

SAMB for “Cs1”

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- Group: No. 6 $C_s^1 Pm$ (b-axis setting) [monoclinic]
 - Associated point group: No. 4 $C_s m$ (b-axis setting) [monoclinic]
 - Generation condition
 - model type: **tight_binding**
 - time-reversal type: **electric**
 - irrep: [A']
 - **spinful**
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- Unit cell:
 - $a = 1.0$, $b = 1.0$, $c = 1.0$, $\alpha = 90.0$, $\beta = 90.0$, $\gamma = 90.0$
- Lattice vectors:
 - $\mathbf{a}_1 = (1.0 \ 0 \ 0)$
 - $\mathbf{a}_2 = (0 \ 1.0 \ 0)$
 - $\mathbf{a}_3 = (0 \ 0 \ 1.0)$

Table 1: High-symmetry line: Γ -X.

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

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- Kets: dimension = 4

Table 2: Hilbert space for full matrix.

| No. | ket | No. | ket | No. | ket | No. | ket |
|-----|-----------------------|-----|-------------------------|-----|-----------------------|-----|-------------------------|
| 1 | $(p_x, \uparrow)@A_1$ | 2 | $(p_x, \downarrow)@A_1$ | 3 | $(p_y, \uparrow)@A_1$ | 4 | $(p_y, \downarrow)@A_1$ |

- Sites in (primitive) unit cell:

Table 3: Site-clusters.

| | site | position | mapping |
|------------------------|----------------|---|---------|
| S ₁ [1a: m] | A ₁ | $\begin{pmatrix} 0 & 0 & 0 \end{pmatrix}$ | [1,2] |

- Bonds in (primitive) unit cell:

Table 4: Bond-clusters.

| | bond | tail | head | n | # | $\mathbf{b}@c$ | mapping |
|------------------------|----------------|----------------|----------------|-----|---|---|---------|
| B ₁ [1a: m] | b ₁ | A ₁ | A ₁ | 1 | 1 | $\begin{pmatrix} -1 & 0 & 0 \end{pmatrix} @ \begin{pmatrix} \frac{1}{2} & 0 & 0 \end{pmatrix}$ | [1,2] |
| B ₂ [1b: m] | b ₂ | A ₁ | A ₁ | 1 | 2 | $\begin{pmatrix} 0 & 1 & 0 \end{pmatrix} @ \begin{pmatrix} 0 & \frac{1}{2} & 0 \end{pmatrix}$ | [1,-2] |
| B ₃ [1a: m] | b ₃ | A ₁ | A ₁ | 1 | 3 | $\begin{pmatrix} 0 & 0 & 1 \end{pmatrix} @ \begin{pmatrix} 0 & 0 & \frac{1}{2} \end{pmatrix}$ | [1,2] |
| B ₄ [1b: m] | b ₄ | A ₁ | A ₁ | 2 | 1 | $\begin{pmatrix} -1 & 1 & 0 \end{pmatrix} @ \begin{pmatrix} \frac{1}{2} & \frac{1}{2} & 0 \end{pmatrix}$ | [1] |
| | b ₅ | A ₁ | A ₁ | 2 | 1 | $\begin{pmatrix} -1 & -1 & 0 \end{pmatrix} @ \begin{pmatrix} \frac{1}{2} & \frac{1}{2} & 0 \end{pmatrix}$ | [2] |
| B ₅ [1b: m] | b ₆ | A ₁ | A ₁ | 2 | 2 | $\begin{pmatrix} 0 & 1 & -1 \end{pmatrix} @ \begin{pmatrix} 0 & \frac{1}{2} & \frac{1}{2} \end{pmatrix}$ | [1] |
| | b ₇ | A ₁ | A ₁ | 2 | 2 | $\begin{pmatrix} 0 & -1 & -1 \end{pmatrix} @ \begin{pmatrix} 0 & \frac{1}{2} & \frac{1}{2} \end{pmatrix}$ | [2] |
| B ₆ [1a: m] | b ₈ | A ₁ | A ₁ | 2 | 3 | $\begin{pmatrix} 1 & 0 & 1 \end{pmatrix} @ \begin{pmatrix} \frac{1}{2} & 0 & \frac{1}{2} \end{pmatrix}$ | [1,2] |
| B ₇ [1a: m] | b ₉ | A ₁ | A ₁ | 2 | 4 | $\begin{pmatrix} 1 & 0 & -1 \end{pmatrix} @ \begin{pmatrix} \frac{1}{2} & 0 & \frac{1}{2} \end{pmatrix}$ | [1,2] |

- SAMB:

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

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

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

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

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

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

$$\boxed{\text{No. 4}} \quad \hat{\mathbb{Q}}_2^{(A',3)}(1, -1) \text{ [M}_1, \text{S}_1]$$

$$\hat{\mathbb{Z}}_4 = \mathbb{X}_4[\mathbb{Q}_2^{(a,A',3)}(1, -1)] \otimes \mathbb{Y}_1[\mathbb{Q}_0^{(s,A')}]$$

$$\boxed{\text{No. 5}} \quad \hat{\mathbb{Q}}_0^{(A')} \text{ [M}_1, \text{B}_1]$$

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

$$\boxed{\text{No. 6}} \quad \hat{\mathbb{Q}}_2^{(A',2)} \text{ [M}_1, \text{B}_1]$$

