

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: 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 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] |

- Bonds in (primitive) unit cell:

Table 4: Bond-clusters.

| bond | tail | head | n | # | $\mathbf{b@c}$ | mapping | |
|----------------|----------------|----------------|----------------|---|----------------|--|--|
| B ₁ | b ₁ | A ₁ | A ₁ | 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 ₂ | A ₁ | A ₁ | 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 ₂ | b ₃ | A ₁ | A ₁ | 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 ₄ | A ₁ | A ₁ | 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 ₃ | b ₅ | A ₁ | A ₁ | 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 ₄ | b ₆ | A ₁ | A ₁ | 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 ₇ | A ₁ | A ₁ | 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 ₈ | A ₁ | A ₁ | 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 ₉ | A ₁ | A ₁ | 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:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

$$\boxed{\text{No. 8}} \quad \hat{\mathbb{Q}}_2^{(A_{1g})} [\mathbb{M}_3, \mathbb{B}_1]$$

$$\hat{\mathbb{Z}}_8 = \mathbb{X}_3[\mathbb{Q}_2^{(a,A_{1g})}] \otimes \mathbb{Y}_2[\mathbb{Q}_0^{(b,A_{1g})}]$$

$$\hat{\mathbb{Z}}_8(\mathbf{k}) = \mathbb{X}_3[\mathbb{Q}_2^{(a,A_{1g})}] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_{1g})}] \otimes \mathbb{F}_1[\mathbb{Q}_0^{(k,A_{1g})}]$$

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

$$\hat{\mathbb{Z}}_9 = \mathbb{X}_6[\mathbb{Q}_2^{(a,B_{1g})}] \otimes \mathbb{Y}_3[\mathbb{Q}_2^{(b,B_{1g})}]$$

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

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

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

$$\hat{\mathbb{Z}}_{10}(\mathbf{k}) = \mathbb{X}_4[\mathbb{Q}_0^{(a,A_{1g})}(1, 1)] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_{1g})}] \otimes \mathbb{F}_1[\mathbb{Q}_0^{(k,A_{1g})}]$$

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

$$\hat{\mathbb{Z}}_{11} = \mathbb{X}_5[\mathbb{Q}_2^{(a,A_{1g})}(1, -1)] \otimes \mathbb{Y}_2[\mathbb{Q}_0^{(b,A_{1g})}]$$

$$\hat{\mathbb{Z}}_{11}(\mathbf{k}) = \mathbb{X}_5[\mathbb{Q}_2^{(a,A_{1g})}(1, -1)] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_{1g})}] \otimes \mathbb{F}_1[\mathbb{Q}_0^{(k,A_{1g})}]$$

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

$$\hat{\mathbb{Z}}_{12} = \mathbb{X}_{10}[\mathbb{Q}_2^{(a,B_{1g})}(1, -1)] \otimes \mathbb{Y}_3[\mathbb{Q}_2^{(b,B_{1g})}]$$

$$\hat{Z}_{12}(\mathbf{k}) = \mathbb{X}_{10}[\mathbb{Q}_2^{(a,B_{1g})}(1, -1)] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_{1g})}] \otimes \mathbb{F}_2[\mathbb{Q}_2^{(k,B_{1g})}]$$

$$\boxed{\text{No. 13}} \quad \hat{\mathbb{Q}}_0^{(A_{1g})} [\text{M}_1, \text{B}_2]$$

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

$$\hat{Z}_{13}(\mathbf{k}) = \mathbb{X}_1[\mathbb{Q}_0^{(a,A_{1g})}] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_{1g})}] \otimes \mathbb{F}_3[\mathbb{Q}_0^{(k,A_{1g})}]$$

$$\boxed{\text{No. 14}} \quad \hat{\mathbb{Q}}_0^{(A_{1g})} [\text{M}_3, \text{B}_2]$$

$$\hat{Z}_{14} = \mathbb{X}_2[\mathbb{Q}_0^{(a,A_{1g})}] \otimes \mathbb{Y}_4[\mathbb{Q}_0^{(b,A_{1g})}]$$

$$\hat{Z}_{14}(\mathbf{k}) = \mathbb{X}_2[\mathbb{Q}_0^{(a,A_{1g})}] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_{1g})}] \otimes \mathbb{F}_3[\mathbb{Q}_0^{(k,A_{1g})}]$$

