form
$\mathbb{Y}_{12}$	$\mathbb{Q}_0^{(b,A_{1g})}$	$B_4$	$\begin{pmatrix} \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \end{pmatrix}$
$\mathbb{Y}_{13}$	$\mathbb{Q}_2^{(b,B_{1g})}$	$B_4$	$\begin{pmatrix} \frac{1}{2} & \frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} \end{pmatrix}$
$\mathbb{Y}_{14}$	$\mathbb{Q}_{2,0}^{(b,E_g)}$	$B_4$	$\begin{pmatrix} \frac{\sqrt{2}}{2} & -\frac{\sqrt{2}}{2} & 0 & 0 \end{pmatrix}$
$\mathbb{Y}_{15}$	$\mathbb{Q}_{2,1}^{(b,E_g)}$	$B_4$	$\begin{pmatrix} 0 & 0 & -\frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2} \end{pmatrix}$
$\mathbb{Y}_{16}$	$\mathbb{T}_1^{(b,A_{2u})}$	$B_4$	$\begin{pmatrix} \frac{i}{2} & -\frac{i}{2} & -\frac{i}{2} & \frac{i}{2} \end{pmatrix}$
$\mathbb{Y}_{17}$	$\mathbb{T}_{1,0}^{(b,E_u)}$	$B_4$	$\begin{pmatrix} 0 & 0 & \frac{\sqrt{2}i}{2} & \frac{\sqrt{2}i}{2} \end{pmatrix}$
$\mathbb{Y}_{18}$	$\mathbb{T}_{1,1}^{(b,E_u)}$	$B_4$	$\begin{pmatrix} \frac{\sqrt{2}i}{2} & \frac{\sqrt{2}i}{2} & 0 & 0 \end{pmatrix}$
$\mathbb{Y}_{19}$	$\mathbb{T}_3^{(b,B_{2u})}$	$B_4$	$\begin{pmatrix} \frac{i}{2} & -\frac{i}{2} & \frac{i}{2} & -\frac{i}{2} \end{pmatrix}$

Table 8: Polar harmonics.

No.	symbol	rank	irrep.	mul.	comp.	form
1	$\mathbb{Q}_0^{(A_{1g})}$	0	$A_{1g}$	—	—	1
2	$\mathbb{Q}_1^{(A_{2u})}$	1	$A_{2u}$	—	—	$z$
3	$\mathbb{Q}_{1,0}^{(E_u)}$	1	$E_u$	—	0	$x$
4	$\mathbb{Q}_{1,1}^{(E_u)}$	1	$E_u$	—	1	$y$
5	$\mathbb{Q}_2^{(A_{1g})}$	2	$A_{1g}$	—	—	$-\frac{x^2}{2} - \frac{y^2}{2} + z^2$
6	$\mathbb{Q}_2^{(B_{1g})}$	2	$B_{1g}$	—	—	$\frac{\sqrt{3}(x-y)(x+y)}{2}$
7	$\mathbb{Q}_2^{(B_{2g})}$	2	$B_{2g}$	—	—	$\sqrt{3}xy$
8	$\mathbb{Q}_{2,0}^{(E_g)}$	2	$E_g$	—	0	$\sqrt{3}yz$
9	$\mathbb{Q}_{2,1}^{(E_g)}$	2	$E_g$	—	1	$\sqrt{3}xz$
10	$\mathbb{Q}_3^{(B_{2u})}$	3	$B_{2u}$	—	—	$\frac{\sqrt{15}z(x-y)(x+y)}{2}$

Table 9: Axial harmonics.

No.	symbol	rank	irrep.	mul.	comp.	form
1	$\mathbb{G}_{1,0}^{(E_g)}$	1	$E_g$	—	0	$X$
2	$\mathbb{G}_{1,1}^{(E_g)}$	1	$E_g$	—	1	$Y$
3	$\mathbb{G}_2^{(B_{2u})}$	2	$B_{2u}$	—	—	$\sqrt{3}XY$
4	$\mathbb{G}_{2,0}^{(E_u)}$	2	$E_u$	—	0	$\sqrt{3}YZ$
5	$\mathbb{G}_{2,1}^{(E_u)}$	2	$E_u$	—	1	$\sqrt{3}XZ$

- 
- Group info.: Generator =  $\{2_{001}|0\}$ ,  $\{4_{001}^+|0\}$ ,  $\{2_{010}|0\}$ ,  $\{-1|0\}$

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

rep. SO	symmetry operations
$\{1 0\}$	$\{1 0\}$
$\{2_{001} 0\}$	$\{2_{001} 0\}$
$\{2_{100} 0\}$	$\{2_{100} 0\}$ , $\{2_{010} 0\}$
$\{2_{110} 0\}$	$\{2_{110} 0\}$ , $\{2_{1-10} 0\}$
$\{4_{001}^+ 0\}$	$\{4_{001}^+ 0\}$ , $\{4_{001}^- 0\}$
$\{-1 0\}$	$\{-1 0\}$
$\{\mathbf{m}_{001} 0\}$	$\{\mathbf{m}_{001} 0\}$
$\{\mathbf{m}_{100} 0\}$	$\{\mathbf{m}_{100} 0\}$ , $\{\mathbf{m}_{010} 0\}$
$\{\mathbf{m}_{110} 0\}$	$\{\mathbf{m}_{110} 0\}$ , $\{\mathbf{m}_{1-10} 0\}$
$\{-4_{001}^+ 0\}$	$\{-4_{001}^+ 0\}$ , $\{-4_{001}^- 0\}$