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

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

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

$$\boxed{\text{No. 8}} \quad \hat{\mathbb{Q}}_2^{(A',3)}(1, -1) \text{ [M}_1, \text{B}_1]$$

$$\hat{\mathbb{Z}}_8 = \mathbb{X}_4[\mathbb{Q}_2^{(a,A',3)}(1, -1)] \otimes \mathbb{Y}_2[\mathbb{Q}_0^{(b,A')}]$$

$$\boxed{\text{No. 9}} \quad \hat{\mathbb{G}}_1^{(A')}(1, 1) \text{ [M}_1, \text{B}_1]$$

$$\hat{\mathbb{Z}}_9 = \mathbb{X}_7[\mathbb{M}_1^{(a,A')}(1, 1)] \otimes \mathbb{Y}_3[\mathbb{T}_0^{(b,A')}]$$

$$\boxed{\text{No. 10}} \quad \hat{\mathbb{G}}_1^{(A')} (1, -1) \text{ } [M_1, B_1]$$

$$\hat{\mathbb{Z}}_{10} = \mathbb{X}_8[\mathbb{M}_1^{(a, A')} (1, -1)] \otimes \mathbb{Y}_3[\mathbb{T}_0^{(b, A')}]$$

$$\boxed{\text{No. 11}} \quad \hat{\mathbb{G}}_3^{(A', 1)} (1, -1) \text{ } [M_1, B_1]$$

$$\hat{\mathbb{Z}}_{11} = \mathbb{X}_9[\mathbb{M}_3^{(a, A', 1)} (1, -1)] \otimes \mathbb{Y}_3[\mathbb{T}_0^{(b, A')}]$$

$$\boxed{\text{No. 12}} \quad \hat{\mathbb{G}}_3^{(A', 2)} (1, -1) \text{ } [M_1, B_1]$$

$$\hat{\mathbb{Z}}_{12} = \mathbb{X}_{10}[\mathbb{M}_3^{(a, A', 2)} (1, -1)] \otimes \mathbb{Y}_3[\mathbb{T}_0^{(b, A')}]$$

$$\boxed{\text{No. 13}} \quad \hat{\mathbb{Q}}_0^{(A')} \text{ } [M_1, B_2]$$

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

$$\boxed{\text{No. 14}} \quad \hat{\mathbb{Q}}_2^{(A', 2)} \text{ } [M_1, B_2]$$

$$\hat{\mathbb{Z}}_{14} = \mathbb{X}_2[\mathbb{Q}_2^{(a, A', 2)}] \otimes \mathbb{Y}_4[\mathbb{Q}_0^{(b, A')}]$$

$$\boxed{\text{No. 15}} \quad \hat{\mathbb{Q}}_0^{(A')} (1, 1) \text{ } [M_1, B_2]$$

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

$$\boxed{\text{No. 16}} \quad \hat{\mathbb{Q}}_2^{(A', 3)} (1, -1) \text{ } [M_1, B_2]$$

$$\hat{\mathbb{Z}}_{16} = \mathbb{X}_4[\mathbb{Q}_2^{(a, A', 3)} (1, -1)] \otimes \mathbb{Y}_4[\mathbb{Q}_0^{(b, A')}]$$

$$\boxed{\text{No. 17}} \quad \hat{\mathbb{Q}}_1^{(A', 1)} (1, 1) \text{ } [M_1, B_2]$$

$$\hat{\mathbb{Z}}_{17} = -\mathbb{X}_{12}[\mathbb{M}_1^{(a, A'', 2)} (1, 1)] \otimes \mathbb{Y}_5[\mathbb{T}_1^{(b, A'')}]$$

$$\boxed{\text{No. 18}} \quad \hat{\mathbb{Q}}_1^{(A', 2)} (1, 1) \text{ } [M_1, B_2]$$

$$\hat{\mathbb{Z}}_{18} = \mathbb{X}_{11}[\mathbb{M}_1^{(a, A'', 1)} (1, 1)] \otimes \mathbb{Y}_5[\mathbb{T}_1^{(b, A'')}]$$

$$\boxed{\text{No. 19}} \quad \hat{\mathbb{Q}}_1^{(A',2)}(1, -1) \text{ } [M_1, B_2]$$

$$\hat{Z}_{19} = \mathbb{X}_{13}[\mathbb{M}_1^{(a,A'',1)}(1, -1)] \otimes \mathbb{Y}_5[\mathbb{T}_1^{(b,A'')}]$$

$$\boxed{\text{No. 20}} \quad \hat{\mathbb{G}}_2^{(A',1)}(1, -1) \text{ } [M_1, B_2]$$

$$\hat{Z}_{20} = -\mathbb{X}_{15}[\mathbb{M}_3^{(a,A'',4)}(1, -1)] \otimes \mathbb{Y}_5[\mathbb{T}_1^{(b,A'')}]$$

$$\boxed{\text{No. 21}} \quad \hat{\mathbb{G}}_2^{(A',2)}(1, -1) \text{ } [M_1, B_2]$$

$$\hat{Z}_{21} = -\mathbb{X}_{14}[\mathbb{M}_3^{(a,A'',1)}(1, -1)] \otimes \mathbb{Y}_5[\mathbb{T}_1^{(b,A'')}]$$

$$\boxed{\text{No. 22}} \quad \hat{\mathbb{Q}}_1^{(A',1)} \text{ } [M_1, B_2]$$

$$\hat{Z}_{22} = -\mathbb{X}_{16}[\mathbb{M}_1^{(a,A'',2)}] \otimes \mathbb{Y}_5[\mathbb{T}_1^{(b,A'')}]$$

$$\boxed{\text{No. 23}} \quad \hat{\mathbb{Q}}_0^{(A')} \text{ } [M_1, B_3]$$

$$\hat{Z}_{23} = \mathbb{X}_1[\mathbb{Q}_0^{(a,A')}] \otimes \mathbb{Y}_6[\mathbb{Q}_0^{(b,A')}]$$

$$\boxed{\text{No. 24}} \quad \hat{\mathbb{Q}}_2^{(A',2)} \text{ } [M_1, B_3]$$

$$\hat{Z}_{24} = \mathbb{X}_2[\mathbb{Q}_2^{(a,A',2)}] \otimes \mathbb{Y}_6[\mathbb{Q}_0^{(b,A')}]$$

$$\boxed{\text{No. 25}} \quad \hat{\mathbb{Q}}_0^{(A')}(1, 1) \text{ } [M_1, B_3]$$

$$\hat{Z}_{25} = \mathbb{X}_3[\mathbb{Q}_0^{(a,A')}(1, 1)] \otimes \mathbb{Y}_6[\mathbb{Q}_0^{(b,A')}]$$

$$\boxed{\text{No. 26}} \quad \hat{\mathbb{Q}}_2^{(A',3)}(1, -1) \text{ } [M_1, B_3]$$

$$\hat{Z}_{26} = \mathbb{X}_4[\mathbb{Q}_2^{(a,A',3)}(1, -1)] \otimes \mathbb{Y}_6[\mathbb{Q}_0^{(b,A')}]$$

