

# SAMB for “D2h1”

Generated on 2023-05-24 22:50 by MultiPie 1.1.1

- 
- Group: No. 47  $D_{2h}^1$   $Pmmm$  [ orthorhombic ]
  - Associated point group: No. 8  $D_{2h}$   $mmm$  [ orthorhombic ]
  - Generation condition
    - model type: **tight\_binding**
    - time-reversal type: **electric**
    - irrep: [Ag]
    - spinful
- 

- Unit cell:
  - $a = 1.0$ ,  $b = 1.2$ ,  $c = 1.5$ ,  $\alpha = 90.0$ ,  $\beta = 90.0$ ,  $\gamma = 90.0$
- Lattice vectors:
  - $\mathbf{a}_1 = (1.0 \ 0 \ 0)$
  - $\mathbf{a}_2 = (0 \ 1.2 \ 0)$
  - $\mathbf{a}_3 = (0 \ 0 \ 1.5)$

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

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

- 
- 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> A <sub>1</sub>	$\begin{pmatrix} 0 & 0 & 0 \end{pmatrix}$	[1,2,3,4,5,6,7,8]

- Bonds in (primitive) unit cell:

Table 4: Bond-clusters.

bond	tail	head	$n$	#	$\mathbf{b}@c$	mapping
B <sub>1</sub> b <sub>1</sub>	A <sub>1</sub>	A <sub>1</sub>	1	1	$\begin{pmatrix} 1 & 0 & 0 \end{pmatrix} @ \begin{pmatrix} \frac{1}{2} & 0 & 0 \end{pmatrix}$	[1,-2,-3,4,-5,6,7,-8]
B <sub>2</sub> b <sub>2</sub>	A <sub>1</sub>	A <sub>1</sub>	2	1	$\begin{pmatrix} 0 & 1 & 0 \end{pmatrix} @ \begin{pmatrix} 0 & \frac{1}{2} & 0 \end{pmatrix}$	[1,-2,3,-4,-5,6,-7,8]
B <sub>3</sub> b <sub>3</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]
B <sub>4</sub> b <sub>4</sub>	A <sub>1</sub>	A <sub>1</sub>	4	1	$\begin{pmatrix} 1 & 1 & 0 \end{pmatrix} @ \begin{pmatrix} \frac{1}{2} & \frac{1}{2} & 0 \end{pmatrix}$	[1,-2,-5,6]
b <sub>5</sub>	A <sub>1</sub>	A <sub>1</sub>	4	1	$\begin{pmatrix} 1 & -1 & 0 \end{pmatrix} @ \begin{pmatrix} \frac{1}{2} & \frac{1}{2} & 0 \end{pmatrix}$	[-3,4,7,-8]

- SAMB:

$$\boxed{\text{No. 1}} \quad \hat{Q}_0^{(A_g)} [M_1, S_1]$$

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

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

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

$$\hat{\mathbb{Z}}_2 = \mathbb{X}_5[\mathbb{Q}_0^{(a, A_g)}] \otimes \mathbb{Y}_1[\mathbb{Q}_0^{(s, A_g)}]$$

$$\hat{\mathbb{Z}}_2(\mathbf{k}) = \mathbb{X}_5[\mathbb{Q}_0^{(a, A_g)}] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s, A_g)}]$$

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

$$\hat{\mathbb{Z}}_3 = \mathbb{X}_6[\mathbb{Q}_2^{(a, A_g, 1)}] \otimes \mathbb{Y}_1[\mathbb{Q}_0^{(s, A_g)}]$$

$$\hat{\mathbb{Z}}_3(\mathbf{k}) = \mathbb{X}_6[\mathbb{Q}_2^{(a, A_g, 1)}] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s, A_g)}]$$

$$\boxed{\text{No. 4}} \quad \hat{\mathbb{Q}}_2^{(A_g, 2)} [\text{M}_3, \text{S}_1]$$

$$\hat{\mathbb{Z}}_4 = \mathbb{X}_7[\mathbb{Q}_2^{(a, A_g, 2)}] \otimes \mathbb{Y}_1[\mathbb{Q}_0^{(s, A_g)}]$$

$$\hat{\mathbb{Z}}_4(\mathbf{k}) = \mathbb{X}_7[\mathbb{Q}_2^{(a, A_g, 2)}] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s, A_g)}]$$

$$\boxed{\text{No. 5}} \quad \hat{\mathbb{Q}}_0^{(A_g)}(1, 1) [\text{M}_3, \text{S}_1]$$

$$\hat{\mathbb{Z}}_5 = \mathbb{X}_8[\mathbb{Q}_0^{(a, A_g)}(1, 1)] \otimes \mathbb{Y}_1[\mathbb{Q}_0^{(s, A_g)}]$$

$$\hat{\mathbb{Z}}_5(\mathbf{k}) = \mathbb{X}_8[\mathbb{Q}_0^{(a, A_g)}(1, 1)] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s, A_g)}]$$

$$\boxed{\text{No. 6}} \quad \hat{\mathbb{Q}}_2^{(A_g, 1)}(1, -1) [\text{M}_3, \text{S}_1]$$

$$\hat{\mathbb{Z}}_6 = \mathbb{X}_9[\mathbb{Q}_2^{(a, A_g, 1)}(1, -1)] \otimes \mathbb{Y}_1[\mathbb{Q}_0^{(s, A_g)}]$$

$$\hat{\mathbb{Z}}_6(\mathbf{k}) = \mathbb{X}_9[\mathbb{Q}_2^{(a, A_g, 1)}(1, -1)] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s, A_g)}]$$

$$\boxed{\text{No. 7}} \quad \hat{\mathbb{Q}}_2^{(A_g, 2)}(1, -1) [\text{M}_3, \text{S}_1]$$

$$\hat{\mathbb{Z}}_7 = \mathbb{X}_{10}[\mathbb{Q}_2^{(a, A_g, 2)}(1, -1)] \otimes \mathbb{Y}_1[\mathbb{Q}_0^{(s, A_g)}]$$

$$\hat{\mathbb{Z}}_7(\mathbf{k}) = \mathbb{X}_{10}[\mathbb{Q}_2^{(a,A_g,2)}(1,-1)] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_g)}]$$

