

SAMB for “0h1”

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

Table 1: High-symmetry line: Γ -X.

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

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- Kets: dimension = 8

Table 2: Hilbert space for full matrix.

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

- Sites in (primitive) unit cell:

Table 3: Site-clusters.

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

- Bonds in (primitive) unit cell:

Table 4: Bond-clusters.

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

- SAMB:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

$$\boxed{\text{No. 6}} \quad \hat{\mathbb{Q}}_0^{(A_{1g})}(1, 1) [\text{M}_3, \text{B}_1]$$

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

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

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

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

$$\hat{\mathbb{Z}}_7(\mathbf{k}) = \frac{\sqrt{2}\mathbb{X}_4[\mathbb{Q}_{2,0}^{(a,E_g)}] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_{1g})}] \otimes \mathbb{F}_2[\mathbb{Q}_{2,0}^{(k,E_g)}]}{2} + \frac{\sqrt{2}\mathbb{X}_5[\mathbb{Q}_{2,1}^{(a,E_g)}] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_{1g})}] \otimes \mathbb{F}_3[\mathbb{Q}_{2,1}^{(k,E_g)}]}{2}$$

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

$$\hat{\mathbb{Z}}_8 = \frac{\sqrt{2}\mathbb{X}_{10}[\mathbb{Q}_{2,1}^{(a,E_g)}(1,-1)] \otimes \mathbb{Y}_4[\mathbb{Q}_{2,1}^{(b,E_g)}]}{2} + \frac{\sqrt{2}\mathbb{X}_9[\mathbb{Q}_{2,0}^{(a,E_g)}(1,-1)] \otimes \mathbb{Y}_3[\mathbb{Q}_{2,0}^{(b,E_g)}]}{2}$$

$$\hat{\mathbb{Z}}_8(\mathbf{k}) = \frac{\sqrt{2}\mathbb{X}_{10}[\mathbb{Q}_{2,1}^{(a,E_g)}(1,-1)] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_{1g})}] \otimes \mathbb{F}_3[\mathbb{Q}_{2,1}^{(k,E_g)}]}{2} + \frac{\sqrt{2}\mathbb{X}_9[\mathbb{Q}_{2,0}^{(a,E_g)}(1,-1)] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_{1g})}] \otimes \mathbb{F}_2[\mathbb{Q}_{2,0}^{(k,E_g)}]}{2}$$

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

$$\hat{\mathbb{Z}}_9 = \mathbb{X}_1[\mathbb{Q}_0^{(a,A_{1g})}] \otimes \mathbb{Y}_5[\mathbb{Q}_0^{(b,A_{1g})}]$$

$$\hat{\mathbb{Z}}_9(\mathbf{k}) = \mathbb{X}_1[\mathbb{Q}_0^{(a,A_{1g})}] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_{1g})}] \otimes \mathbb{F}_4[\mathbb{Q}_0^{(k,A_{1g})}]$$

$$\boxed{\text{No. 10}} \quad \hat{\mathbb{Q}}_0^{(A_{1g})} [\text{M}_3, \text{B}_2]$$

$$\hat{\mathbb{Z}}_{10} = \mathbb{X}_2[\mathbb{Q}_0^{(a,A_{1g})}] \otimes \mathbb{Y}_5[\mathbb{Q}_0^{(b,A_{1g})}]$$

$$\hat{\mathbb{Z}}_{10}(\mathbf{k}) = \mathbb{X}_2[\mathbb{Q}_0^{(a,A_{1g})}] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_{1g})}] \otimes \mathbb{F}_4[\mathbb{Q}_0^{(k,A_{1g})}]$$

$$\boxed{\text{No. 11}} \quad \hat{\mathbb{Q}}_0^{(A_{1g})}(1,1) [\text{M}_3, \text{B}_2]$$

$$\hat{\mathbb{Z}}_{11} = \mathbb{X}_3[\mathbb{Q}_0^{(a,A_{1g})}(1,1)] \otimes \mathbb{Y}_5[\mathbb{Q}_0^{(b,A_{1g})}]$$

$$\hat{\mathbb{Z}}_{11}(\mathbf{k}) = \mathbb{X}_3[\mathbb{Q}_0^{(a,A_{1g})}(1,1)] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_{1g})}] \otimes \mathbb{F}_4[\mathbb{Q}_0^{(k,A_{1g})}]$$

$$\boxed{\text{No. 12}} \quad \hat{\mathbb{Q}}_0^{(A_{1g})} [\text{M}_3, \text{B}_2]$$

$$\hat{\mathbb{Z}}_{12} = \frac{\sqrt{5}\mathbb{X}_4[\mathbb{Q}_{2,0}^{(a,E_g)}] \otimes \mathbb{Y}_6[\mathbb{Q}_{2,0}^{(b,E_g)}]}{5} + \frac{\sqrt{5}\mathbb{X}_5[\mathbb{Q}_{2,1}^{(a,E_g)}] \otimes \mathbb{Y}_7[\mathbb{Q}_{2,1}^{(b,E_g)}]}{5} + \frac{\sqrt{5}\mathbb{X}_6[\mathbb{Q}_{2,0}^{(a,T_{2g})}] \otimes \mathbb{Y}_8[\mathbb{Q}_{2,0}^{(b,T_{2g})}]}{5} + \frac{\sqrt{5}\mathbb{X}_7[\mathbb{Q}_{2,1}^{(a,T_{2g})}] \otimes \mathbb{Y}_9[\mathbb{Q}_{2,1}^{(b,T_{2g})}]}{5} + \frac{\sqrt{5}\mathbb{X}_8[\mathbb{Q}_{2,2}^{(a,T_{2g})}] \otimes \mathbb{Y}_{10}[\mathbb{Q}_{2,2}^{(b,T_{2g})}]}{5}$$