$$\boxed{\text{No. 27}} \quad \hat{\mathbb{G}}_1^{(A')}(1, 1) \text{ } [M_1, B_3]$$

$$\hat{Z}_{27} = \mathbb{X}_7[\mathbb{M}_1^{(a,A')}(1, 1)] \otimes \mathbb{Y}_7[\mathbb{T}_0^{(b,A')}]$$

$$\boxed{\text{No. 28}} \quad \hat{\mathbb{G}}_1^{(A')} (1, -1) \text{ [M}_1, \text{B}_3]$$

$$\hat{\mathbb{Z}}_{28} = \mathbb{X}_8[\mathbb{M}_1^{(a, A')} (1, -1)] \otimes \mathbb{Y}_7[\mathbb{T}_0^{(b, A')}]$$

$$\boxed{\text{No. 29}} \quad \hat{\mathbb{G}}_3^{(A', 1)} (1, -1) \text{ [M}_1, \text{B}_3]$$

$$\hat{\mathbb{Z}}_{29} = \mathbb{X}_9[\mathbb{M}_3^{(a, A', 1)} (1, -1)] \otimes \mathbb{Y}_7[\mathbb{T}_0^{(b, A')}]$$

$$\boxed{\text{No. 30}} \quad \hat{\mathbb{G}}_3^{(A', 2)} (1, -1) \text{ [M}_1, \text{B}_3]$$

$$\hat{\mathbb{Z}}_{30} = \mathbb{X}_{10}[\mathbb{M}_3^{(a, A', 2)} (1, -1)] \otimes \mathbb{Y}_7[\mathbb{T}_0^{(b, A')}]$$

$$\boxed{\text{No. 31}} \quad \hat{\mathbb{Q}}_0^{(A')} \text{ [M}_1, \text{B}_4]$$

$$\hat{\mathbb{Z}}_{31} = \mathbb{X}_1[\mathbb{Q}_0^{(a, A')}] \otimes \mathbb{Y}_8[\mathbb{Q}_0^{(b, A')}]$$

$$\boxed{\text{No. 32}} \quad \hat{\mathbb{Q}}_2^{(A', 2)} \text{ [M}_1, \text{B}_4]$$

$$\hat{\mathbb{Z}}_{32} = \mathbb{X}_2[\mathbb{Q}_2^{(a, A', 2)}] \otimes \mathbb{Y}_8[\mathbb{Q}_0^{(b, A')}]$$

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

$$\hat{\mathbb{Z}}_{33} = \mathbb{X}_5[\mathbb{Q}_2^{(a, A'', 2)}] \otimes \mathbb{Y}_9[\mathbb{Q}_1^{(b, A'')}]$$

$$\boxed{\text{No. 34}} \quad \hat{\mathbb{Q}}_0^{(A')} (1, 1) \text{ [M}_1, \text{B}_4]$$

$$\hat{\mathbb{Z}}_{34} = \mathbb{X}_3[\mathbb{Q}_0^{(a, A')} (1, 1)] \otimes \mathbb{Y}_8[\mathbb{Q}_0^{(b, A')}]$$

$$\boxed{\text{No. 35}} \quad \hat{\mathbb{Q}}_2^{(A', 3)} (1, -1) \text{ [M}_1, \text{B}_4]$$

$$\hat{\mathbb{Z}}_{35} = \mathbb{X}_4[\mathbb{Q}_2^{(a, A', 3)} (1, -1)] \otimes \mathbb{Y}_8[\mathbb{Q}_0^{(b, A')}]$$

$$\boxed{\text{No. 36}} \quad \hat{\mathbb{Q}}_1^{(A', 2)} (1, -1) \text{ [M}_1, \text{B}_4]$$

$$\hat{\mathbb{Z}}_{36} = \mathbb{X}_6[\mathbb{Q}_2^{(a, A'', 1)} (1, -1)] \otimes \mathbb{Y}_9[\mathbb{Q}_1^{(b, A'')}]$$

$$\boxed{\text{No. 37}} \quad \hat{\mathbb{G}}_1^{(A')}(1, 1) \text{ [M}_1, \text{B}_4]$$

$$\hat{\mathbb{Z}}_{37} = \mathbb{X}_7[\mathbb{M}_1^{(a, A')}(1, 1)] \otimes \mathbb{Y}_{10}[\mathbb{T}_0^{(b, A')}]$$

$$\boxed{\text{No. 38}} \quad \hat{\mathbb{Q}}_1^{(A', 1)}(1, 1) \text{ [M}_1, \text{B}_4]$$

$$\hat{\mathbb{Z}}_{38} = -\mathbb{X}_{12}[\mathbb{M}_1^{(a, A'', 2)}(1, 1)] \otimes \mathbb{Y}_{11}[\mathbb{T}_1^{(b, A'')}]$$

$$\boxed{\text{No. 39}} \quad \hat{\mathbb{Q}}_1^{(A', 2)}(1, 1) \text{ [M}_1, \text{B}_4]$$

$$\hat{\mathbb{Z}}_{39} = \mathbb{X}_{11}[\mathbb{M}_1^{(a, A'', 1)}(1, 1)] \otimes \mathbb{Y}_{11}[\mathbb{T}_1^{(b, A'')}]$$

$$\boxed{\text{No. 40}} \quad \hat{\mathbb{G}}_1^{(A')}(1, -1) \text{ [M}_1, \text{B}_4]$$

$$\hat{\mathbb{Z}}_{40} = \mathbb{X}_8[\mathbb{M}_1^{(a, A')}(1, -1)] \otimes \mathbb{Y}_{10}[\mathbb{T}_0^{(b, A')}]$$

$$\boxed{\text{No. 41}} \quad \hat{\mathbb{Q}}_1^{(A', 2)}(1, -1) \text{ [M}_1, \text{B}_4]$$

$$\hat{\mathbb{Z}}_{41} = \mathbb{X}_{13}[\mathbb{M}_1^{(a, A'', 1)}(1, -1)] \otimes \mathbb{Y}_{11}[\mathbb{T}_1^{(b, A'')}]$$