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

$$\hat{\mathbb{Z}}_8 = \mathbb{X}_1[\mathbb{Q}_0^{(a,A_g)}] \otimes \mathbb{Y}_2[\mathbb{Q}_0^{(b,A_g)}]$$

$$\hat{\mathbb{Z}}_8(\mathbf{k}) = \mathbb{X}_1[\mathbb{Q}_0^{(a,A_g)}] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_g)}] \otimes \mathbb{F}_1[\mathbb{Q}_0^{(k,A_g)}]$$

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

$$\hat{\mathbb{Z}}_9 = -\mathbb{X}_4[\mathbb{M}_2^{(a,B_{3u})}(1,-1)] \otimes \mathbb{Y}_3[\mathbb{T}_1^{(b,B_{3u})}]$$

$$\hat{\mathbb{Z}}_9(\mathbf{k}) = -\mathbb{X}_4[\mathbb{M}_2^{(a,B_{3u})}(1,-1)] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_g)}] \otimes \mathbb{F}_2[\mathbb{T}_1^{(k,B_{3u})}]$$

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

$$\hat{\mathbb{Z}}_{10} = \mathbb{X}_5[\mathbb{Q}_0^{(a,A_g)}] \otimes \mathbb{Y}_2[\mathbb{Q}_0^{(b,A_g)}]$$

$$\hat{\mathbb{Z}}_{10}(\mathbf{k}) = \mathbb{X}_5[\mathbb{Q}_0^{(a,A_g)}] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_g)}] \otimes \mathbb{F}_1[\mathbb{Q}_0^{(k,A_g)}]$$

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

$$\hat{\mathbb{Z}}_{11} = \mathbb{X}_6[\mathbb{Q}_2^{(a,A_g,1)}] \otimes \mathbb{Y}_2[\mathbb{Q}_0^{(b,A_g)}]$$

$$\hat{\mathbb{Z}}_{11}(\mathbf{k}) = \mathbb{X}_6[\mathbb{Q}_2^{(a,A_g,1)}] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_g)}] \otimes \mathbb{F}_1[\mathbb{Q}_0^{(k,A_g)}]$$

$$\boxed{\text{No. 12}} \quad \hat{\mathbb{Q}}_2^{(A_g,2)} [\mathbb{M}_3, \mathbb{B}_1]$$

$$\hat{\mathbb{Z}}_{12} = \mathbb{X}_7[\mathbb{Q}_2^{(a,A_g,2)}] \otimes \mathbb{Y}_2[\mathbb{Q}_0^{(b,A_g)}]$$

$$\hat{\mathbb{Z}}_{12}(\mathbf{k}) = \mathbb{X}_7[\mathbb{Q}_2^{(a,A_g,2)}] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_g)}] \otimes \mathbb{F}_1[\mathbb{Q}_0^{(k,A_g)}]$$

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

$$\hat{\mathbb{Z}}_{13} = \mathbb{X}_8[\mathbb{Q}_0^{(a,A_g)}(1,1)] \otimes \mathbb{Y}_2[\mathbb{Q}_0^{(b,A_g)}]$$

$$\hat{Z}_{13}(\mathbf{k}) = \mathbb{X}_8[\mathbb{Q}_0^{(a,A_g)}(1,1)] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_g)}] \otimes \mathbb{F}_1[\mathbb{Q}_0^{(k,A_g)}]$$

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

$$\hat{Z}_{14} = \mathbb{X}_9[\mathbb{Q}_2^{(a,A_g,1)}(1,-1)] \otimes \mathbb{Y}_2[\mathbb{Q}_0^{(b,A_g)}]$$

$$\hat{Z}_{14}(\mathbf{k}) = \mathbb{X}_9[\mathbb{Q}_2^{(a,A_g,1)}(1,-1)] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_g)}] \otimes \mathbb{F}_1[\mathbb{Q}_0^{(k,A_g)}]$$

$$\boxed{\text{No. 15}} \quad \hat{\mathbb{Q}}_2^{(A_g,2)}(1,-1) [\text{M}_3, \text{B}_1]$$

$$\hat{Z}_{15} = \mathbb{X}_{10}[\mathbb{Q}_2^{(a,A_g,2)}(1,-1)] \otimes \mathbb{Y}_2[\mathbb{Q}_0^{(b,A_g)}]$$

$$\hat{Z}_{15}(\mathbf{k}) = \mathbb{X}_{10}[\mathbb{Q}_2^{(a,A_g,2)}(1,-1)] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_g)}] \otimes \mathbb{F}_1[\mathbb{Q}_0^{(k,A_g)}]$$

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

$$\hat{Z}_{16} = \mathbb{X}_1[\mathbb{Q}_0^{(a,A_g)}] \otimes \mathbb{Y}_4[\mathbb{Q}_0^{(b,A_g)}]$$

$$\hat{Z}_{16}(\mathbf{k}) = \mathbb{X}_1[\mathbb{Q}_0^{(a,A_g)}] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_g)}] \otimes \mathbb{F}_3[\mathbb{Q}_0^{(k,A_g)}]$$

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

$$\hat{Z}_{17} = \mathbb{X}_3[\mathbb{M}_2^{(a,B_{2u})}(1,-1)] \otimes \mathbb{Y}_5[\mathbb{T}_1^{(b,B_{2u})}]$$

$$\hat{Z}_{17}(\mathbf{k}) = \mathbb{X}_3[\mathbb{M}_2^{(a,B_{2u})}(1,-1)] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_g)}] \otimes \mathbb{F}_4[\mathbb{T}_1^{(k,B_{2u})}]$$

$$\boxed{\text{No. 18}} \quad \hat{\mathbb{Q}}_0^{(A_g)} [\text{M}_3, \text{B}_2]$$

$$\hat{Z}_{18} = \mathbb{X}_5[\mathbb{Q}_0^{(a,A_g)}] \otimes \mathbb{Y}_4[\mathbb{Q}_0^{(b,A_g)}]$$

$$\hat{Z}_{18}(\mathbf{k}) = \mathbb{X}_5[\mathbb{Q}_0^{(a,A_g)}] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_g)}] \otimes \mathbb{F}_3[\mathbb{Q}_0^{(k,A_g)}]$$