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

$$\hat{Z}_{15} = \mathbb{X}_3[\mathbb{Q}_2^{(a,A_{1g})}] \otimes \mathbb{Y}_4[\mathbb{Q}_0^{(b,A_{1g})}]$$

$$\hat{Z}_{15}(\mathbf{k}) = \mathbb{X}_3[\mathbb{Q}_2^{(a,A_{1g})}] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_{1g})}] \otimes \mathbb{F}_3[\mathbb{Q}_0^{(k,A_{1g})}]$$

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

$$\hat{Z}_{16} = \mathbb{X}_7[\mathbb{Q}_2^{(a,B_{2g})}] \otimes \mathbb{Y}_5[\mathbb{Q}_2^{(b,B_{2g})}]$$

$$\hat{Z}_{16}(\mathbf{k}) = \mathbb{X}_7[\mathbb{Q}_2^{(a,B_{2g})}] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_{1g})}] \otimes \mathbb{F}_4[\mathbb{Q}_2^{(k,B_{2g})}]$$

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

$$\hat{Z}_{17} = \mathbb{X}_4[\mathbb{Q}_0^{(a,A_{1g})}(1, 1)] \otimes \mathbb{Y}_4[\mathbb{Q}_0^{(b,A_{1g})}]$$

$$\hat{Z}_{17}(\mathbf{k}) = \mathbb{X}_4[\mathbb{Q}_0^{(a,A_{1g})}(1, 1)] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_{1g})}] \otimes \mathbb{F}_3[\mathbb{Q}_0^{(k,A_{1g})}]$$

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

$$\hat{Z}_{18} = \mathbb{X}_5[\mathbb{Q}_2^{(a,A_{1g})}(1, -1)] \otimes \mathbb{Y}_4[\mathbb{Q}_0^{(b,A_{1g})}]$$

$$\hat{Z}_{18}(\mathbf{k}) = \mathbb{X}_5[\mathbb{Q}_2^{(a,A_{1g})}(1, -1)] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_{1g})}] \otimes \mathbb{F}_3[\mathbb{Q}_0^{(k,A_{1g})}]$$

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

$$\hat{Z}_{19} = \mathbb{X}_{11}[\mathbb{Q}_2^{(a,B_{2g})}(1, -1)] \otimes \mathbb{Y}_5[\mathbb{Q}_2^{(b,B_{2g})}]$$

$$\hat{Z}_{19}(\mathbf{k}) = \mathbb{X}_{11}[\mathbb{Q}_2^{(a,B_{2g})}(1, -1)] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_{1g})}] \otimes \mathbb{F}_4[\mathbb{Q}_2^{(k,B_{2g})}]$$

$$\boxed{\text{No. 20}} \quad \hat{\mathbb{Q}}_0^{(A_{1g})} \text{ [M}_1, \text{B}_3]$$

$$\hat{Z}_{20} = \mathbb{X}_1[\mathbb{Q}_0^{(a,A_{1g})}] \otimes \mathbb{Y}_6[\mathbb{Q}_0^{(b,A_{1g})}]$$

$$\hat{Z}_{20}(\mathbf{k}) = \mathbb{X}_1[\mathbb{Q}_0^{(a,A_{1g})}] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_{1g})}] \otimes \mathbb{F}_5[\mathbb{Q}_0^{(k,A_{1g})}]$$

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

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

$$\hat{Z}_{21}(\mathbf{k}) = \mathbb{X}_2[\mathbb{Q}_0^{(a,A_{1g})}] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_{1g})}] \otimes \mathbb{F}_5[\mathbb{Q}_0^{(k,A_{1g})}]$$