$$\boxed{\text{No. 42}} \quad \hat{\mathbb{G}}_3^{(A', 1)}(1, -1) \text{ [M}_1, \text{B}_4]$$

$$\hat{\mathbb{Z}}_{42} = \mathbb{X}_9[\mathbb{M}_3^{(a, A', 1)}(1, -1)] \otimes \mathbb{Y}_{10}[\mathbb{T}_0^{(b, A')}]$$

$$\boxed{\text{No. 43}} \quad \hat{\mathbb{G}}_3^{(A', 2)}(1, -1) \text{ [M}_1, \text{B}_4]$$

$$\hat{\mathbb{Z}}_{43} = \mathbb{X}_{10}[\mathbb{M}_3^{(a, A', 2)}(1, -1)] \otimes \mathbb{Y}_{10}[\mathbb{T}_0^{(b, A')}]$$

$$\boxed{\text{No. 44}} \quad \hat{\mathbb{G}}_2^{(A', 1)}(1, -1) \text{ [M}_1, \text{B}_4]$$

$$\hat{\mathbb{Z}}_{44} = -\mathbb{X}_{15}[\mathbb{M}_3^{(a, A'', 4)}(1, -1)] \otimes \mathbb{Y}_{11}[\mathbb{T}_1^{(b, A'')}]$$

$$\boxed{\text{No. 45}} \quad \hat{\mathbb{G}}_2^{(A', 2)}(1, -1) \text{ [M}_1, \text{B}_4]$$

$$\hat{\mathbb{Z}}_{45} = -\mathbb{X}_{14}[\mathbb{M}_3^{(a, A'', 1)}(1, -1)] \otimes \mathbb{Y}_{11}[\mathbb{T}_1^{(b, A'')}]$$

$$\boxed{\text{No. 46}} \quad \hat{\mathbb{Q}}_1^{(A',1)} \text{ [M}_1, \text{B}_4]$$

$$\hat{\mathbb{Z}}_{46} = -\mathbb{X}_{16}[\mathbb{M}_1^{(a,A'',2)}] \otimes \mathbb{Y}_{11}[\mathbb{T}_1^{(b,A'')}]$$

$$\boxed{\text{No. 47}} \quad \hat{\mathbb{Q}}_0^{(A')} \text{ [M}_1, \text{B}_5]$$

$$\hat{\mathbb{Z}}_{47} = \mathbb{X}_1[\mathbb{Q}_0^{(a,A')}] \otimes \mathbb{Y}_{12}[\mathbb{Q}_0^{(b,A')}]$$

$$\boxed{\text{No. 48}} \quad \hat{\mathbb{Q}}_2^{(A',2)} \text{ [M}_1, \text{B}_5]$$

$$\hat{\mathbb{Z}}_{48} = \mathbb{X}_2[\mathbb{Q}_2^{(a,A',2)}] \otimes \mathbb{Y}_{12}[\mathbb{Q}_0^{(b,A')}]$$

$$\boxed{\text{No. 49}} \quad \hat{\mathbb{Q}}_1^{(A',1)} \text{ [M}_1, \text{B}_5]$$

$$\hat{\mathbb{Z}}_{49} = \mathbb{X}_5[\mathbb{Q}_2^{(a,A'',2)}] \otimes \mathbb{Y}_{13}[\mathbb{Q}_1^{(b,A'')}]$$

$$\boxed{\text{No. 50}} \quad \hat{\mathbb{Q}}_0^{(A')}(1, 1) \text{ [M}_1, \text{B}_5]$$

$$\hat{\mathbb{Z}}_{50} = \mathbb{X}_3[\mathbb{Q}_0^{(a,A')}(1, 1)] \otimes \mathbb{Y}_{12}[\mathbb{Q}_0^{(b,A')}]$$

$$\boxed{\text{No. 51}} \quad \hat{\mathbb{Q}}_2^{(A',3)}(1, -1) \text{ [M}_1, \text{B}_5]$$

$$\hat{\mathbb{Z}}_{51} = \mathbb{X}_4[\mathbb{Q}_2^{(a,A',3)}(1, -1)] \otimes \mathbb{Y}_{12}[\mathbb{Q}_0^{(b,A')}]$$

$$\boxed{\text{No. 52}} \quad \hat{\mathbb{Q}}_1^{(A',2)}(1, -1) \text{ [M}_1, \text{B}_5]$$

$$\hat{\mathbb{Z}}_{52} = \mathbb{X}_6[\mathbb{Q}_2^{(a,A'',1)}(1, -1)] \otimes \mathbb{Y}_{13}[\mathbb{Q}_1^{(b,A'')}]$$

$$\boxed{\text{No. 53}} \quad \hat{\mathbb{G}}_1^{(A')}(1, 1) \text{ [M}_1, \text{B}_5]$$

$$\hat{\mathbb{Z}}_{53} = \mathbb{X}_7[\mathbb{M}_1^{(a,A')}(1, 1)] \otimes \mathbb{Y}_{14}[\mathbb{T}_0^{(b,A')}]$$

$$\boxed{\text{No. 54}} \quad \hat{\mathbb{Q}}_1^{(A',1)}(1, 1) \text{ [M}_1, \text{B}_5]$$

$$\hat{\mathbb{Z}}_{54} = -\mathbb{X}_{12}[\mathbb{M}_1^{(a,A'',2)}(1, 1)] \otimes \mathbb{Y}_{15}[\mathbb{T}_1^{(b,A'')}]$$

$$\boxed{\text{No. 55}} \quad \hat{\mathbb{Q}}_1^{(A',2)}(1,1) \text{ [M}_1, \text{B}_5]$$

$$\hat{\mathbb{Z}}_{55} = \mathbb{X}_{11}[\mathbb{M}_1^{(a,A'',1)}(1,1)] \otimes \mathbb{Y}_{15}[\mathbb{T}_1^{(b,A'')}]$$

$$\boxed{\text{No. 56}} \quad \hat{\mathbb{G}}_1^{(A')}(1,-1) \text{ [M}_1, \text{B}_5]$$

$$\hat{\mathbb{Z}}_{56} = \mathbb{X}_8[\mathbb{M}_1^{(a,A')}(1,-1)] \otimes \mathbb{Y}_{14}[\mathbb{T}_0^{(b,A')}]$$