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

$$\hat{Z}_{19} = \mathbb{X}_6[\mathbb{Q}_2^{(a,A_g,1)}] \otimes \mathbb{Y}_4[\mathbb{Q}_0^{(b,A_g)}]$$

$$\hat{\mathbb{Z}}_{19}(\mathbf{k}) = \mathbb{X}_6[\mathbb{Q}_2^{(a,A_g,1)}] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_g)}] \otimes \mathbb{F}_3[\mathbb{Q}_0^{(k,A_g)}]$$

$$\boxed{\text{No. 20}} \quad \hat{\mathbb{Q}}_2^{(A_g,2)} [\text{M}_3, \text{B}_2]$$

$$\hat{\mathbb{Z}}_{20} = \mathbb{X}_7[\mathbb{Q}_2^{(a,A_g,2)}] \otimes \mathbb{Y}_4[\mathbb{Q}_0^{(b,A_g)}]$$

$$\hat{\mathbb{Z}}_{20}(\mathbf{k}) = \mathbb{X}_7[\mathbb{Q}_2^{(a,A_g,2)}] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_g)}] \otimes \mathbb{F}_3[\mathbb{Q}_0^{(k,A_g)}]$$

$$\boxed{\text{No. 21}} \quad \hat{\mathbb{Q}}_0^{(A_g)}(1, 1) [\text{M}_3, \text{B}_2]$$

$$\hat{\mathbb{Z}}_{21} = \mathbb{X}_8[\mathbb{Q}_0^{(a,A_g)}(1, 1)] \otimes \mathbb{Y}_4[\mathbb{Q}_0^{(b,A_g)}]$$

$$\hat{\mathbb{Z}}_{21}(\mathbf{k}) = \mathbb{X}_8[\mathbb{Q}_0^{(a,A_g)}(1, 1)] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_g)}] \otimes \mathbb{F}_3[\mathbb{Q}_0^{(k,A_g)}]$$

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

$$\hat{\mathbb{Z}}_{22} = \mathbb{X}_9[\mathbb{Q}_2^{(a,A_g,1)}(1, -1)] \otimes \mathbb{Y}_4[\mathbb{Q}_0^{(b,A_g)}]$$

$$\hat{\mathbb{Z}}_{22}(\mathbf{k}) = \mathbb{X}_9[\mathbb{Q}_2^{(a,A_g,1)}(1, -1)] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_g)}] \otimes \mathbb{F}_3[\mathbb{Q}_0^{(k,A_g)}]$$

$$\boxed{\text{No. 23}} \quad \hat{\mathbb{Q}}_2^{(A_g,2)}(1, -1) [\text{M}_3, \text{B}_2]$$

$$\hat{\mathbb{Z}}_{23} = \mathbb{X}_{10}[\mathbb{Q}_2^{(a,A_g,2)}(1, -1)] \otimes \mathbb{Y}_4[\mathbb{Q}_0^{(b,A_g)}]$$

$$\hat{\mathbb{Z}}_{23}(\mathbf{k}) = \mathbb{X}_{10}[\mathbb{Q}_2^{(a,A_g,2)}(1, -1)] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_g)}] \otimes \mathbb{F}_3[\mathbb{Q}_0^{(k,A_g)}]$$

$$\boxed{\text{No. 24}} \quad \hat{\mathbb{Q}}_0^{(A_g)} [\text{M}_1, \text{B}_3]$$

$$\hat{\mathbb{Z}}_{24} = \mathbb{X}_1[\mathbb{Q}_0^{(a,A_g)}] \otimes \mathbb{Y}_6[\mathbb{Q}_0^{(b,A_g)}]$$

$$\hat{\mathbb{Z}}_{24}(\mathbf{k}) = \mathbb{X}_1[\mathbb{Q}_0^{(a,A_g)}] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_g)}] \otimes \mathbb{F}_5[\mathbb{Q}_0^{(k,A_g)}]$$

$$\boxed{\text{No. 25}} \quad \hat{\mathbb{Q}}_2^{(A_g,2)}(1, -1) [\text{M}_2, \text{B}_3]$$

$$\hat{\mathbb{Z}}_{25} = \mathbb{X}_2[\mathbb{M}_2^{(a,B_{1u})}(1, -1)] \otimes \mathbb{Y}_7[\mathbb{T}_1^{(b,B_{1u})}]$$

$$\hat{\mathbb{Z}}_{25}(\mathbf{k}) = \mathbb{X}_2[\mathbb{M}_2^{(a, B_{1u})}(1, -1)] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s, A_g)}] \otimes \mathbb{F}_6[\mathbb{T}_1^{(k, B_{1u})}]$$

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

$$\hat{\mathbb{Z}}_{26} = \mathbb{X}_5[\mathbb{Q}_0^{(a, A_g)}] \otimes \mathbb{Y}_6[\mathbb{Q}_0^{(b, A_g)}]$$

$$\hat{\mathbb{Z}}_{26}(\mathbf{k}) = \mathbb{X}_5[\mathbb{Q}_0^{(a, A_g)}] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s, A_g)}] \otimes \mathbb{F}_5[\mathbb{Q}_0^{(k, A_g)}]$$

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

$$\hat{\mathbb{Z}}_{27} = \mathbb{X}_6[\mathbb{Q}_2^{(a, A_g, 1)}] \otimes \mathbb{Y}_6[\mathbb{Q}_0^{(b, A_g)}]$$

$$\hat{\mathbb{Z}}_{27}(\mathbf{k}) = \mathbb{X}_6[\mathbb{Q}_2^{(a, A_g, 1)}] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s, A_g)}] \otimes \mathbb{F}_5[\mathbb{Q}_0^{(k, A_g)}]$$

$$\boxed{\text{No. 28}} \quad \hat{\mathbb{Q}}_2^{(A_g, 2)} [\text{M}_3, \text{B}_3]$$

$$\hat{\mathbb{Z}}_{28} = \mathbb{X}_7[\mathbb{Q}_2^{(a, A_g, 2)}] \otimes \mathbb{Y}_6[\mathbb{Q}_0^{(b, A_g)}]$$

$$\hat{\mathbb{Z}}_{28}(\mathbf{k}) = \mathbb{X}_7[\mathbb{Q}_2^{(a, A_g, 2)}] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s, A_g)}] \otimes \mathbb{F}_5[\mathbb{Q}_0^{(k, A_g)}]$$

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

$$\hat{\mathbb{Z}}_{29} = \mathbb{X}_8[\mathbb{Q}_0^{(a, A_g)}(1, 1)] \otimes \mathbb{Y}_6[\mathbb{Q}_0^{(b, A_g)}]$$

$$\hat{\mathbb{Z}}_{29}(\mathbf{k}) = \mathbb{X}_8[\mathbb{Q}_0^{(a, A_g)}(1, 1)] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s, A_g)}] \otimes \mathbb{F}_5[\mathbb{Q}_0^{(k, A_g)}]$$