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

$$\hat{Z}_{22} = \mathbb{X}_3[\mathbb{Q}_2^{(a,A_{1g})}] \otimes \mathbb{Y}_6[\mathbb{Q}_0^{(b,A_{1g})}]$$

$$\hat{Z}_{22}(\mathbf{k}) = \mathbb{X}_3[\mathbb{Q}_2^{(a,A_{1g})}] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_{1g})}] \otimes \mathbb{F}_5[\mathbb{Q}_0^{(k,A_{1g})}]$$

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

$$\hat{Z}_{23} = \mathbb{X}_4[\mathbb{Q}_0^{(a,A_{1g})}(1, 1)] \otimes \mathbb{Y}_6[\mathbb{Q}_0^{(b,A_{1g})}]$$

$$\hat{Z}_{23}(\mathbf{k}) = \mathbb{X}_4[\mathbb{Q}_0^{(a,A_{1g})}(1, 1)] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_{1g})}] \otimes \mathbb{F}_5[\mathbb{Q}_0^{(k,A_{1g})}]$$

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

$$\hat{Z}_{24} = \mathbb{X}_5[\mathbb{Q}_2^{(a,A_{1g})}(1, -1)] \otimes \mathbb{Y}_6[\mathbb{Q}_0^{(b,A_{1g})}]$$

$$\hat{\mathbb{Z}}_{24}(\mathbf{k}) = \mathbb{X}_5[\mathbb{Q}_2^{(a,A_{1g})}(1, -1)] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_{1g})}] \otimes \mathbb{F}_5[\mathbb{Q}_0^{(k,A_{1g})}]$$

$$\boxed{\text{No. 25}} \quad \hat{\mathbb{Q}}_0^{(A_{1g})} [\text{M}_1, \text{B}_4]$$

$$\hat{\mathbb{Z}}_{25} = \mathbb{X}_1[\mathbb{Q}_0^{(a,A_{1g})}] \otimes \mathbb{Y}_7[\mathbb{Q}_0^{(b,A_{1g})}]$$

$$\hat{\mathbb{Z}}_{25}(\mathbf{k}) = \mathbb{X}_1[\mathbb{Q}_0^{(a,A_{1g})}] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_{1g})}] \otimes \mathbb{F}_6[\mathbb{Q}_0^{(k,A_{1g})}]$$

$$\boxed{\text{No. 26}} \quad \hat{\mathbb{Q}}_0^{(A_{1g})} [\text{M}_3, \text{B}_4]$$

$$\hat{\mathbb{Z}}_{26} = \mathbb{X}_2[\mathbb{Q}_0^{(a,A_{1g})}] \otimes \mathbb{Y}_7[\mathbb{Q}_0^{(b,A_{1g})}]$$

$$\hat{\mathbb{Z}}_{26}(\mathbf{k}) = \mathbb{X}_2[\mathbb{Q}_0^{(a,A_{1g})}] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_{1g})}] \otimes \mathbb{F}_6[\mathbb{Q}_0^{(k,A_{1g})}]$$

$$\boxed{\text{No. 27}} \quad \hat{\mathbb{Q}}_2^{(A_{1g})} [\text{M}_3, \text{B}_4]$$

$$\hat{\mathbb{Z}}_{27} = \mathbb{X}_3[\mathbb{Q}_2^{(a,A_{1g})}] \otimes \mathbb{Y}_7[\mathbb{Q}_0^{(b,A_{1g})}]$$

$$\hat{\mathbb{Z}}_{27}(\mathbf{k}) = \mathbb{X}_3[\mathbb{Q}_2^{(a,A_{1g})}] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_{1g})}] \otimes \mathbb{F}_6[\mathbb{Q}_0^{(k,A_{1g})}]$$

$$\boxed{\text{No. 28}} \quad \hat{\mathbb{Q}}_0^{(A_{1g})} [\text{M}_3, \text{B}_4]$$