$$\boxed{\text{No. 57}} \quad \hat{\mathbb{Q}}_1^{(A',2)}(1,-1) \text{ [M}_1, \text{B}_5]$$

$$\hat{\mathbb{Z}}_{57} = \mathbb{X}_{13}[\mathbb{M}_1^{(a,A'',1)}(1,-1)] \otimes \mathbb{Y}_{15}[\mathbb{T}_1^{(b,A'')}]$$

$$\boxed{\text{No. 58}} \quad \hat{\mathbb{G}}_3^{(A',1)}(1,-1) \text{ [M}_1, \text{B}_5]$$

$$\hat{\mathbb{Z}}_{58} = \mathbb{X}_9[\mathbb{M}_3^{(a,A',1)}(1,-1)] \otimes \mathbb{Y}_{14}[\mathbb{T}_0^{(b,A')}]$$

$$\boxed{\text{No. 59}} \quad \hat{\mathbb{G}}_3^{(A',2)}(1,-1) \text{ [M}_1, \text{B}_5]$$

$$\hat{\mathbb{Z}}_{59} = \mathbb{X}_{10}[\mathbb{M}_3^{(a,A',2)}(1,-1)] \otimes \mathbb{Y}_{14}[\mathbb{T}_0^{(b,A')}]$$

$$\boxed{\text{No. 60}} \quad \hat{\mathbb{G}}_2^{(A',1)}(1,-1) \text{ [M}_1, \text{B}_5]$$

$$\hat{\mathbb{Z}}_{60} = -\mathbb{X}_{15}[\mathbb{M}_3^{(a,A'',4)}(1,-1)] \otimes \mathbb{Y}_{15}[\mathbb{T}_1^{(b,A'')}]$$

$$\boxed{\text{No. 61}} \quad \hat{\mathbb{G}}_2^{(A',2)}(1,-1) \text{ [M}_1, \text{B}_5]$$

$$\hat{\mathbb{Z}}_{61} = -\mathbb{X}_{14}[\mathbb{M}_3^{(a,A'',1)}(1,-1)] \otimes \mathbb{Y}_{15}[\mathbb{T}_1^{(b,A'')}]$$

$$\boxed{\text{No. 62}} \quad \hat{\mathbb{Q}}_1^{(A',1)} \text{ [M}_1, \text{B}_5]$$

$$\hat{\mathbb{Z}}_{62} = -\mathbb{X}_{16}[\mathbb{M}_1^{(a,A'',2)}] \otimes \mathbb{Y}_{15}[\mathbb{T}_1^{(b,A'')}]$$

$$\boxed{\text{No. 63}} \quad \hat{\mathbb{Q}}_0^{(A')} \text{ [M}_1, \text{B}_6]$$

$$\hat{\mathbb{Z}}_{63} = \mathbb{X}_1[\mathbb{Q}_0^{(a,A')}] \otimes \mathbb{Y}_{16}[\mathbb{Q}_0^{(b,A')}]$$

$$\boxed{\text{No. 64}} \quad \hat{\mathbb{Q}}_2^{(A',2)} \text{ } [M_1, B_6]$$

$$\hat{Z}_{64} = \mathbb{X}_2[\mathbb{Q}_2^{(a,A',2)}] \otimes \mathbb{Y}_{16}[\mathbb{Q}_0^{(b,A')}]$$

$$\boxed{\text{No. 65}} \quad \hat{\mathbb{Q}}_0^{(A')} (1, 1) \text{ } [M_1, B_6]$$

$$\hat{Z}_{65} = \mathbb{X}_3[\mathbb{Q}_0^{(a,A')} (1, 1)] \otimes \mathbb{Y}_{16}[\mathbb{Q}_0^{(b,A')}]$$

$$\boxed{\text{No. 66}} \quad \hat{\mathbb{Q}}_2^{(A',3)} (1, -1) \text{ } [M_1, B_6]$$

$$\hat{Z}_{66} = \mathbb{X}_4[\mathbb{Q}_2^{(a,A',3)} (1, -1)] \otimes \mathbb{Y}_{16}[\mathbb{Q}_0^{(b,A')}]$$

$$\boxed{\text{No. 67}} \quad \hat{\mathbb{G}}_1^{(A')} (1, 1) \text{ } [M_1, B_6]$$

$$\hat{Z}_{67} = \mathbb{X}_7[\mathbb{M}_1^{(a,A')} (1, 1)] \otimes \mathbb{Y}_{17}[\mathbb{T}_0^{(b,A')}]$$

$$\boxed{\text{No. 68}} \quad \hat{\mathbb{G}}_1^{(A')} (1, -1) \text{ } [M_1, B_6]$$

$$\hat{Z}_{68} = \mathbb{X}_8[\mathbb{M}_1^{(a,A')} (1, -1)] \otimes \mathbb{Y}_{17}[\mathbb{T}_0^{(b,A')}]$$

$$\boxed{\text{No. 69}} \quad \hat{\mathbb{G}}_3^{(A',1)} (1, -1) \text{ } [M_1, B_6]$$

$$\hat{Z}_{69} = \mathbb{X}_9[\mathbb{M}_3^{(a,A',1)} (1, -1)] \otimes \mathbb{Y}_{17}[\mathbb{T}_0^{(b,A')}]$$

$$\boxed{\text{No. 70}} \quad \hat{\mathbb{G}}_3^{(A',2)} (1, -1) \text{ } [M_1, B_6]$$

$$\hat{Z}_{70} = \mathbb{X}_{10}[\mathbb{M}_3^{(a,A',2)} (1, -1)] \otimes \mathbb{Y}_{17}[\mathbb{T}_0^{(b,A')}]$$

$$\boxed{\text{No. 71}} \quad \hat{\mathbb{Q}}_0^{(A')} \text{ } [M_1, B_7]$$

$$\hat{Z}_{71} = \mathbb{X}_1[\mathbb{Q}_0^{(a,A')}] \otimes \mathbb{Y}_{18}[\mathbb{Q}_0^{(b,A')}]$$