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

$$\hat{\mathbb{Z}}_{30} = \mathbb{X}_9[\mathbb{Q}_2^{(a, A_g, 1)}(1, -1)] \otimes \mathbb{Y}_6[\mathbb{Q}_0^{(b, A_g)}]$$

$$\hat{\mathbb{Z}}_{30}(\mathbf{k}) = \mathbb{X}_9[\mathbb{Q}_2^{(a, A_g, 1)}(1, -1)] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s, A_g)}] \otimes \mathbb{F}_5[\mathbb{Q}_0^{(k, A_g)}]$$

$$\boxed{\text{No. 31}} \quad \hat{\mathbb{Q}}_2^{(A_g, 2)}(1, -1) [\text{M}_3, \text{B}_3]$$

$$\hat{\mathbb{Z}}_{31} = \mathbb{X}_{10}[\mathbb{Q}_2^{(a, A_g, 2)}(1, -1)] \otimes \mathbb{Y}_6[\mathbb{Q}_0^{(b, A_g)}]$$

$$\hat{Z}_{31}(\mathbf{k}) = \mathbb{X}_{10}[\mathbb{Q}_2^{(a,A_g,2)}(1,-1)] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_g)}] \otimes \mathbb{F}_5[\mathbb{Q}_0^{(k,A_g)}]$$

$$\boxed{\text{No. 32}} \quad \hat{\mathbb{Q}}_0^{(A_g)} [\text{M}_1, \text{B}_4]$$

$$\hat{Z}_{32} = \mathbb{X}_1[\mathbb{Q}_0^{(a,A_g)}] \otimes \mathbb{Y}_8[\mathbb{Q}_0^{(b,A_g)}]$$

$$\hat{Z}_{32}(\mathbf{k}) = \mathbb{X}_1[\mathbb{Q}_0^{(a,A_g)}] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_g)}] \otimes \mathbb{F}_7[\mathbb{Q}_0^{(k,A_g)}]$$

$$\boxed{\text{No. 33}} \quad \hat{\mathbb{Q}}_2^{(A_g,1)}(1,-1) [\text{M}_2, \text{B}_4]$$

$$\hat{Z}_{33} = \frac{\sqrt{2}\mathbb{X}_3[\mathbb{M}_2^{(a,B_{2u})}(1,-1)] \otimes \mathbb{Y}_{10}[\mathbb{T}_1^{(b,B_{2u})}]}{2} - \frac{\sqrt{2}\mathbb{X}_4[\mathbb{M}_2^{(a,B_{3u})}(1,-1)] \otimes \mathbb{Y}_{11}[\mathbb{T}_1^{(b,B_{3u})}]}{2}$$

$$\hat{Z}_{33}(\mathbf{k}) = \frac{\sqrt{2}\mathbb{X}_3[\mathbb{M}_2^{(a,B_{2u})}(1,-1)] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_g)}] \otimes \mathbb{F}_9[\mathbb{T}_1^{(k,B_{2u})}]}{2} - \frac{\sqrt{2}\mathbb{X}_4[\mathbb{M}_2^{(a,B_{3u})}(1,-1)] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_g)}] \otimes \mathbb{F}_{10}[\mathbb{T}_1^{(k,B_{3u})}]}{2}$$

$$\boxed{\text{No. 34}} \quad \hat{\mathbb{Q}}_2^{(A_g,2)}(1,-1) [\text{M}_2, \text{B}_4]$$

$$\hat{Z}_{34} = -\frac{\sqrt{2}\mathbb{X}_3[\mathbb{M}_2^{(a,B_{2u})}(1,-1)] \otimes \mathbb{Y}_{10}[\mathbb{T}_1^{(b,B_{2u})}]}{2} - \frac{\sqrt{2}\mathbb{X}_4[\mathbb{M}_2^{(a,B_{3u})}(1,-1)] \otimes \mathbb{Y}_{11}[\mathbb{T}_1^{(b,B_{3u})}]}{2}$$

$$\hat{Z}_{34}(\mathbf{k}) = -\frac{\sqrt{2}\mathbb{X}_3[\mathbb{M}_2^{(a,B_{2u})}(1,-1)] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_g)}] \otimes \mathbb{F}_9[\mathbb{T}_1^{(k,B_{2u})}]}{2} - \frac{\sqrt{2}\mathbb{X}_4[\mathbb{M}_2^{(a,B_{3u})}(1,-1)] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_g)}] \otimes \mathbb{F}_{10}[\mathbb{T}_1^{(k,B_{3u})}]}{2}$$

$$\boxed{\text{No. 35}} \quad \hat{\mathbb{Q}}_0^{(A_g)} [\text{M}_3, \text{B}_4]$$

$$\hat{Z}_{35} = \mathbb{X}_5[\mathbb{Q}_0^{(a,A_g)}] \otimes \mathbb{Y}_8[\mathbb{Q}_0^{(b,A_g)}]$$

$$\hat{Z}_{35}(\mathbf{k}) = \mathbb{X}_5[\mathbb{Q}_0^{(a,A_g)}] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_g)}] \otimes \mathbb{F}_7[\mathbb{Q}_0^{(k,A_g)}]$$

$$\boxed{\text{No. 36}} \quad \hat{\mathbb{Q}}_2^{(A_g,1)} [\text{M}_3, \text{B}_4]$$

$$\hat{Z}_{36} = \mathbb{X}_6[\mathbb{Q}_2^{(a,A_g,1)}] \otimes \mathbb{Y}_8[\mathbb{Q}_0^{(b,A_g)}]$$

$$\hat{Z}_{36}(\mathbf{k}) = \mathbb{X}_6[\mathbb{Q}_2^{(a,A_g,1)}] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_g)}] \otimes \mathbb{F}_7[\mathbb{Q}_0^{(k,A_g)}]$$



$$\boxed{\text{No. 37}} \quad \hat{\mathbb{Q}}_2^{(A_g, 2)} [\text{M}_3, \text{B}_4]$$

$$\hat{\mathbb{Z}}_{37} = \mathbb{X}_7[\mathbb{Q}_2^{(a, A_g, 2)}] \otimes \mathbb{Y}_8[\mathbb{Q}_0^{(b, A_g)}]$$