$$\begin{aligned} \hat{\mathbb{Z}}_{12}(\mathbf{k}) = & \frac{\sqrt{5}\mathbb{X}_4[\mathbb{Q}_{2,0}^{(a,E_g)}] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_{1g})}] \otimes \mathbb{F}_5[\mathbb{Q}_{2,0}^{(k,E_g)}]}{5} + \frac{\sqrt{5}\mathbb{X}_5[\mathbb{Q}_{2,1}^{(a,E_g)}] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_{1g})}] \otimes \mathbb{F}_6[\mathbb{Q}_{2,1}^{(k,E_g)}]}{5} + \frac{\sqrt{5}\mathbb{X}_6[\mathbb{Q}_{2,0}^{(a,T_{2g})}] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_{1g})}] \otimes \mathbb{F}_7[\mathbb{Q}_{2,0}^{(k,T_{2g})}]}{5} \\ & + \frac{\sqrt{5}\mathbb{X}_7[\mathbb{Q}_{2,1}^{(a,T_{2g})}] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_{1g})}] \otimes \mathbb{F}_8[\mathbb{Q}_{2,1}^{(k,T_{2g})}]}{5} + \frac{\sqrt{5}\mathbb{X}_8[\mathbb{Q}_{2,2}^{(a,T_{2g})}] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_{1g})}] \otimes \mathbb{F}_9[\mathbb{Q}_{2,2}^{(k,T_{2g})}]}{5} \end{aligned}$$

$$\boxed{\text{No. 13}} \quad \hat{\mathbb{Q}}_4^{(A_{1g})} [\text{M}_3, \text{B}_2]$$

$$\begin{aligned} \hat{\mathbb{Z}}_{13} = & \frac{\sqrt{30}\mathbb{X}_4[\mathbb{Q}_{2,0}^{(a,E_g)}] \otimes \mathbb{Y}_6[\mathbb{Q}_{2,0}^{(b,E_g)}]}{10} + \frac{\sqrt{30}\mathbb{X}_5[\mathbb{Q}_{2,1}^{(a,E_g)}] \otimes \mathbb{Y}_7[\mathbb{Q}_{2,1}^{(b,E_g)}]}{10} - \frac{\sqrt{30}\mathbb{X}_6[\mathbb{Q}_{2,0}^{(a,T_{2g})}] \otimes \mathbb{Y}_8[\mathbb{Q}_{2,0}^{(b,T_{2g})}]}{15} \\ & - \frac{\sqrt{30}\mathbb{X}_7[\mathbb{Q}_{2,1}^{(a,T_{2g})}] \otimes \mathbb{Y}_9[\mathbb{Q}_{2,1}^{(b,T_{2g})}]}{15} - \frac{\sqrt{30}\mathbb{X}_8[\mathbb{Q}_{2,2}^{(a,T_{2g})}] \otimes \mathbb{Y}_{10}[\mathbb{Q}_{2,2}^{(b,T_{2g})}]}{15} \end{aligned}$$

$$\begin{aligned} \hat{\mathbb{Z}}_{13}(\mathbf{k}) = & \frac{\sqrt{30}\mathbb{X}_4[\mathbb{Q}_{2,0}^{(a,E_g)}] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_{1g})}] \otimes \mathbb{F}_5[\mathbb{Q}_{2,0}^{(k,E_g)}]}{10} + \frac{\sqrt{30}\mathbb{X}_5[\mathbb{Q}_{2,1}^{(a,E_g)}] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_{1g})}] \otimes \mathbb{F}_6[\mathbb{Q}_{2,1}^{(k,E_g)}]}{10} - \frac{\sqrt{30}\mathbb{X}_6[\mathbb{Q}_{2,0}^{(a,T_{2g})}] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_{1g})}] \otimes \mathbb{F}_7[\mathbb{Q}_{2,0}^{(k,T_{2g})}]}{15} \\ & - \frac{\sqrt{30}\mathbb{X}_7[\mathbb{Q}_{2,1}^{(a,T_{2g})}] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_{1g})}] \otimes \mathbb{F}_8[\mathbb{Q}_{2,1}^{(k,T_{2g})}]}{15} - \frac{\sqrt{30}\mathbb{X}_8[\mathbb{Q}_{2,2}^{(a,T_{2g})}] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_{1g})}] \otimes \mathbb{F}_9[\mathbb{Q}_{2,2}^{(k,T_{2g})}]}{15} \end{aligned}$$