$$\hat{\mathbb{Z}}_{28} = \frac{\sqrt{3}\mathbb{X}_6[\mathbb{Q}_2^{(a,B_{1g})}] \otimes \mathbb{Y}_8[\mathbb{Q}_2^{(b,B_{1g})}]}{3} + \frac{\sqrt{3}\mathbb{X}_8[\mathbb{Q}_{2,0}^{(a,E_g)}] \otimes \mathbb{Y}_9[\mathbb{Q}_{2,0}^{(b,E_g)}]}{3} + \frac{\sqrt{3}\mathbb{X}_9[\mathbb{Q}_{2,1}^{(a,E_g)}] \otimes \mathbb{Y}_{10}[\mathbb{Q}_{2,1}^{(b,E_g)}]}{3}$$

$$\hat{\mathbb{Z}}_{28}(\mathbf{k}) = \frac{\sqrt{3}\mathbb{X}_6[\mathbb{Q}_2^{(a,B_{1g})}] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_{1g})}] \otimes \mathbb{F}_7[\mathbb{Q}_2^{(k,B_{1g})}]}{3} + \frac{\sqrt{3}\mathbb{X}_8[\mathbb{Q}_{2,0}^{(a,E_g)}] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_{1g})}] \otimes \mathbb{F}_8[\mathbb{Q}_{2,0}^{(k,E_g)}]}{3} + \frac{\sqrt{3}\mathbb{X}_9[\mathbb{Q}_{2,1}^{(a,E_g)}] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_{1g})}] \otimes \mathbb{F}_9[\mathbb{Q}_{2,1}^{(k,E_g)}]}{3}$$

$$\boxed{\text{No. 29}} \quad \hat{\mathbb{Q}}_2^{(A_{1g})} [\text{M}_3, \text{B}_4]$$

$$\hat{\mathbb{Z}}_{29} = -\frac{\sqrt{6}\mathbb{X}_6[\mathbb{Q}_2^{(a,B_{1g})}] \otimes \mathbb{Y}_8[\mathbb{Q}_2^{(b,B_{1g})}]}{3} + \frac{\sqrt{6}\mathbb{X}_8[\mathbb{Q}_{2,0}^{(a,E_g)}] \otimes \mathbb{Y}_9[\mathbb{Q}_{2,0}^{(b,E_g)}]}{6} + \frac{\sqrt{6}\mathbb{X}_9[\mathbb{Q}_{2,1}^{(a,E_g)}] \otimes \mathbb{Y}_{10}[\mathbb{Q}_{2,1}^{(b,E_g)}]}{6}$$

$$\hat{\mathbb{Z}}_{29}(\mathbf{k}) = -\frac{\sqrt{6}\mathbb{X}_6[\mathbb{Q}_2^{(a,B_{1g})}] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_{1g})}] \otimes \mathbb{F}_7[\mathbb{Q}_2^{(k,B_{1g})}]}{3} + \frac{\sqrt{6}\mathbb{X}_8[\mathbb{Q}_{2,0}^{(a,E_g)}] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_{1g})}] \otimes \mathbb{F}_8[\mathbb{Q}_{2,0}^{(k,E_g)}]}{6} + \frac{\sqrt{6}\mathbb{X}_9[\mathbb{Q}_{2,1}^{(a,E_g)}] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_{1g})}] \otimes \mathbb{F}_9[\mathbb{Q}_{2,1}^{(k,E_g)}]}{6}$$

$$\boxed{\text{No. 30}} \quad \hat{\mathbb{Q}}_0^{(A_{1g})}(1, 1) \text{ [M}_3, \text{B}_4]$$

$$\hat{\mathbb{Z}}_{30} = \mathbb{X}_4[\mathbb{Q}_0^{(a, A_{1g})}(1, 1)] \otimes \mathbb{Y}_7[\mathbb{Q}_0^{(b, A_{1g})}]$$

$$\hat{\mathbb{Z}}_{30}(\mathbf{k}) = \mathbb{X}_4[\mathbb{Q}_0^{(a, A_{1g})}(1, 1)] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s, A_{1g})}] \otimes \mathbb{F}_6[\mathbb{Q}_0^{(k, A_{1g})}]$$