$$\hat{\mathbb{Z}}_{37}(\mathbf{k}) = \mathbb{X}_7[\mathbb{Q}_2^{(a, A_g, 2)}] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s, A_g)}] \otimes \mathbb{F}_7[\mathbb{Q}_0^{(k, A_g)}]$$

$$\boxed{\text{No. 38}} \quad \hat{\mathbb{Q}}_0^{(A_g)} [\text{M}_3, \text{B}_4]$$

$$\hat{\mathbb{Z}}_{38} = \mathbb{X}_{11}[\mathbb{Q}_2^{(a, B_{1g})}] \otimes \mathbb{Y}_9[\mathbb{Q}_2^{(b, B_{1g})}]$$

$$\hat{\mathbb{Z}}_{38}(\mathbf{k}) = \mathbb{X}_{11}[\mathbb{Q}_2^{(a, B_{1g})}] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s, A_g)}] \otimes \mathbb{F}_8[\mathbb{Q}_2^{(k, B_{1g})}]$$

$$\boxed{\text{No. 39}} \quad \hat{\mathbb{Q}}_0^{(A_g)}(1, 1) [\text{M}_3, \text{B}_4]$$

$$\hat{\mathbb{Z}}_{39} = \mathbb{X}_8[\mathbb{Q}_0^{(a, A_g)}(1, 1)] \otimes \mathbb{Y}_8[\mathbb{Q}_0^{(b, A_g)}]$$

$$\hat{\mathbb{Z}}_{39}(\mathbf{k}) = \mathbb{X}_8[\mathbb{Q}_0^{(a, A_g)}(1, 1)] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s, A_g)}] \otimes \mathbb{F}_7[\mathbb{Q}_0^{(k, A_g)}]$$

$$\boxed{\text{No. 40}} \quad \hat{\mathbb{Q}}_2^{(A_g, 1)}(1, -1) [\text{M}_3, \text{B}_4]$$

$$\hat{\mathbb{Z}}_{40} = \mathbb{X}_9[\mathbb{Q}_2^{(a, A_g, 1)}(1, -1)] \otimes \mathbb{Y}_8[\mathbb{Q}_0^{(b, A_g)}]$$

$$\hat{\mathbb{Z}}_{40}(\mathbf{k}) = \mathbb{X}_9[\mathbb{Q}_2^{(a, A_g, 1)}(1, -1)] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s, A_g)}] \otimes \mathbb{F}_7[\mathbb{Q}_0^{(k, A_g)}]$$

$$\boxed{\text{No. 41}} \quad \hat{\mathbb{Q}}_2^{(A_g, 2)}(1, -1) [\text{M}_3, \text{B}_4]$$

$$\hat{\mathbb{Z}}_{41} = \mathbb{X}_{10}[\mathbb{Q}_2^{(a, A_g, 2)}(1, -1)] \otimes \mathbb{Y}_8[\mathbb{Q}_0^{(b, A_g)}]$$

$$\hat{\mathbb{Z}}_{41}(\mathbf{k}) = \mathbb{X}_{10}[\mathbb{Q}_2^{(a, A_g, 2)}(1, -1)] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s, A_g)}] \otimes \mathbb{F}_7[\mathbb{Q}_0^{(k, A_g)}]$$

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

$$\hat{\mathbb{Z}}_{42} = \mathbb{X}_{12}[\mathbb{Q}_2^{(a, B_{1g})}(1, -1)] \otimes \mathbb{Y}_9[\mathbb{Q}_2^{(b, B_{1g})}]$$

$$\hat{\mathbb{Z}}_{42}(\mathbf{k}) = \mathbb{X}_{12}[\mathbb{Q}_2^{(a, B_{1g})}(1, -1)] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s, A_g)}] \otimes \mathbb{F}_8[\mathbb{Q}_2^{(k, B_{1g})}]$$

$$\boxed{\text{No. 43}} \quad \hat{\mathbb{Q}}_2^{(A_g, 2)}(1, 0) [\text{M}_3, \text{B}_4]$$

$$\hat{\mathbb{Z}}_{43} = -\mathbb{X}_{13}[\mathbb{G}_1^{(a, B_{1g})}(1, 0)] \otimes \mathbb{Y}_9[\mathbb{Q}_2^{(b, B_{1g})}]$$

$$\hat{\mathbb{Z}}_{43}(\mathbf{k}) = -\mathbb{X}_{13}[\mathbb{G}_1^{(a, B_{1g})}(1, 0)] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s, A_g)}] \otimes \mathbb{F}_8[\mathbb{Q}_2^{(k, B_{1g})}]$$

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
$\mathbb{X}_1$	$\mathbb{Q}_0^{(a, A_g)}$	M <sub>1</sub>	$\begin{pmatrix} \frac{\sqrt{2}}{2} & 0 \\ 0 & \frac{\sqrt{2}}{2} \end{pmatrix}$
$\mathbb{X}_2$	$\mathbb{M}_2^{(a, B_{1u})}(1, -1)$	M <sub>2</sub>	$\begin{pmatrix} 0 & -\frac{i}{2} & 0 & \frac{1}{2} & 0 & 0 \\ \frac{i}{2} & 0 & \frac{1}{2} & 0 & 0 & 0 \\ \frac{1}{2} & 0 & 0 & 0 & 0 & \frac{1}{2} \\ 0 & -\frac{1}{2} & 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & \frac{1}{2} & 0 & 0 & -\frac{i}{2} \\ 0 & 0 & 0 & -\frac{1}{2} & \frac{i}{2} & 0 \end{pmatrix}$
$\mathbb{X}_3$	$\mathbb{M}_2^{(a, B_{2u})}(1, -1)$	M <sub>2</sub>	$\begin{pmatrix} 0 & -\frac{i}{2} & 0 & \frac{1}{2} & 0 & 0 \\ \frac{i}{2} & 0 & \frac{1}{2} & 0 & 0 & 0 \\ \frac{1}{2} & 0 & 0 & 0 & 0 & \frac{1}{2} \\ 0 & -\frac{1}{2} & 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & \frac{1}{2} & 0 & 0 & -\frac{i}{2} \\ 0 & 0 & 0 & -\frac{1}{2} & \frac{i}{2} & 0 \end{pmatrix}$
$\mathbb{X}_4$	$\mathbb{M}_2^{(a, B_{3u})}(1, -1)$	M <sub>2</sub>	$\begin{pmatrix} 0 & 0 & \frac{1}{2} & 0 & 0 & -\frac{i}{2} \\ 0 & 0 & 0 & -\frac{1}{2} & \frac{i}{2} & 0 \end{pmatrix}$
$\mathbb{X}_5$	$\mathbb{Q}_0^{(a, A_g)}$	M <sub>3</sub>	$\begin{pmatrix} \frac{\sqrt{6}}{6} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{6}}{6} & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{6}}{6} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{6}}{6} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{6}}{6} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{6}}{6} \end{pmatrix}$
$\mathbb{X}_6$	$\mathbb{Q}_2^{(a, A_g, 1)}$	M <sub>3</sub>	$\begin{pmatrix} -\frac{\sqrt{3}}{6} & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{3}}{6} & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{3}}{6} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{3}}{6} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{3}}{3} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{3}}{3} \end{pmatrix}$