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

$$\begin{aligned} \hat{\mathbb{Z}}_{14} = & \frac{\sqrt{5}\mathbb{X}_{10}[\mathbb{Q}_{2,1}^{(a,E_g)}(1, -1)] \otimes \mathbb{Y}_7[\mathbb{Q}_{2,1}^{(b,E_g)}]}{5} + \frac{\sqrt{5}\mathbb{X}_{11}[\mathbb{Q}_{2,0}^{(a,T_{2g})}(1, -1)] \otimes \mathbb{Y}_8[\mathbb{Q}_{2,0}^{(b,T_{2g})}]}{5} + \frac{\sqrt{5}\mathbb{X}_{12}[\mathbb{Q}_{2,1}^{(a,T_{2g})}(1, -1)] \otimes \mathbb{Y}_9[\mathbb{Q}_{2,1}^{(b,T_{2g})}]}{5} \\ & + \frac{\sqrt{5}\mathbb{X}_{13}[\mathbb{Q}_{2,2}^{(a,T_{2g})}(1, -1)] \otimes \mathbb{Y}_{10}[\mathbb{Q}_{2,2}^{(b,T_{2g})}]}{5} + \frac{\sqrt{5}\mathbb{X}_9[\mathbb{Q}_{2,0}^{(a,E_g)}(1, -1)] \otimes \mathbb{Y}_6[\mathbb{Q}_{2,0}^{(b,E_g)}]}{5} \end{aligned}$$

$$\begin{aligned} \hat{\mathbb{Z}}_{14}(\mathbf{k}) = & \frac{\sqrt{5}\mathbb{X}_{10}[\mathbb{Q}_{2,1}^{(a,E_g)}(1, -1)] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_{1g})}] \otimes \mathbb{F}_6[\mathbb{Q}_{2,1}^{(k,E_g)}]}{5} + \frac{\sqrt{5}\mathbb{X}_{11}[\mathbb{Q}_{2,0}^{(a,T_{2g})}(1, -1)] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_{1g})}] \otimes \mathbb{F}_7[\mathbb{Q}_{2,0}^{(k,T_{2g})}]}{5} \\ & + \frac{\sqrt{5}\mathbb{X}_{12}[\mathbb{Q}_{2,1}^{(a,T_{2g})}(1, -1)] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_{1g})}] \otimes \mathbb{F}_8[\mathbb{Q}_{2,1}^{(k,T_{2g})}]}{5} + \frac{\sqrt{5}\mathbb{X}_{13}[\mathbb{Q}_{2,2}^{(a,T_{2g})}(1, -1)] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_{1g})}] \otimes \mathbb{F}_9[\mathbb{Q}_{2,2}^{(k,T_{2g})}]}{5} \\ & + \frac{\sqrt{5}\mathbb{X}_9[\mathbb{Q}_{2,0}^{(a,E_g)}(1, -1)] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_{1g})}] \otimes \mathbb{F}_5[\mathbb{Q}_{2,0}^{(k,E_g)}]}{5} \end{aligned}$$

$$\boxed{\text{No. 15}} \quad \hat{\mathbb{Q}}_4^{(A_{1g})}(1, -1) [\text{M}_3, \text{B}_2]$$

$$\begin{aligned} \hat{\mathbb{Z}}_{15} = & \frac{\sqrt{30}\mathbb{X}_{10}[\mathbb{Q}_{2,1}^{(a,E_g)}(1, -1)] \otimes \mathbb{Y}_7[\mathbb{Q}_{2,1}^{(b,E_g)}]}{10} - \frac{\sqrt{30}\mathbb{X}_{11}[\mathbb{Q}_{2,0}^{(a,T_{2g})}(1, -1)] \otimes \mathbb{Y}_8[\mathbb{Q}_{2,0}^{(b,T_{2g})}]}{15} - \frac{\sqrt{30}\mathbb{X}_{12}[\mathbb{Q}_{2,1}^{(a,T_{2g})}(1, -1)] \otimes \mathbb{Y}_9[\mathbb{Q}_{2,1}^{(b,T_{2g})}]}{15} \\ & - \frac{\sqrt{30}\mathbb{X}_{13}[\mathbb{Q}_{2,2}^{(a,T_{2g})}(1, -1)] \otimes \mathbb{Y}_{10}[\mathbb{Q}_{2,2}^{(b,T_{2g})}]}{15} + \frac{\sqrt{30}\mathbb{X}_9[\mathbb{Q}_{2,0}^{(a,E_g)}(1, -1)] \otimes \mathbb{Y}_6[\mathbb{Q}_{2,0}^{(b,E_g)}]}{10} \\ \\ \hat{\mathbb{Z}}_{15}(\mathbf{k}) = & \frac{\sqrt{30}\mathbb{X}_{10}[\mathbb{Q}_{2,1}^{(a,E_g)}(1, -1)] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_{1g})}] \otimes \mathbb{F}_6[\mathbb{Q}_{2,1}^{(k,E_g)}]}{10} - \frac{\sqrt{30}\mathbb{X}_{11}[\mathbb{Q}_{2,0}^{(a,T_{2g})}(1, -1)] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_{1g})}] \otimes \mathbb{F}_7[\mathbb{Q}_{2,0}^{(k,T_{2g})}]}{15} \\ & - \frac{\sqrt{30}\mathbb{X}_{12}[\mathbb{Q}_{2,1}^{(a,T_{2g})}(1, -1)] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_{1g})}] \otimes \mathbb{F}_8[\mathbb{Q}_{2,1}^{(k,T_{2g})}]}{15} - \frac{\sqrt{30}\mathbb{X}_{13}[\mathbb{Q}_{2,2}^{(a,T_{2g})}(1, -1)] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_{1g})}] \otimes \mathbb{F}_9[\mathbb{Q}_{2,2}^{(k,T_{2g})}]}{15} \\ & + \frac{\sqrt{30}\mathbb{X}_9[\mathbb{Q}_{2,0}^{(a,E_g)}(1, -1)] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_{1g})}] \otimes \mathbb{F}_5[\mathbb{Q}_{2,0}^{(k,E_g)}]}{10} \end{aligned}$$