$$\boxed{\text{No. 31}} \quad \hat{\mathbb{Q}}_2^{(A_{1g})}(1, -1) \text{ [M}_3, \text{B}_4]$$

$$\hat{\mathbb{Z}}_{31} = \mathbb{X}_5[\mathbb{Q}_2^{(a, A_{1g})}(1, -1)] \otimes \mathbb{Y}_7[\mathbb{Q}_0^{(b, A_{1g})}]$$

$$\hat{\mathbb{Z}}_{31}(\mathbf{k}) = \mathbb{X}_5[\mathbb{Q}_2^{(a, A_{1g})}(1, -1)] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s, A_{1g})}] \otimes \mathbb{F}_6[\mathbb{Q}_0^{(k, A_{1g})}]$$

$$\boxed{\text{No. 32}} \quad \hat{\mathbb{Q}}_0^{(A_{1g})}(1, -1) \text{ [M}_3, \text{B}_4]$$

$$\hat{\mathbb{Z}}_{32} = \frac{\sqrt{3}\mathbb{X}_{10}[\mathbb{Q}_2^{(a, B_{1g})}(1, -1)] \otimes \mathbb{Y}_8[\mathbb{Q}_2^{(b, B_{1g})}]}{3} + \frac{\sqrt{3}\mathbb{X}_{12}[\mathbb{Q}_{2,0}^{(a, E_g)}(1, -1)] \otimes \mathbb{Y}_9[\mathbb{Q}_{2,0}^{(b, E_g)}]}{3} + \frac{\sqrt{3}\mathbb{X}_{13}[\mathbb{Q}_{2,1}^{(a, E_g)}(1, -1)] \otimes \mathbb{Y}_{10}[\mathbb{Q}_{2,1}^{(b, E_g)}]}{3}$$

$$\begin{aligned} \hat{\mathbb{Z}}_{32}(\mathbf{k}) = & \frac{\sqrt{3}\mathbb{X}_{10}[\mathbb{Q}_2^{(a, B_{1g})}(1, -1)] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s, A_{1g})}] \otimes \mathbb{F}_7[\mathbb{Q}_2^{(k, B_{1g})}]}{3} + \frac{\sqrt{3}\mathbb{X}_{12}[\mathbb{Q}_{2,0}^{(a, E_g)}(1, -1)] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s, A_{1g})}] \otimes \mathbb{F}_8[\mathbb{Q}_{2,0}^{(k, E_g)}]}{3} \\ & + \frac{\sqrt{3}\mathbb{X}_{13}[\mathbb{Q}_{2,1}^{(a, E_g)}(1, -1)] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s, A_{1g})}] \otimes \mathbb{F}_9[\mathbb{Q}_{2,1}^{(k, E_g)}]}{3} \end{aligned}$$

$$\boxed{\text{No. 33}} \quad \hat{\mathbb{Q}}_2^{(A_{1g})}(1, -1) \text{ [M}_3, \text{B}_4]$$

$$\hat{\mathbb{Z}}_{33} = -\frac{\sqrt{6}\mathbb{X}_{10}[\mathbb{Q}_2^{(a, B_{1g})}(1, -1)] \otimes \mathbb{Y}_8[\mathbb{Q}_2^{(b, B_{1g})}]}{3} + \frac{\sqrt{6}\mathbb{X}_{12}[\mathbb{Q}_{2,0}^{(a, E_g)}(1, -1)] \otimes \mathbb{Y}_9[\mathbb{Q}_{2,0}^{(b, E_g)}]}{6} + \frac{\sqrt{6}\mathbb{X}_{13}[\mathbb{Q}_{2,1}^{(a, E_g)}(1, -1)] \otimes \mathbb{Y}_{10}[\mathbb{Q}_{2,1}^{(b, E_g)}]}{6}$$