continued ...

Table 6

symbol	type	group	form
$\mathbb{X}_7$	$\mathbb{Q}_2^{(a, A_g, 2)}$	$M_3$	$\begin{pmatrix} \frac{1}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{1}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$
$\mathbb{X}_8$	$\mathbb{Q}_0^{(a, A_g)}(1, 1)$	$M_3$	$\begin{pmatrix} 0 & 0 & -\frac{\sqrt{3}i}{6} & 0 & 0 & \frac{\sqrt{3}}{6} \\ 0 & 0 & 0 & \frac{\sqrt{3}i}{6} & -\frac{\sqrt{3}}{6} & 0 \\ \frac{\sqrt{3}i}{6} & 0 & 0 & 0 & 0 & -\frac{\sqrt{3}i}{6} \\ 0 & -\frac{\sqrt{3}i}{6} & 0 & 0 & -\frac{\sqrt{3}}{6} & 0 \\ 0 & -\frac{\sqrt{3}}{6} & 0 & \frac{\sqrt{3}i}{6} & 0 & 0 \\ \frac{\sqrt{3}}{6} & 0 & \frac{\sqrt{3}i}{6} & 0 & 0 & 0 \end{pmatrix}$
$\mathbb{X}_9$	$\mathbb{Q}_2^{(a, A_g, 1)}(1, -1)$	$M_3$	$\begin{pmatrix} 0 & 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 & -\frac{\sqrt{6}}{12} \\ 0 & 0 & 0 & \frac{\sqrt{6}i}{6} & \frac{\sqrt{6}}{12} & 0 \\ \frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 & \frac{\sqrt{6}i}{12} \\ 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 & \frac{\sqrt{6}}{12} & 0 \\ 0 & \frac{\sqrt{6}}{12} & 0 & -\frac{\sqrt{6}i}{12} & 0 & 0 \\ -\frac{\sqrt{6}}{12} & 0 & -\frac{\sqrt{6}i}{12} & 0 & 0 & 0 \end{pmatrix}$
$\mathbb{X}_{10}$	$\mathbb{Q}_2^{(a, A_g, 2)}(1, -1)$	$M_3$	$\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{2}}{4} \\ 0 & 0 & 0 & 0 & \frac{\sqrt{2}}{4} & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{2}i}{4} \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{2}i}{4} & 0 \\ 0 & \frac{\sqrt{2}}{4} & 0 & \frac{\sqrt{2}i}{4} & 0 & 0 \\ -\frac{\sqrt{2}}{4} & 0 & \frac{\sqrt{2}i}{4} & 0 & 0 & 0 \end{pmatrix}$
$\mathbb{X}_{11}$	$\mathbb{Q}_2^{(a, B_{1g})}$	$M_3$	$\begin{pmatrix} 0 & 0 & \frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2} & 0 & 0 \\ \frac{1}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$

continued ...

Table 6

symbol	type	group	form
$\mathbb{X}_{12}$	$\mathbb{Q}_2^{(a, B_{1g})}(1, -1)$	$M_3$	$\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{2}i}{4} \\ 0 & 0 & 0 & 0 & \frac{\sqrt{2}i}{4} & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{2}}{4} \\ 0 & 0 & 0 & 0 & \frac{\sqrt{2}}{4} & 0 \\ 0 & -\frac{\sqrt{2}i}{4} & 0 & \frac{\sqrt{2}}{4} & 0 & 0 \\ -\frac{\sqrt{2}i}{4} & 0 & -\frac{\sqrt{2}}{4} & 0 & 0 & 0 \end{pmatrix}$
$\mathbb{X}_{13}$	$\mathbb{G}_1^{(a, B_{1g})}(1, 0)$	$M_3$	$\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{2}i}{4} \\ 0 & 0 & 0 & 0 & \frac{\sqrt{2}i}{4} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{2}}{4} \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{2}}{4} & 0 \\ 0 & -\frac{\sqrt{2}i}{4} & 0 & -\frac{\sqrt{2}}{4} & 0 & 0 \\ -\frac{\sqrt{2}i}{4} & 0 & \frac{\sqrt{2}}{4} & 0 & 0 & 0 \end{pmatrix}$

Table 7: Cluster SAMB.

symbol	type	cluster	form
$\mathbb{Y}_1$	$\mathbb{Q}_0^{(s, A_g)}$	$S_1$	$\begin{pmatrix} 1 \end{pmatrix}$
$\mathbb{Y}_2$	$\mathbb{Q}_0^{(b, A_g)}$	$B_1$	$\begin{pmatrix} 1 \end{pmatrix}$
$\mathbb{Y}_3$	$\mathbb{T}_1^{(b, B_{3u})}$	$B_1$	$\begin{pmatrix} i \end{pmatrix}$
$\mathbb{Y}_4$	$\mathbb{Q}_0^{(b, A_g)}$	$B_2$	$\begin{pmatrix} 1 \end{pmatrix}$
$\mathbb{Y}_5$	$\mathbb{T}_1^{(b, B_{2u})}$	$B_2$	$\begin{pmatrix} i \end{pmatrix}$
$\mathbb{Y}_6$	$\mathbb{Q}_0^{(b, A_g)}$	$B_3$	$\begin{pmatrix} 1 \end{pmatrix}$
$\mathbb{Y}_7$	$\mathbb{T}_1^{(b, B_{1u})}$	$B_3$	$\begin{pmatrix} i \end{pmatrix}$
$\mathbb{Y}_8$	$\mathbb{Q}_0^{(b, A_g)}$	$B_4$	$\begin{pmatrix} \frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2} \end{pmatrix}$
$\mathbb{Y}_9$	$\mathbb{Q}_2^{(b, B_{1g})}$	$B_4$	$\begin{pmatrix} \frac{\sqrt{2}}{2} & -\frac{\sqrt{2}}{2} \end{pmatrix}$
$\mathbb{Y}_{10}$	$\mathbb{T}_1^{(b, B_{2u})}$	$B_4$	$\begin{pmatrix} \frac{\sqrt{2}i}{2} & -\frac{\sqrt{2}i}{2} \end{pmatrix}$
$\mathbb{Y}_{11}$	$\mathbb{T}_1^{(b, B_{3u})}$	$B_4$	$\begin{pmatrix} \frac{\sqrt{2}i}{2} & \frac{\sqrt{2}i}{2} \end{pmatrix}$