Table 5: Atomic SAMB group.

| group | bra | ket |
|----------------|--|--|
| M ₁ | (s, ↑), (s, ↓) | (s, ↑), (s, ↓) |
| M ₂ | (s, ↑), (s, ↓) | (p _x , ↑), (p _x , ↓), (p _y , ↑), (p _y , ↓), (p _z , ↑), (p _z , ↓) |
| M ₃ | (p _x , ↑), (p _x , ↓), (p _y , ↑), (p _y , ↓), (p _z , ↑), (p _z , ↓) | (p _x , ↑), (p _x , ↓), (p _y , ↑), (p _y , ↓), (p _z , ↑), (p _z , ↓) |

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 | $\begin{pmatrix} \frac{\sqrt{6}}{6} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{6}}{6} & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{6}}{6} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{6}}{6} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{6}}{6} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{6}}{6} \end{pmatrix}$ |

continued ...

Table 6

| symbol | type | group | form |
|----------------|----------------------------------|-------|--|
| \mathbb{X}_3 | $\mathbb{Q}_0^{(a,A_{1g})}(1,1)$ | M_3 | $\begin{pmatrix} 0 & 0 & -\frac{\sqrt{3}i}{6} & 0 & 0 & \frac{\sqrt{3}}{6} \\ 0 & 0 & 0 & \frac{\sqrt{3}i}{6} & -\frac{\sqrt{3}}{6} & 0 \\ \frac{\sqrt{3}i}{6} & 0 & 0 & 0 & 0 & -\frac{\sqrt{3}i}{6} \\ 0 & -\frac{\sqrt{3}i}{6} & 0 & 0 & -\frac{\sqrt{3}i}{6} & 0 \\ 0 & -\frac{\sqrt{3}}{6} & 0 & \frac{\sqrt{3}i}{6} & 0 & 0 \\ \frac{\sqrt{3}}{6} & 0 & \frac{\sqrt{3}i}{6} & 0 & 0 & 0 \end{pmatrix}$ |
| \mathbb{X}_4 | $\mathbb{Q}_{2,0}^{(a,E_g)}$ | M_3 | $\begin{pmatrix} -\frac{\sqrt{3}}{6} & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{3}}{6} & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{3}}{6} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{3}}{6} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{3}}{3} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{3}}{3} \end{pmatrix}$ |
| \mathbb{X}_5 | $\mathbb{Q}_{2,1}^{(a,E_g)}$ | M_3 | $\begin{pmatrix} \frac{1}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{1}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$ |
| \mathbb{X}_6 | $\mathbb{Q}_{2,0}^{(a,T_{2g})}$ | M_3 | $\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{2} \\ 0 & 0 & \frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2} & 0 & 0 \end{pmatrix}$ |
| \mathbb{X}_7 | $\mathbb{Q}_{2,1}^{(a,T_{2g})}$ | M_3 | $\begin{pmatrix} 0 & 0 & 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{2} \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{1}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 & 0 & 0 \end{pmatrix}$ |

continued ...

Table 6

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

continued ...

Table 6

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

Table 7: Cluster SAMB.

| symbol | type | cluster | form |
|-------------------|---------------------------------|---------|---|
| \mathbb{Y}_1 | $\mathbb{Q}_0^{(s,A_{1g})}$ | S_1 | $\begin{pmatrix} 1 \end{pmatrix}$ |
| \mathbb{Y}_2 | $\mathbb{Q}_0^{(b,A_{1g})}$ | B_1 | $\begin{pmatrix} \frac{\sqrt{3}}{3} & \frac{\sqrt{3}}{3} & \frac{\sqrt{3}}{3} \end{pmatrix}$ |
| \mathbb{Y}_3 | $\mathbb{Q}_{2,0}^{(b,E_g)}$ | B_1 | $\begin{pmatrix} -\frac{\sqrt{6}}{3} & \frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} \end{pmatrix}$ |
| \mathbb{Y}_4 | $\mathbb{Q}_{2,1}^{(b,E_g)}$ | B_1 | $\begin{pmatrix} 0 & -\frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2} \end{pmatrix}$ |
| \mathbb{Y}_5 | $\mathbb{Q}_0^{(b,A_{1g})}$ | B_2 | $\begin{pmatrix} \frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} \end{pmatrix}$ |
| \mathbb{Y}_6 | $\mathbb{Q}_{2,0}^{(b,E_g)}$ | B_2 | $\begin{pmatrix} -\frac{\sqrt{3}}{6} & -\frac{\sqrt{3}}{6} & -\frac{\sqrt{3}}{6} & \frac{\sqrt{3}}{3} & -\frac{\sqrt{3}}{6} & \frac{\sqrt{3}}{3} \end{pmatrix}$ |
| \mathbb{Y}_7 | $\mathbb{Q}_{2,1}^{(b,E_g)}$ | B_2 | $\begin{pmatrix} \frac{1}{2} & \frac{1}{2} & -\frac{1}{2} & 0 & -\frac{1}{2} & 0 \end{pmatrix}$ |
| \mathbb{Y}_8 | $\mathbb{Q}_{2,0}^{(b,T_{2g})}$ | B_2 | $\begin{pmatrix} \frac{\sqrt{2}}{2} & -\frac{\sqrt{2}}{2} & 0 & 0 & 0 & 0 \end{pmatrix}$ |
| \mathbb{Y}_9 | $\mathbb{Q}_{2,1}^{(b,T_{2g})}$ | B_2 | $\begin{pmatrix} 0 & 0 & -\frac{\sqrt{2}}{2} & 0 & \frac{\sqrt{2}}{2} & 0 \end{pmatrix}$ |
| \mathbb{Y}_{10} | $\mathbb{Q}_{2,2}^{(b,T_{2g})}$ | B_2 | $\begin{pmatrix} 0 & 0 & 0 & -\frac{\sqrt{2}}{2} & 0 & \frac{\sqrt{2}}{2} \end{pmatrix}$ |