$$\begin{aligned} \hat{\mathbb{Z}}_{33}(\mathbf{k}) = & -\frac{\sqrt{6}\mathbb{X}_{10}[\mathbb{Q}_2^{(a, B_{1g})}(1, -1)] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s, A_{1g})}] \otimes \mathbb{F}_7[\mathbb{Q}_2^{(k, B_{1g})}]}{3} + \frac{\sqrt{6}\mathbb{X}_{12}[\mathbb{Q}_{2,0}^{(a, E_g)}(1, -1)] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s, A_{1g})}] \otimes \mathbb{F}_8[\mathbb{Q}_{2,0}^{(k, E_g)}]}{6} \\ & + \frac{\sqrt{6}\mathbb{X}_{13}[\mathbb{Q}_{2,1}^{(a, E_g)}(1, -1)] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s, A_{1g})}] \otimes \mathbb{F}_9[\mathbb{Q}_{2,1}^{(k, E_g)}]}{6} \end{aligned}$$

$$\boxed{\text{No. 34}} \quad \hat{\mathbb{Q}}_2^{(A_{1g})}(1, 0) \text{ [M}_3, \text{B}_4]$$

$$\hat{\mathbb{Z}}_{34} = \frac{\sqrt{2}\mathbb{X}_{14}[\mathbb{G}_{1,0}^{(a, E_g)}(1, 0)] \otimes \mathbb{Y}_9[\mathbb{Q}_{2,0}^{(b, E_g)}]}{2} - \frac{\sqrt{2}\mathbb{X}_{15}[\mathbb{G}_{1,1}^{(a, E_g)}(1, 0)] \otimes \mathbb{Y}_{10}[\mathbb{Q}_{2,1}^{(b, E_g)}]}{2}$$

$$\hat{\mathbb{Z}}_{34}(\mathbf{k}) = \frac{\sqrt{2}\mathbb{X}_{14}[\mathbb{G}_{1,0}^{(a, E_g)}(1, 0)] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s, A_{1g})}] \otimes \mathbb{F}_8[\mathbb{Q}_{2,0}^{(k, E_g)}]}{2} - \frac{\sqrt{2}\mathbb{X}_{15}[\mathbb{G}_{1,1}^{(a, E_g)}(1, 0)] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s, A_{1g})}] \otimes \mathbb{F}_9[\mathbb{Q}_{2,1}^{(k, E_g)}]}{2}$$

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 | $\mathbb{Q}_0^{(a, A_{1g})}$ | 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}_3 | $\mathbb{Q}_2^{(a, A_{1g})}$ | M ₃ | $\begin{pmatrix} -\frac{\sqrt{3}}{6} & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{3}}{6} & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{3}}{6} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{3}}{6} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{3}}{3} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{3}}{3} \end{pmatrix}$ |
| \mathbb{X}_4 | $\mathbb{Q}_0^{(a, A_{1g})}(1, 1)$ | 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}_5 | $\mathbb{Q}_2^{(a,A_{1g})}(1,-1)$ | M_3 | $\begin{pmatrix} 0 & 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 & -\frac{\sqrt{6}}{12} \\ 0 & 0 & 0 & \frac{\sqrt{6}i}{6} & \frac{\sqrt{6}}{12} & 0 \\ \frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 & \frac{\sqrt{6}i}{12} \\ 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 & \frac{\sqrt{6}i}{12} & 0 \\ 0 & \frac{\sqrt{6}}{12} & 0 & -\frac{\sqrt{6}i}{12} & 0 & 0 \\ -\frac{\sqrt{6}}{12} & 0 & -\frac{\sqrt{6}i}{12} & 0 & 0 & 0 \end{pmatrix}$ |
| \mathbb{X}_6 | $\mathbb{Q}_2^{(a,B_{1g})}$ | 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}_7 | $\mathbb{Q}_2^{(a,B_{2g})}$ | 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}_8 | $\mathbb{Q}_{2,0}^{(a,E_g)}$ | M_3 | $\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{2} \\ 0 & 0 & \frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2} & 0 & 0 \end{pmatrix}$ |
| \mathbb{X}_9 | $\mathbb{Q}_{2,1}^{(a,E_g)}$ | M_3 | $\begin{pmatrix} 0 & 0 & 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{2} \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{1}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 & 0 & 0 \end{pmatrix}$ |

continued ...