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	$\{2_{1-10} 0\}$	7	$\{4^+_{001} 0\}$	8	$\{4^-_{001} 0\}$	9	$\{-1 0\}$	10	$\{m_{001} 0\}$
11	$\{m_{100} 0\}$	12	$\{m_{010} 0\}$	13	$\{m_{110} 0\}$	14	$\{m_{1-10} 0\}$	15	$\{-4^+_{001} 0\}$
16	$\{-4^-_{001} 0\}$								

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

	1	2 <sub>001</sub>	2 <sub>100</sub>	2 <sub>110</sub>	4 <sup>+</sup> <sub>001</sub>	-1	m <sub>001</sub>	m <sub>100</sub>	m <sub>110</sub>	-4 <sup>+</sup> <sub>001</sub>
$A_{1g}$	1	1	1	1	1	1	1	1	1	1
$A_{2g}$	1	1	-1	-1	1	1	1	-1	-1	1
$B_{1g}$	1	1	1	-1	-1	1	1	1	-1	-1
$B_{2g}$	1	1	-1	1	-1	1	1	-1	1	-1
$E_g$	2	-2	0	0	0	2	-2	0	0	0
$A_{1u}$	1	1	1	1	1	-1	-1	-1	-1	-1
$A_{2u}$	1	1	-1	-1	1	-1	-1	1	1	-1
$B_{1u}$	1	1	1	-1	-1	-1	-1	-1	1	1
$B_{2u}$	1	1	-1	1	-1	-1	-1	1	-1	1
$E_u$	2	-2	0	0	0	-2	2	0	0	0

Table 13: Parity conversion.

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

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

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

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

$A_{1g}$	$A_{2g}$	$B_{1g}$	$B_{2g}$	$E_g$	$A_{1u}$	$A_{2u}$	$B_{1u}$	$B_{2u}$	$E_u$
-	-	-	-	$A_{2g}$	-	-	-	-	$A_{2g}$

Table 16: Virtual-cluster sites.

No.	position	No.	position	No.	position	No.	position
1	$\begin{pmatrix} 2 & 1 & 1 \end{pmatrix}$	2	$\begin{pmatrix} -2 & -1 & 1 \end{pmatrix}$	3	$\begin{pmatrix} 2 & -1 & -1 \end{pmatrix}$	4	$\begin{pmatrix} -2 & 1 & -1 \end{pmatrix}$
5	$\begin{pmatrix} 1 & 2 & -1 \end{pmatrix}$	6	$\begin{pmatrix} -1 & -2 & -1 \end{pmatrix}$	7	$\begin{pmatrix} -1 & 2 & 1 \end{pmatrix}$	8	$\begin{pmatrix} 1 & -2 & 1 \end{pmatrix}$
9	$\begin{pmatrix} -2 & -1 & -1 \end{pmatrix}$	10	$\begin{pmatrix} 2 & 1 & -1 \end{pmatrix}$	11	$\begin{pmatrix} -2 & 1 & 1 \end{pmatrix}$	12	$\begin{pmatrix} 2 & -1 & 1 \end{pmatrix}$
13	$\begin{pmatrix} -1 & -2 & 1 \end{pmatrix}$	14	$\begin{pmatrix} 1 & 2 & 1 \end{pmatrix}$	15	$\begin{pmatrix} 1 & -2 & -1 \end{pmatrix}$	16	$\begin{pmatrix} -1 & 2 & -1 \end{pmatrix}$



Table 17: Virtual-cluster basis.

symbol	1	2	3	4	5	6	7	8	9	10
$\mathbb{Q}_0^{(A_{1g})}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$
$\mathbb{Q}_1^{(A_{2u})}$	$\frac{1}{4}$	$\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$
$\mathbb{Q}_{1,0}^{(E_u)}$	$\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{10}$
$\mathbb{Q}_{1,1}^{(E_u)}$	$-\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{20}$
$\mathbb{Q}_2^{(B_{1g})}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$
$\mathbb{Q}_2^{(B_{2g})}$	$\frac{1}{4}$	$\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$
$\mathbb{Q}_{2,0}^{(E_g)}$	$\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{20}$
$\mathbb{Q}_{2,1}^{(E_g)}$	$\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{10}$
$\mathbb{Q}_3^{(B_{1u})}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$
$\mathbb{Q}_3^{(B_{2u})}$	$\frac{1}{4}$	$\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$
$\mathbb{Q}_{3,0}^{(E_{u,1})}$	$\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{20}$
$\mathbb{Q}_{3,1}^{(E_{u,1})}$	$-\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{10}$
$\mathbb{Q}_4^{(A_{2g})}$	$\frac{1}{4}$	$\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$
$\mathbb{Q}_{4,0}^{(E_{g,1})}$	$-\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{10}$
$\mathbb{Q}_{4,1}^{(E_{g,1})}$	$\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{20}$

continued ...

Table 17

symbol	1	2	3	4	5	6	7	8	9	10
	$-\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{10}$				
$\mathbb{Q}_5^{(A_{1u})}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$
	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$				