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 | $\frac{\sqrt{6}c_{001}}{3} + \frac{\sqrt{6}c_{002}}{3} + \frac{\sqrt{6}c_{003}}{3}$ |
| \mathbb{F}_2 | $\mathbb{Q}_{2,0}^{(k, E_g)}$ | B_1 | $-\frac{2\sqrt{3}c_{001}}{3} + \frac{\sqrt{3}c_{002}}{3} + \frac{\sqrt{3}c_{003}}{3}$ |
| \mathbb{F}_3 | $\mathbb{Q}_{2,1}^{(k, E_g)}$ | B_1 | $-c_{002} + c_{003}$ |
| \mathbb{F}_4 | $\mathbb{Q}_0^{(k, A_{1g})}$ | B_2 | $\frac{\sqrt{3}c_{004}}{3} + \frac{\sqrt{3}c_{005}}{3} + \frac{\sqrt{3}c_{006}}{3} + \frac{\sqrt{3}c_{007}}{3} + \frac{\sqrt{3}c_{008}}{3} + \frac{\sqrt{3}c_{009}}{3}$ |
| \mathbb{F}_5 | $\mathbb{Q}_{2,0}^{(k, E_g)}$ | B_2 | $-\frac{\sqrt{6}c_{004}}{6} - \frac{\sqrt{6}c_{005}}{6} - \frac{\sqrt{6}c_{006}}{6} + \frac{\sqrt{6}c_{007}}{3} - \frac{\sqrt{6}c_{008}}{6} + \frac{\sqrt{6}c_{009}}{3}$ |
| \mathbb{F}_6 | $\mathbb{Q}_{2,1}^{(k, E_g)}$ | B_2 | $\frac{\sqrt{2}c_{004}}{2} + \frac{\sqrt{2}c_{005}}{2} - \frac{\sqrt{2}c_{006}}{2} - \frac{\sqrt{2}c_{008}}{2}$ |
| \mathbb{F}_7 | $\mathbb{Q}_{2,0}^{(k, T_{2g})}$ | B_2 | $c_{004} - c_{005}$ |
| \mathbb{F}_8 | $\mathbb{Q}_{2,1}^{(k, T_{2g})}$ | B_2 | $-c_{006} + c_{008}$ |
| \mathbb{F}_9 | $\mathbb{Q}_{2,2}^{(k, T_{2g})}$ | B_2 | $-c_{007} + c_{009}$ |

Table 10: Polar harmonics.

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

continued ...

Table 10

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

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

Table 11: Conjugacy class (point-group part).

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

Table 12: Symmetry operations.

| No. | SO | No. | SO | No. | SO | No. | SO | No. | SO |
|-----|---------------------|-----|---------------------|-----|---------------------|-----|---------------------|-----|--------------------|
| 1 | $\{1 0\}$ | 2 | $\{2_{001} 0\}$ | 3 | $\{2_{100} 0\}$ | 4 | $\{2_{010} 0\}$ | 5 | $\{2_{110} 0\}$ |
| 6 | $\{2_{101} 0\}$ | 7 | $\{2_{011} 0\}$ | 8 | $\{2_{1-10} 0\}$ | 9 | $\{2_{-101} 0\}$ | 10 | $\{2_{01-1} 0\}$ |
| 11 | $\{3_{111}^+ 0\}$ | 12 | $\{3_{1-1-1}^+ 0\}$ | 13 | $\{3_{-11-1}^+ 0\}$ | 14 | $\{3_{-1-11}^+ 0\}$ | 15 | $\{3_{-111}^- 0\}$ |
| 16 | $\{3_{1-1-1}^- 0\}$ | 17 | $\{3_{-11-1}^- 0\}$ | 18 | $\{3_{-1-11}^- 0\}$ | 19 | $\{4_{001}^+ 0\}$ | 20 | $\{4_{100}^+ 0\}$ |

continued ...