$$\boxed{\text{No. 72}} \quad \hat{\mathbb{Q}}_2^{(A',2)} \text{ } [M_1, B_7]$$

$$\hat{Z}_{72} = \mathbb{X}_2[\mathbb{Q}_2^{(a,A',2)}] \otimes \mathbb{Y}_{18}[\mathbb{Q}_0^{(b,A')}]$$

$$\boxed{\text{No. 73}} \quad \hat{\mathbb{Q}}_0^{(A')}(1, 1) \text{ [M}_1, \text{B}_7]$$

$$\hat{\mathbb{Z}}_{73} = \mathbb{X}_3[\mathbb{Q}_0^{(a, A')}(1, 1)] \otimes \mathbb{Y}_{18}[\mathbb{Q}_0^{(b, A')}]$$

$$\boxed{\text{No. 74}} \quad \hat{\mathbb{Q}}_2^{(A', 3)}(1, -1) \text{ [M}_1, \text{B}_7]$$

$$\hat{\mathbb{Z}}_{74} = \mathbb{X}_4[\mathbb{Q}_2^{(a, A', 3)}(1, -1)] \otimes \mathbb{Y}_{18}[\mathbb{Q}_0^{(b, A')}]$$

$$\boxed{\text{No. 75}} \quad \hat{\mathbb{G}}_1^{(A')}(1, 1) \text{ [M}_1, \text{B}_7]$$

$$\hat{\mathbb{Z}}_{75} = \mathbb{X}_7[\mathbb{M}_1^{(a, A')}(1, 1)] \otimes \mathbb{Y}_{19}[\mathbb{T}_0^{(b, A')}]$$

$$\boxed{\text{No. 76}} \quad \hat{\mathbb{G}}_1^{(A')}(1, -1) \text{ [M}_1, \text{B}_7]$$

$$\hat{\mathbb{Z}}_{76} = \mathbb{X}_8[\mathbb{M}_1^{(a, A')}(1, -1)] \otimes \mathbb{Y}_{19}[\mathbb{T}_0^{(b, A')}]$$

$$\boxed{\text{No. 77}} \quad \hat{\mathbb{G}}_3^{(A', 1)}(1, -1) \text{ [M}_1, \text{B}_7]$$

$$\hat{\mathbb{Z}}_{77} = \mathbb{X}_9[\mathbb{M}_3^{(a, A', 1)}(1, -1)] \otimes \mathbb{Y}_{19}[\mathbb{T}_0^{(b, A')}]$$

$$\boxed{\text{No. 78}} \quad \hat{\mathbb{G}}_3^{(A', 2)}(1, -1) \text{ [M}_1, \text{B}_7]$$

$$\hat{\mathbb{Z}}_{78} = \mathbb{X}_{10}[\mathbb{M}_3^{(a, A', 2)}(1, -1)] \otimes \mathbb{Y}_{19}[\mathbb{T}_0^{(b, A')}]$$

Table 5: Atomic SAMB group.

| group | bra | ket |
|----------------|--|--|
| M ₁ | $(p_x, \uparrow), (p_x, \downarrow), (p_y, \uparrow), (p_y, \downarrow)$ | $(p_x, \uparrow), (p_x, \downarrow), (p_y, \uparrow), (p_y, \downarrow)$ |

Table 6: Atomic SAMB.

| symbol | type | group | form |
|----------------|----------------------------------|-------|--|
| \mathbb{X}_1 | $\mathbb{Q}_0^{(a,A')}$ | M_1 | $\begin{pmatrix} \frac{1}{2} & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 \\ 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & \frac{1}{2} \end{pmatrix}$ |
| \mathbb{X}_2 | $\mathbb{Q}_2^{(a,A',2)}$ | M_1 | $\begin{pmatrix} \frac{1}{2} & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 \\ 0 & 0 & -\frac{1}{2} & 0 \\ 0 & 0 & 0 & -\frac{1}{2} \end{pmatrix}$ |
| \mathbb{X}_3 | $\mathbb{Q}_0^{(a,A')}(1,1)$ | M_1 | $\begin{pmatrix} 0 & 0 & -\frac{i}{2} & 0 \\ 0 & 0 & 0 & \frac{i}{2} \\ \frac{i}{2} & 0 & 0 & 0 \\ 0 & -\frac{i}{2} & 0 & 0 \end{pmatrix}$ |
| \mathbb{X}_4 | $\mathbb{Q}_2^{(a,A',3)}(1,-1)$ | M_1 | $\begin{pmatrix} 0 & 0 & 0 & -\frac{i}{2} \\ 0 & 0 & -\frac{i}{2} & 0 \\ 0 & \frac{i}{2} & 0 & 0 \\ \frac{i}{2} & 0 & 0 & 0 \end{pmatrix}$ |
| \mathbb{X}_5 | $\mathbb{Q}_2^{(a,A'',2)}$ | M_1 | $\begin{pmatrix} 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & \frac{1}{2} \\ \frac{1}{2} & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 \end{pmatrix}$ |
| \mathbb{X}_6 | $\mathbb{Q}_2^{(a,A'',1)}(1,-1)$ | M_1 | $\begin{pmatrix} 0 & 0 & 0 & -\frac{1}{2} \\ 0 & 0 & \frac{1}{2} & 0 \\ 0 & \frac{1}{2} & 0 & 0 \\ -\frac{1}{2} & 0 & 0 & 0 \end{pmatrix}$ |
| \mathbb{X}_7 | $\mathbb{M}_1^{(a,A')}(1,1)$ | M_1 | $\begin{pmatrix} 0 & \frac{\sqrt{19}i}{19} & 0 & \frac{3\sqrt{19}}{38} \\ -\frac{\sqrt{19}i}{19} & 0 & \frac{3\sqrt{19}}{38} & 0 \\ 0 & \frac{3\sqrt{19}}{38} & 0 & -\frac{2\sqrt{19}i}{19} \\ \frac{3\sqrt{19}}{38} & 0 & \frac{2\sqrt{19}i}{19} & 0 \end{pmatrix}$ |
| \mathbb{X}_8 | $\mathbb{M}_1^{(a,A')}(1,-1)$ | M_1 | $\begin{pmatrix} 0 & -\frac{7\sqrt{38}i}{76} & 0 & -\frac{\sqrt{38}}{76} \\ \frac{7\sqrt{38}i}{76} & 0 & -\frac{\sqrt{38}}{76} & 0 \\ 0 & -\frac{\sqrt{38}}{76} & 0 & -\frac{5\sqrt{38}i}{76} \\ -\frac{\sqrt{38}}{76} & 0 & \frac{5\sqrt{38}i}{76} & 0 \end{pmatrix}$ |

continued ...