Table 8: Uniform SAMB.

symbol	type	cluster	form
$\mathbb{U}_1$	$\mathbb{Q}_0^{(s, A_g)}$	$S_1$	$(1)$

Table 9: Structure SAMB.

symbol	type	cluster	form
$\mathbb{F}_1$	$\mathbb{Q}_0^{(k, A_g)}$	$B_1$	$\sqrt{2}c_{001}$
$\mathbb{F}_2$	$\mathbb{T}_1^{(k, B_{3u})}$	$B_1$	$\sqrt{2}s_{001}$
$\mathbb{F}_3$	$\mathbb{Q}_0^{(k, A_g)}$	$B_2$	$\sqrt{2}c_{002}$
$\mathbb{F}_4$	$\mathbb{T}_1^{(k, B_{2u})}$	$B_2$	$\sqrt{2}s_{002}$
$\mathbb{F}_5$	$\mathbb{Q}_0^{(k, A_g)}$	$B_3$	$\sqrt{2}c_{003}$
$\mathbb{F}_6$	$\mathbb{T}_1^{(k, B_{1u})}$	$B_3$	$\sqrt{2}s_{003}$
$\mathbb{F}_7$	$\mathbb{Q}_0^{(k, A_g)}$	$B_4$	$c_{004} + c_{005}$
$\mathbb{F}_8$	$\mathbb{Q}_2^{(k, B_{1g})}$	$B_4$	$c_{004} - c_{005}$
$\mathbb{F}_9$	$\mathbb{T}_1^{(k, B_{2u})}$	$B_4$	$s_{004} - s_{005}$
$\mathbb{F}_{10}$	$\mathbb{T}_1^{(k, B_{3u})}$	$B_4$	$s_{004} + s_{005}$

Table 10: Polar harmonics.

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

*continued ...*

Table 10

No.	symbol	rank	irrep.	mul.	comp.	form
2	$\mathbb{Q}_1^{(B_{1u})}$	1	$B_{1u}$	—	—	$z$
3	$\mathbb{Q}_1^{(B_{2u})}$	1	$B_{2u}$	—	—	$y$
4	$\mathbb{Q}_1^{(B_{3u})}$	1	$B_{3u}$	—	—	$x$
5	$\mathbb{Q}_2^{(A_g,1)}$	2	$A_g$	1	—	$-\frac{x^2}{2} - \frac{y^2}{2} + z^2$
6	$\mathbb{Q}_2^{(A_g,2)}$	2	$A_g$	2	—	$\frac{\sqrt{3}(x-y)(x+y)}{2}$
7	$\mathbb{Q}_2^{(B_{1g})}$	2	$B_{1g}$	—	—	$\sqrt{3}xy$

Table 11: Axial harmonics.

No.	symbol	rank	irrep.	mul.	comp.	form
1	$\mathbb{G}_1^{(B_{1g})}$	1	$B_{1g}$	—	—	$Z$
2	$\mathbb{G}_2^{(B_{1u})}$	2	$B_{1u}$	—	—	$\sqrt{3}XY$
3	$\mathbb{G}_2^{(B_{2u})}$	2	$B_{2u}$	—	—	$\sqrt{3}XZ$
4	$\mathbb{G}_2^{(B_{3u})}$	2	$B_{3u}$	—	—	$\sqrt{3}YZ$

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

Table 12: Conjugacy class (point-group part).

rep. SO	symmetry operations
$\{1 0\}$	$\{1 0\}$
$\{2_{001} 0\}$	$\{2_{001} 0\}$
$\{2_{010} 0\}$	$\{2_{010} 0\}$
$\{2_{100} 0\}$	$\{2_{100} 0\}$
$\{-1 0\}$	$\{-1 0\}$

*continued ...*

Table 12

rep. SO	symmetry operations
$\{m_{001} 0\}$	$\{m_{001} 0\}$
$\{m_{010} 0\}$	$\{m_{010} 0\}$
$\{m_{100} 0\}$	$\{m_{100} 0\}$

Table 13: Symmetry operations.

No.	SO	No.	SO	No.	SO	No.	SO	No.	SO
1	$\{1 0\}$	2	$\{2_{001} 0\}$	3	$\{2_{010} 0\}$	4	$\{2_{100} 0\}$	5	$\{-1 0\}$
6	$\{m_{001} 0\}$	7	$\{m_{010} 0\}$	8	$\{m_{100} 0\}$				

Table 14: Character table (point-group part).

	1	2 <sub>001</sub>	2 <sub>010</sub>	2 <sub>100</sub>	-1	m <sub>001</sub>	m <sub>010</sub>	m <sub>100</sub>
$A_g$	1	1	1	1	1	1	1	1
$B_{1g}$	1	1	-1	-1	1	1	-1	-1
$B_{2g}$	1	-1	1	-1	1	-1	1	-1
$B_{3g}$	1	-1	-1	1	1	-1	-1	1
$A_u$	1	1	1	1	-1	-1	-1	-1
$B_{1u}$	1	1	-1	-1	-1	-1	1	1
$B_{2u}$	1	-1	1	-1	-1	1	-1	1
$B_{3u}$	1	-1	-1	1	-1	1	1	-1

Table 15: Parity conversion.