Table 12

| No. | SO | No. | SO | No. | SO | No. | SO | No. | SO |
|-----|----------------------|-----|----------------------|-----|----------------------|-----|--------------------|-----|----------------------|
| 21 | $\{4^+_{010} 0\}$ | 22 | $\{4^-_{001} 0\}$ | 23 | $\{4^-_{100} 0\}$ | 24 | $\{4^-_{010} 0\}$ | 25 | $\{-1 0\}$ |
| 26 | $\{m_{001} 0\}$ | 27 | $\{m_{100} 0\}$ | 28 | $\{m_{010} 0\}$ | 29 | $\{m_{110} 0\}$ | 30 | $\{m_{101} 0\}$ |
| 31 | $\{m_{011} 0\}$ | 32 | $\{m_{1-10} 0\}$ | 33 | $\{m_{-101} 0\}$ | 34 | $\{m_{01-1} 0\}$ | 35 | $\{-3^+_{111} 0\}$ |
| 36 | $\{-3^+_{1-1-1} 0\}$ | 37 | $\{-3^+_{-11-1} 0\}$ | 38 | $\{-3^+_{-1-11} 0\}$ | 39 | $\{-3^-_{111} 0\}$ | 40 | $\{-3^-_{1-1-1} 0\}$ |
| 41 | $\{-3^-_{-11-1} 0\}$ | 42 | $\{-3^-_{-1-11} 0\}$ | 43 | $\{-4^+_{001} 0\}$ | 44 | $\{-4^+_{100} 0\}$ | 45 | $\{-4^+_{010} 0\}$ |
| 46 | $\{-4^-_{001} 0\}$ | 47 | $\{-4^-_{100} 0\}$ | 48 | $\{-4^-_{010} 0\}$ | | | | |

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

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

Table 14: Parity conversion.

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

Table 15: Symmetric product, $[\Gamma \otimes \Gamma']_+$.

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

Table 16: Anti-symmetric product, $[\Gamma \otimes \Gamma]_-$.

| A_{1g} | A_{2g} | E_g | T_{1g} | T_{2g} | A_{1u} | A_{2u} | E_u | T_{1u} | T_{2u} |
|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|
| $-$ | $-$ | A_{2g} | T_{1g} | T_{1g} | $-$ | $-$ | A_{2g} | T_{1g} | T_{1g} |

Table 17: Virtual-cluster sites.

| No. | position | No. | position | No. | position | No. | position |
|-----|--|-----|--|-----|---|-----|--|
| 1 | $\begin{pmatrix} 3 & 2 & 1 \end{pmatrix}$ | 2 | $\begin{pmatrix} -3 & -2 & 1 \end{pmatrix}$ | 3 | $\begin{pmatrix} 3 & -2 & -1 \end{pmatrix}$ | 4 | $\begin{pmatrix} -3 & 2 & -1 \end{pmatrix}$ |
| 5 | $\begin{pmatrix} 2 & 3 & -1 \end{pmatrix}$ | 6 | $\begin{pmatrix} 1 & -2 & 3 \end{pmatrix}$ | 7 | $\begin{pmatrix} -3 & 1 & 2 \end{pmatrix}$ | 8 | $\begin{pmatrix} -2 & -3 & -1 \end{pmatrix}$ |
| 9 | $\begin{pmatrix} -1 & -2 & -3 \end{pmatrix}$ | 10 | $\begin{pmatrix} -3 & -1 & -2 \end{pmatrix}$ | 11 | $\begin{pmatrix} 1 & 3 & 2 \end{pmatrix}$ | 12 | $\begin{pmatrix} -1 & -3 & 2 \end{pmatrix}$ |
| 13 | $\begin{pmatrix} 1 & -3 & -2 \end{pmatrix}$ | 14 | $\begin{pmatrix} -1 & 3 & -2 \end{pmatrix}$ | 15 | $\begin{pmatrix} 2 & 1 & 3 \end{pmatrix}$ | 16 | $\begin{pmatrix} -2 & 1 & -3 \end{pmatrix}$ |
| 17 | $\begin{pmatrix} -2 & -1 & 3 \end{pmatrix}$ | 18 | $\begin{pmatrix} 2 & -1 & -3 \end{pmatrix}$ | 19 | $\begin{pmatrix} -2 & 3 & 1 \end{pmatrix}$ | 20 | $\begin{pmatrix} 3 & -1 & 2 \end{pmatrix}$ |
| 21 | $\begin{pmatrix} 1 & 2 & -3 \end{pmatrix}$ | 22 | $\begin{pmatrix} 2 & -3 & 1 \end{pmatrix}$ | 23 | $\begin{pmatrix} 3 & 1 & -2 \end{pmatrix}$ | 24 | $\begin{pmatrix} -1 & 2 & 3 \end{pmatrix}$ |
| 25 | $\begin{pmatrix} -3 & -2 & -1 \end{pmatrix}$ | 26 | $\begin{pmatrix} 3 & 2 & -1 \end{pmatrix}$ | 27 | $\begin{pmatrix} -3 & 2 & 1 \end{pmatrix}$ | 28 | $\begin{pmatrix} 3 & -2 & 1 \end{pmatrix}$ |

continued ...