Table 6

| symbol | type | group | form |
|-------------------|----------------------------------|-------|--|
| \mathbb{X}_9 | $\mathbb{M}_3^{(a,A',1)}(1,-1)$ | M_1 | $\begin{pmatrix} 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & -\frac{1}{2} \\ \frac{1}{2} & 0 & 0 & 0 \\ 0 & -\frac{1}{2} & 0 & 0 \end{pmatrix}$ |
| \mathbb{X}_{10} | $\mathbb{M}_3^{(a,A',2)}(1,-1)$ | M_1 | $\begin{pmatrix} 0 & \frac{\sqrt{2}i}{4} & 0 & -\frac{\sqrt{2}}{4} \\ -\frac{\sqrt{2}i}{4} & 0 & -\frac{\sqrt{2}}{4} & 0 \\ 0 & -\frac{\sqrt{2}}{4} & 0 & -\frac{\sqrt{2}i}{4} \\ -\frac{\sqrt{2}}{4} & 0 & \frac{\sqrt{2}i}{4} & 0 \end{pmatrix}$ |
| \mathbb{X}_{11} | $\mathbb{M}_1^{(a,A'',1)}(1,1)$ | M_1 | $\begin{pmatrix} 0 & \frac{2\sqrt{19}}{19} & 0 & -\frac{3\sqrt{19}i}{38} \\ \frac{2\sqrt{19}}{19} & 0 & \frac{3\sqrt{19}i}{38} & 0 \\ 0 & -\frac{3\sqrt{19}i}{38} & 0 & -\frac{\sqrt{19}}{19} \\ \frac{3\sqrt{19}i}{38} & 0 & -\frac{\sqrt{19}}{19} & 0 \end{pmatrix}$ |
| \mathbb{X}_{12} | $\mathbb{M}_1^{(a,A'',2)}(1,1)$ | M_1 | $\begin{pmatrix} -\frac{1}{2} & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 \\ 0 & 0 & -\frac{1}{2} & 0 \\ 0 & 0 & 0 & \frac{1}{2} \end{pmatrix}$ |
| \mathbb{X}_{13} | $\mathbb{M}_1^{(a,A'',1)}(1,-1)$ | M_1 | $\begin{pmatrix} 0 & \frac{5\sqrt{38}}{76} & 0 & \frac{\sqrt{38}i}{76} \\ \frac{5\sqrt{38}}{76} & 0 & -\frac{\sqrt{38}i}{76} & 0 \\ 0 & \frac{\sqrt{38}i}{76} & 0 & \frac{7\sqrt{38}}{76} \\ -\frac{\sqrt{38}i}{76} & 0 & \frac{7\sqrt{38}}{76} & 0 \end{pmatrix}$ |
| \mathbb{X}_{14} | $\mathbb{M}_3^{(a,A'',1)}(1,-1)$ | M_1 | $\begin{pmatrix} 0 & \frac{\sqrt{2}}{4} & 0 & \frac{\sqrt{2}i}{4} \\ \frac{\sqrt{2}}{4} & 0 & -\frac{\sqrt{2}i}{4} & 0 \\ 0 & \frac{\sqrt{2}i}{4} & 0 & -\frac{\sqrt{2}}{4} \\ -\frac{\sqrt{2}i}{4} & 0 & -\frac{\sqrt{2}}{4} & 0 \end{pmatrix}$ |
| \mathbb{X}_{15} | $\mathbb{M}_3^{(a,A'',4)}(1,-1)$ | M_1 | $\begin{pmatrix} \frac{1}{2} & 0 & 0 & 0 \\ 0 & -\frac{1}{2} & 0 & 0 \\ 0 & 0 & -\frac{1}{2} & 0 \\ 0 & 0 & 0 & \frac{1}{2} \end{pmatrix}$ |
| \mathbb{X}_{16} | $\mathbb{M}_1^{(a,A'',2)}$ | M_1 | $\begin{pmatrix} 0 & 0 & -\frac{i}{2} & 0 \\ 0 & 0 & 0 & -\frac{i}{2} \\ \frac{i}{2} & 0 & 0 & 0 \\ 0 & \frac{i}{2} & 0 & 0 \end{pmatrix}$ |

Table 7: Cluster SAMB.