$\leftrightarrow$	$\leftrightarrow$	$\leftrightarrow$	$\leftrightarrow$	$\leftrightarrow$
$A_g (A_u)$	$B_{3g} (B_{3u})$	$B_{2g} (B_{2u})$	$B_{1g} (B_{1u})$	$A_u (A_g)$
<i>continued ...</i>				

Table 15

$\leftrightarrow$	$\leftrightarrow$	$\leftrightarrow$	$\leftrightarrow$	$\leftrightarrow$
$B_{3u} (B_{3g})$	$B_{2u} (B_{2g})$	$B_{1u} (B_{1g})$		

Table 16: Symmetric product,  $[\Gamma \otimes \Gamma']_+$ .

	$A_g$	$B_{1g}$	$B_{2g}$	$B_{3g}$	$A_u$	$B_{1u}$	$B_{2u}$	$B_{3u}$
$A_g$	$A_g$	$B_{1g}$	$B_{2g}$	$B_{3g}$	$A_u$	$B_{1u}$	$B_{2u}$	$B_{3u}$
$B_{1g}$		$A_g$	$B_{3g}$	$B_{2g}$	$B_{1u}$	$A_u$	$B_{3u}$	$B_{2u}$
$B_{2g}$			$A_g$	$B_{1g}$	$B_{2u}$	$B_{3u}$	$A_u$	$B_{1u}$
$B_{3g}$				$A_g$	$B_{3u}$	$B_{2u}$	$B_{1u}$	$A_u$
$A_u$					$A_g$	$B_{1g}$	$B_{2g}$	$B_{3g}$
$B_{1u}$						$A_g$	$B_{3g}$	$B_{2g}$
$B_{2u}$							$A_g$	$B_{1g}$
$B_{3u}$								$A_g$

Table 17: Anti-symmetric product,  $[\Gamma \otimes \Gamma']_-$ .

$A_g$	$B_{1g}$	$B_{2g}$	$B_{3g}$	$A_u$	$B_{1u}$	$B_{2u}$	$B_{3u}$
-	-	-	-	-	-	-	-

Table 18: Virtual-cluster sites.

No.	position	No.	position	No.	position	No.	position
1	$\begin{pmatrix} 1 & 1 & 1 \end{pmatrix}$	2	$\begin{pmatrix} -1 & -1 & 1 \end{pmatrix}$	3	$\begin{pmatrix} -1 & 1 & -1 \end{pmatrix}$	4	$\begin{pmatrix} 1 & -1 & -1 \end{pmatrix}$
5	$\begin{pmatrix} -1 & -1 & -1 \end{pmatrix}$	6	$\begin{pmatrix} 1 & 1 & -1 \end{pmatrix}$	7	$\begin{pmatrix} 1 & -1 & 1 \end{pmatrix}$	8	$\begin{pmatrix} -1 & 1 & 1 \end{pmatrix}$



Table 19: Virtual-cluster basis.

symbol	1	2	3	4	5	6	7	8
$\mathbb{Q}_0^{(Ag)}$	$\frac{\sqrt{2}}{4}$	$\frac{\sqrt{2}}{4}$	$\frac{\sqrt{2}}{4}$	$\frac{\sqrt{2}}{4}$	$\frac{\sqrt{2}}{4}$	$\frac{\sqrt{2}}{4}$	$\frac{\sqrt{2}}{4}$	$\frac{\sqrt{2}}{4}$
$\mathbb{Q}_1^{(B1u)}$	$\frac{\sqrt{2}}{4}$	$\frac{\sqrt{2}}{4}$	$-\frac{\sqrt{2}}{4}$	$-\frac{\sqrt{2}}{4}$	$-\frac{\sqrt{2}}{4}$	$-\frac{\sqrt{2}}{4}$	$\frac{\sqrt{2}}{4}$	$\frac{\sqrt{2}}{4}$
$\mathbb{Q}_1^{(B2u)}$	$\frac{\sqrt{2}}{4}$	$-\frac{\sqrt{2}}{4}$	$\frac{\sqrt{2}}{4}$	$-\frac{\sqrt{2}}{4}$	$-\frac{\sqrt{2}}{4}$	$\frac{\sqrt{2}}{4}$	$-\frac{\sqrt{2}}{4}$	$\frac{\sqrt{2}}{4}$
$\mathbb{Q}_1^{(B3u)}$	$\frac{\sqrt{2}}{4}$	$-\frac{\sqrt{2}}{4}$	$-\frac{\sqrt{2}}{4}$	$\frac{\sqrt{2}}{4}$	$-\frac{\sqrt{2}}{4}$	$\frac{\sqrt{2}}{4}$	$\frac{\sqrt{2}}{4}$	$-\frac{\sqrt{2}}{4}$
$\mathbb{Q}_2^{(B1g)}$	$\frac{\sqrt{2}}{4}$	$\frac{\sqrt{2}}{4}$	$-\frac{\sqrt{2}}{4}$	$-\frac{\sqrt{2}}{4}$	$\frac{\sqrt{2}}{4}$	$\frac{\sqrt{2}}{4}$	$-\frac{\sqrt{2}}{4}$	$-\frac{\sqrt{2}}{4}$
$\mathbb{Q}_2^{(B2g)}$	$\frac{\sqrt{2}}{4}$	$-\frac{\sqrt{2}}{4}$	$\frac{\sqrt{2}}{4}$	$-\frac{\sqrt{2}}{4}$	$\frac{\sqrt{2}}{4}$	$-\frac{\sqrt{2}}{4}$	$\frac{\sqrt{2}}{4}$	$-\frac{\sqrt{2}}{4}$
$\mathbb{Q}_2^{(B3g)}$	$\frac{\sqrt{2}}{4}$	$-\frac{\sqrt{2}}{4}$	$-\frac{\sqrt{2}}{4}$	$\frac{\sqrt{2}}{4}$	$\frac{\sqrt{2}}{4}$	$-\frac{\sqrt{2}}{4}$	$-\frac{\sqrt{2}}{4}$	$\frac{\sqrt{2}}{4}$
$\mathbb{Q}_3^{(Au)}$	$\frac{\sqrt{2}}{4}$	$\frac{\sqrt{2}}{4}$	$\frac{\sqrt{2}}{4}$	$\frac{\sqrt{2}}{4}$	$-\frac{\sqrt{2}}{4}$	$-\frac{\sqrt{2}}{4}$	$-\frac{\sqrt{2}}{4}$	$-\frac{\sqrt{2}}{4}$