Table 17

| No. | position | No. | position | No. | position | No. | position |
|-----|---|-----|---|-----|--|-----|---|
| 29 | $\begin{pmatrix} -2 & -3 & 1 \end{pmatrix}$ | 30 | $\begin{pmatrix} -1 & 2 & -3 \end{pmatrix}$ | 31 | $\begin{pmatrix} 3 & -1 & -2 \end{pmatrix}$ | 32 | $\begin{pmatrix} 2 & 3 & 1 \end{pmatrix}$ |
| 33 | $\begin{pmatrix} 1 & 2 & 3 \end{pmatrix}$ | 34 | $\begin{pmatrix} 3 & 1 & 2 \end{pmatrix}$ | 35 | $\begin{pmatrix} -1 & -3 & -2 \end{pmatrix}$ | 36 | $\begin{pmatrix} 1 & 3 & -2 \end{pmatrix}$ |
| 37 | $\begin{pmatrix} -1 & 3 & 2 \end{pmatrix}$ | 38 | $\begin{pmatrix} 1 & -3 & 2 \end{pmatrix}$ | 39 | $\begin{pmatrix} -2 & -1 & -3 \end{pmatrix}$ | 40 | $\begin{pmatrix} 2 & -1 & 3 \end{pmatrix}$ |
| 41 | $\begin{pmatrix} 2 & 1 & -3 \end{pmatrix}$ | 42 | $\begin{pmatrix} -2 & 1 & 3 \end{pmatrix}$ | 43 | $\begin{pmatrix} 2 & -3 & -1 \end{pmatrix}$ | 44 | $\begin{pmatrix} -3 & 1 & -2 \end{pmatrix}$ |
| 45 | $\begin{pmatrix} -1 & -2 & 3 \end{pmatrix}$ | 46 | $\begin{pmatrix} -2 & 3 & -1 \end{pmatrix}$ | 47 | $\begin{pmatrix} -3 & -1 & 2 \end{pmatrix}$ | 48 | $\begin{pmatrix} 1 & -2 & -3 \end{pmatrix}$ |

Table 18: Virtual-cluster basis.