| symbol | type | cluster | form |
|-------------------|--------------------------|---------|--|
| \mathbb{Y}_1 | $\mathbb{Q}_0^{(s,A')}$ | S_1 | $\begin{pmatrix} 1 \end{pmatrix}$ |
| \mathbb{Y}_2 | $\mathbb{Q}_0^{(b,A')}$ | B_1 | $\begin{pmatrix} 1 \end{pmatrix}$ |
| \mathbb{Y}_3 | $\mathbb{T}_0^{(b,A')}$ | B_1 | $\begin{pmatrix} i \end{pmatrix}$ |
| \mathbb{Y}_4 | $\mathbb{Q}_0^{(b,A')}$ | B_2 | $\begin{pmatrix} 1 \end{pmatrix}$ |
| \mathbb{Y}_5 | $\mathbb{T}_1^{(b,A'')}$ | B_2 | $\begin{pmatrix} i \end{pmatrix}$ |
| \mathbb{Y}_6 | $\mathbb{Q}_0^{(b,A')}$ | B_3 | $\begin{pmatrix} 1 \end{pmatrix}$ |
| \mathbb{Y}_7 | $\mathbb{T}_0^{(b,A')}$ | B_3 | $\begin{pmatrix} i \end{pmatrix}$ |
| \mathbb{Y}_8 | $\mathbb{Q}_0^{(b,A')}$ | B_4 | $\begin{pmatrix} \frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2} \end{pmatrix}$ |
| \mathbb{Y}_9 | $\mathbb{Q}_1^{(b,A'')}$ | B_4 | $\begin{pmatrix} \frac{\sqrt{2}}{2} & -\frac{\sqrt{2}}{2} \end{pmatrix}$ |
| \mathbb{Y}_{10} | $\mathbb{T}_0^{(b,A')}$ | B_4 | $\begin{pmatrix} \frac{\sqrt{2}i}{2} & \frac{\sqrt{2}i}{2} \end{pmatrix}$ |
| \mathbb{Y}_{11} | $\mathbb{T}_1^{(b,A'')}$ | B_4 | $\begin{pmatrix} \frac{\sqrt{2}i}{2} & -\frac{\sqrt{2}i}{2} \end{pmatrix}$ |
| \mathbb{Y}_{12} | $\mathbb{Q}_0^{(b,A')}$ | B_5 | $\begin{pmatrix} \frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2} \end{pmatrix}$ |
| \mathbb{Y}_{13} | $\mathbb{Q}_1^{(b,A'')}$ | B_5 | $\begin{pmatrix} \frac{\sqrt{2}}{2} & -\frac{\sqrt{2}}{2} \end{pmatrix}$ |
| \mathbb{Y}_{14} | $\mathbb{T}_0^{(b,A')}$ | B_5 | $\begin{pmatrix} \frac{\sqrt{2}i}{2} & \frac{\sqrt{2}i}{2} \end{pmatrix}$ |
| \mathbb{Y}_{15} | $\mathbb{T}_1^{(b,A'')}$ | B_5 | $\begin{pmatrix} \frac{\sqrt{2}i}{2} & -\frac{\sqrt{2}i}{2} \end{pmatrix}$ |
| \mathbb{Y}_{16} | $\mathbb{Q}_0^{(b,A')}$ | B_6 | $\begin{pmatrix} 1 \end{pmatrix}$ |
| \mathbb{Y}_{17} | $\mathbb{T}_0^{(b,A')}$ | B_6 | $\begin{pmatrix} i \end{pmatrix}$ |
| \mathbb{Y}_{18} | $\mathbb{Q}_0^{(b,A')}$ | B_7 | $\begin{pmatrix} 1 \end{pmatrix}$ |
| \mathbb{Y}_{19} | $\mathbb{T}_0^{(b,A')}$ | B_7 | $\begin{pmatrix} i \end{pmatrix}$ |

Table 8: Polar harmonics.

| No. | symbol | rank | irrep. | mul. | comp. | form |
|-----|--------------------------|------|--------|------|-------|--------------------------------|
| 1 | $\mathbb{Q}_0^{(A')}$ | 0 | A' | — | — | 1 |
| 2 | $\mathbb{Q}_1^{(A'')}$ | 1 | A'' | — | — | y |
| 3 | $\mathbb{Q}_2^{(A'',1)}$ | 2 | A'' | 1 | — | $\sqrt{3}yz$ |
| 4 | $\mathbb{Q}_2^{(A'',2)}$ | 2 | A'' | 2 | — | $\sqrt{3}xy$ |
| 5 | $\mathbb{Q}_2^{(A',2)}$ | 2 | A' | 2 | — | $\frac{\sqrt{3}(x-y)(x+y)}{2}$ |
| 6 | $\mathbb{Q}_2^{(A',3)}$ | 2 | A' | 3 | — | $\sqrt{3}xz$ |

Table 9: Axial harmonics.

| No. | symbol | rank | irrep. | mul. | comp. | form |
|-----|--------------------------|------|--------|------|-------|----------------------------------|
| 1 | $\mathbb{G}_1^{(A'',1)}$ | 1 | A'' | 1 | — | X |
| 2 | $\mathbb{G}_1^{(A'',2)}$ | 1 | A'' | 2 | — | Z |
| 3 | $\mathbb{G}_1^{(A')}$ | 1 | A' | — | — | Y |
| 4 | $\mathbb{G}_3^{(A'',1)}$ | 3 | A'' | 1 | — | $\frac{X(2X^2-3Y^2-3Z^2)}{2}$ |
| 5 | $\mathbb{G}_3^{(A'',4)}$ | 3 | A'' | 4 | — | $\frac{\sqrt{15}Z(X-Y)(X+Y)}{2}$ |
| 6 | $\mathbb{G}_3^{(A',1)}$ | 3 | A' | 1 | — | $\sqrt{15}XYZ$ |
| 7 | $\mathbb{G}_3^{(A',2)}$ | 3 | A' | 2 | — | $-\frac{Y(3X^2-2Y^2+3Z^2)}{2}$ |

-
- Group info.: Generator = $\{m_{010}|0\}$

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

| rep. SO | symmetry operations |
|-----------------|---------------------|
| $\{1 0\}$ | $\{1 0\}$ |
| $\{m_{010} 0\}$ | $\{m_{010} 0\}$ |

Table 11: Symmetry operations.

| No. | SO | No. | SO | No. | SO | No. | SO | No. | SO |
|-----|-----------|-----|-----------------|-----|----|-----|----|-----|----|
| 1 | $\{1 0\}$ | 2 | $\{m_{010} 0\}$ | | | | | | |

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

| | 1 | m_{010} |
|-------|---|-----------|
| A' | 1 | 1 |
| A'' | 1 | -1 |

Table 13: Parity conversion.

| \leftrightarrow | \leftrightarrow |
|-------------------|-------------------|
| $A' (A'')$ | $A'' (A')$ |

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

| | A' | A'' |
|-------|------|-------|
| A' | A' | A'' |
| A'' | A' | A' |

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

| A' | A'' |
|------|-------|
| $-$ | $-$ |

Table 16: Virtual-cluster sites.

| No. | position | No. | position |
|-----|---|-----|--|
| 1 | $\begin{pmatrix} 0 & 1 & 0 \end{pmatrix}$ | 2 | $\begin{pmatrix} 0 & -1 & 0 \end{pmatrix}$ |

Table 17: Virtual-cluster basis.

| symbol | 1 | 2 |
|---------------|----------------------|-----------------------|
| $Q_0^{(A')}$ | $\frac{\sqrt{2}}{2}$ | $\frac{\sqrt{2}}{2}$ |
| $Q_1^{(A'')}$ | $\frac{\sqrt{2}}{2}$ | $-\frac{\sqrt{2}}{2}$ |