Table 6

| symbol | type | group | form |
|-------------------|--------------------------------------|-------|--|
| \mathbb{X}_{10} | $\mathbb{Q}_2^{(a, B_{1g})}(1, -1)$ | 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}_{11} | $\mathbb{Q}_2^{(a, B_{2g})}(1, -1)$ | 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}_{12} | $\mathbb{Q}_{2,0}^{(a, E_g)}(1, -1)$ | 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}_{13} | $\mathbb{Q}_{2,1}^{(a, E_g)}(1, -1)$ | M_3 | $\begin{pmatrix} 0 & 0 & 0 & -\frac{\sqrt{2}i}{4} & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{2}i}{4} & 0 & 0 & 0 \\ 0 & \frac{\sqrt{2}i}{4} & 0 & 0 & -\frac{\sqrt{2}i}{4} & 0 \\ \frac{\sqrt{2}i}{4} & 0 & 0 & 0 & 0 & \frac{\sqrt{2}i}{4} \\ 0 & 0 & \frac{\sqrt{2}i}{4} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{2}i}{4} & 0 & 0 \end{pmatrix}$ |
| \mathbb{X}_{14} | $\mathbb{G}_{1,0}^{(a, E_g)}(1, 0)$ | M_3 | $\begin{pmatrix} 0 & 0 & 0 & -\frac{\sqrt{2}}{4} & -\frac{\sqrt{2}i}{4} & 0 \\ 0 & 0 & \frac{\sqrt{2}}{4} & 0 & 0 & \frac{\sqrt{2}i}{4} \\ 0 & \frac{\sqrt{2}}{4} & 0 & 0 & 0 & 0 \\ -\frac{\sqrt{2}}{4} & 0 & 0 & 0 & 0 & 0 \\ \frac{\sqrt{2}i}{4} & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{2}i}{4} & 0 & 0 & 0 & 0 \end{pmatrix}$ |

continued ...

Table 6

| symbol | type | group | form |
|-------------------|-----------------------------------|-------|--|
| \mathbb{X}_{15} | $\mathbb{G}_{1,1}^{(a,E_g)}(1,0)$ | 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 | $\mathbb{Q}_0^{(b,A_{1g})}$ | B_2 | $\begin{pmatrix} \frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2} \end{pmatrix}$ |
| \mathbb{Y}_5 | $\mathbb{Q}_2^{(b,B_{2g})}$ | B_2 | $\begin{pmatrix} \frac{\sqrt{2}}{2} & -\frac{\sqrt{2}}{2} \end{pmatrix}$ |
| \mathbb{Y}_6 | $\mathbb{Q}_0^{(b,A_{1g})}$ | B_3 | $\begin{pmatrix} 1 \end{pmatrix}$ |
| \mathbb{Y}_7 | $\mathbb{Q}_0^{(b,A_{1g})}$ | B_4 | $\begin{pmatrix} \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \end{pmatrix}$ |
| \mathbb{Y}_8 | $\mathbb{Q}_2^{(b,B_{1g})}$ | B_4 | $\begin{pmatrix} \frac{1}{2} & \frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} \end{pmatrix}$ |
| \mathbb{Y}_9 | $\mathbb{Q}_{2,0}^{(b,E_g)}$ | B_4 | $\begin{pmatrix} \frac{\sqrt{2}}{2} & -\frac{\sqrt{2}}{2} & 0 & 0 \end{pmatrix}$ |
| \mathbb{Y}_{10} | $\mathbb{Q}_{2,1}^{(b,E_g)}$ | B_4 | $\begin{pmatrix} 0 & 0 & -\frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2} \end{pmatrix}$ |

Table 8: Uniform SAMB.

| symbol | type | cluster | form |
|----------------|------------------------------|---------|-----------------------------------|
| \mathbb{U}_1 | $\mathbb{Q}_0^{(s, A_{1g})}$ | S_1 | $\begin{pmatrix} 1 \end{pmatrix}$ |

Table 9: Structure SAMB.

| symbol | type | cluster | form |
|----------------|-------------------------------|---------|---|
| \mathbb{F}_1 | $\mathbb{Q}_0^{(k, A_{1g})}$ | B_1 | $c_{001} + c_{002}$ |
| \mathbb{F}_2 | $\mathbb{Q}_2^{(k, B_{1g})}$ | B_1 | $c_{001} - c_{002}$ |
| \mathbb{F}_3 | $\mathbb{Q}_0^{(k, A_{1g})}$ | B_2 | $c_{003} + c_{004}$ |
| \mathbb{F}_4 | $\mathbb{Q}_2^{(k, B_{2g})}$ | B_2 | $c_{003} - c_{004}$ |
| \mathbb{F}_5 | $\mathbb{Q}_0^{(k, A_{1g})}$ | B_3 | $\sqrt{2}c_{005}$ |
| \mathbb{F}_6 | $\mathbb{Q}_0^{(k, A_{1g})}$ | B_4 | $\frac{\sqrt{2}c_{006}}{2} + \frac{\sqrt{2}c_{007}}{2} + \frac{\sqrt{2}c_{008}}{2} + \frac{\sqrt{2}c_{009}}{2}$ |
| \mathbb{F}_7 | $\mathbb{Q}_2^{(k, B_{1g})}$ | B_4 | $\frac{\sqrt{2}c_{006}}{2} + \frac{\sqrt{2}c_{007}}{2} - \frac{\sqrt{2}c_{008}}{2} - \frac{\sqrt{2}c_{009}}{2}$ |
| \mathbb{F}_8 | $\mathbb{Q}_{2,0}^{(k, E_g)}$ | B_4 | $c_{006} - c_{007}$ |
| \mathbb{F}_9 | $\mathbb{Q}_{2,1}^{(k, E_g)}$ | B_4 | $-c_{008} + c_{009}$ |

Table 10: Polar harmonics.

| No. | symbol | rank | irrep. | mul. | comp. | form |
|-----|----------------------------|------|----------|------|-------|--|
| 1 | $\mathbb{Q}_0^{(A_{1g})}$ | 0 | A_{1g} | — | — | 1 |
| 2 | $\mathbb{Q}_2^{(A_{1g})}$ | 2 | A_{1g} | — | — | $-\frac{x^2}{2} - \frac{y^2}{2} + z^2$ |
| 3 | $\mathbb{Q}_2^{(B_{1g})}$ | 2 | B_{1g} | — | — | $\frac{\sqrt{3}(x-y)(x+y)}{2}$ |
| 4 | $\mathbb{Q}_2^{(B_{2g})}$ | 2 | B_{2g} | — | — | $\sqrt{3}xy$ |
| 5 | $\mathbb{Q}_{2,0}^{(E_g)}$ | 2 | E_g | — | 0 | $\sqrt{3}yz$ |

continued ...

Table 10

| No. | symbol | rank | irrep. | mul. | comp. | form |
|-----|----------------------------|------|--------|------|-------|--------------|
| 6 | $\mathbb{Q}_{2,1}^{(E_g)}$ | 2 | E_g | — | 1 | $\sqrt{3}xz$ |

Table 11: 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 |

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

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

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

Table 13: 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 14: Character table (point-group part).

| | 1 | 2 ₀₀₁ | 2 ₁₀₀ | 2 ₁₁₀ | 4 ⁺ ₀₀₁ | -1 | m ₀₀₁ | m ₁₀₀ | m ₁₁₀ | -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 |
| 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 15: 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 16: 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 17: 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 18: 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 19: Virtual-cluster basis.

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

continued ...

Table 19

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