| symbol | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
|----------------------|--------------------------|--------------------------|--------------------------|--------------------------|--------------------------|--------------------------|--------------------------|--------------------------|--------------------------|--------------------------|
| $Q_0^{(A_{1g})}$ | $\frac{\sqrt{3}}{12}$ | $\frac{\sqrt{3}}{12}$ | $\frac{\sqrt{3}}{12}$ | $\frac{\sqrt{3}}{12}$ | $\frac{\sqrt{3}}{12}$ | $\frac{\sqrt{3}}{12}$ | $\frac{\sqrt{3}}{12}$ | $\frac{\sqrt{3}}{12}$ | $\frac{\sqrt{3}}{12}$ | $\frac{\sqrt{3}}{12}$ |
| | $\frac{\sqrt{3}}{12}$ | $\frac{\sqrt{3}}{12}$ | $\frac{\sqrt{3}}{12}$ | $\frac{\sqrt{3}}{12}$ | $\frac{\sqrt{3}}{12}$ | $\frac{\sqrt{3}}{12}$ | $\frac{\sqrt{3}}{12}$ | $\frac{\sqrt{3}}{12}$ | $\frac{\sqrt{3}}{12}$ | $\frac{\sqrt{3}}{12}$ |
| | $\frac{\sqrt{3}}{12}$ | $\frac{\sqrt{3}}{12}$ | $\frac{\sqrt{3}}{12}$ | $\frac{\sqrt{3}}{12}$ | $\frac{\sqrt{3}}{12}$ | $\frac{\sqrt{3}}{12}$ | $\frac{\sqrt{3}}{12}$ | $\frac{\sqrt{3}}{12}$ | $\frac{\sqrt{3}}{12}$ | $\frac{\sqrt{3}}{12}$ |
| | $\frac{\sqrt{3}}{12}$ | $\frac{\sqrt{3}}{12}$ | $\frac{\sqrt{3}}{12}$ | $\frac{\sqrt{3}}{12}$ | $\frac{\sqrt{3}}{12}$ | $\frac{\sqrt{3}}{12}$ | $\frac{\sqrt{3}}{12}$ | $\frac{\sqrt{3}}{12}$ | $\frac{\sqrt{3}}{12}$ | $\frac{\sqrt{3}}{12}$ |
| | $\frac{\sqrt{3}}{12}$ | $\frac{\sqrt{3}}{12}$ | $\frac{\sqrt{3}}{12}$ | $\frac{\sqrt{3}}{12}$ | $\frac{\sqrt{3}}{12}$ | $\frac{\sqrt{3}}{12}$ | $\frac{\sqrt{3}}{12}$ | $\frac{\sqrt{3}}{12}$ | $\frac{\sqrt{3}}{12}$ | $\frac{\sqrt{3}}{12}$ |
| $Q_{1,0}^{(T_{1u})}$ | $\frac{3\sqrt{14}}{56}$ | $-\frac{3\sqrt{14}}{56}$ | $\frac{3\sqrt{14}}{56}$ | $-\frac{3\sqrt{14}}{56}$ | $\frac{\sqrt{14}}{28}$ | $\frac{\sqrt{14}}{56}$ | $-\frac{3\sqrt{14}}{56}$ | $-\frac{\sqrt{14}}{28}$ | $-\frac{\sqrt{14}}{56}$ | $-\frac{3\sqrt{14}}{56}$ |
| | $\frac{\sqrt{14}}{56}$ | $-\frac{\sqrt{14}}{56}$ | $\frac{\sqrt{14}}{56}$ | $-\frac{\sqrt{14}}{56}$ | $\frac{\sqrt{14}}{28}$ | $-\frac{\sqrt{14}}{28}$ | $-\frac{\sqrt{14}}{28}$ | $\frac{\sqrt{14}}{28}$ | $-\frac{\sqrt{14}}{28}$ | $\frac{3\sqrt{14}}{56}$ |
| | $\frac{\sqrt{14}}{56}$ | $\frac{\sqrt{14}}{28}$ | $\frac{3\sqrt{14}}{56}$ | $-\frac{\sqrt{14}}{56}$ | $-\frac{3\sqrt{14}}{56}$ | $\frac{3\sqrt{14}}{56}$ | $-\frac{3\sqrt{14}}{56}$ | $\frac{3\sqrt{14}}{56}$ | $-\frac{\sqrt{14}}{28}$ | $-\frac{\sqrt{14}}{56}$ |
| | $\frac{3\sqrt{14}}{56}$ | $\frac{\sqrt{14}}{28}$ | $\frac{\sqrt{14}}{56}$ | $\frac{3\sqrt{14}}{56}$ | $-\frac{\sqrt{14}}{56}$ | $\frac{\sqrt{14}}{56}$ | $-\frac{\sqrt{14}}{56}$ | $\frac{\sqrt{14}}{56}$ | $-\frac{\sqrt{14}}{28}$ | $\frac{\sqrt{14}}{28}$ |
| | $\frac{\sqrt{14}}{28}$ | $-\frac{\sqrt{14}}{28}$ | $\frac{\sqrt{14}}{28}$ | $-\frac{3\sqrt{14}}{56}$ | $-\frac{\sqrt{14}}{56}$ | $-\frac{\sqrt{14}}{28}$ | $-\frac{3\sqrt{14}}{56}$ | $\frac{\sqrt{14}}{56}$ | | |
| $Q_{1,1}^{(T_{1u})}$ | $\frac{\sqrt{14}}{28}$ | $-\frac{\sqrt{14}}{28}$ | $-\frac{\sqrt{14}}{28}$ | $\frac{\sqrt{14}}{28}$ | $\frac{3\sqrt{14}}{56}$ | $-\frac{\sqrt{14}}{28}$ | $\frac{\sqrt{14}}{56}$ | $-\frac{3\sqrt{14}}{56}$ | $-\frac{\sqrt{14}}{28}$ | $-\frac{\sqrt{14}}{56}$ |
| | $\frac{3\sqrt{14}}{56}$ | $-\frac{3\sqrt{14}}{56}$ | $-\frac{3\sqrt{14}}{56}$ | $\frac{3\sqrt{14}}{56}$ | $\frac{\sqrt{14}}{56}$ | $\frac{\sqrt{14}}{56}$ | $-\frac{\sqrt{14}}{56}$ | $-\frac{\sqrt{14}}{56}$ | $\frac{3\sqrt{14}}{56}$ | $-\frac{\sqrt{14}}{56}$ |
| | $\frac{\sqrt{14}}{28}$ | $-\frac{3\sqrt{14}}{56}$ | $\frac{\sqrt{14}}{56}$ | $\frac{\sqrt{14}}{28}$ | $-\frac{\sqrt{14}}{28}$ | $\frac{\sqrt{14}}{28}$ | $\frac{\sqrt{14}}{28}$ | $-\frac{\sqrt{14}}{28}$ | $-\frac{3\sqrt{14}}{56}$ | $\frac{\sqrt{14}}{28}$ |
| | $-\frac{\sqrt{14}}{56}$ | $\frac{3\sqrt{14}}{56}$ | $\frac{\sqrt{14}}{28}$ | $\frac{\sqrt{14}}{56}$ | $-\frac{3\sqrt{14}}{56}$ | $\frac{3\sqrt{14}}{56}$ | $\frac{3\sqrt{14}}{56}$ | $-\frac{3\sqrt{14}}{56}$ | $-\frac{\sqrt{14}}{56}$ | $-\frac{\sqrt{14}}{56}$ |
| | $\frac{\sqrt{14}}{56}$ | $\frac{\sqrt{14}}{56}$ | $-\frac{3\sqrt{14}}{56}$ | $\frac{\sqrt{14}}{56}$ | $-\frac{\sqrt{14}}{28}$ | $\frac{3\sqrt{14}}{56}$ | $-\frac{\sqrt{14}}{56}$ | $-\frac{\sqrt{14}}{28}$ | | |
| $Q_{1,2}^{(T_{1u})}$ | $\frac{\sqrt{14}}{56}$ | $\frac{\sqrt{14}}{56}$ | $-\frac{\sqrt{14}}{56}$ | $-\frac{\sqrt{14}}{56}$ | $-\frac{\sqrt{14}}{56}$ | $\frac{3\sqrt{14}}{56}$ | $\frac{\sqrt{14}}{28}$ | $-\frac{\sqrt{14}}{56}$ | $-\frac{3\sqrt{14}}{56}$ | $-\frac{\sqrt{14}}{28}$ |
| | $\frac{\sqrt{14}}{28}$ | $\frac{\sqrt{14}}{28}$ | $-\frac{\sqrt{14}}{28}$ | $-\frac{\sqrt{14}}{28}$ | $\frac{3\sqrt{14}}{56}$ | $-\frac{3\sqrt{14}}{56}$ | $\frac{3\sqrt{14}}{56}$ | $-\frac{3\sqrt{14}}{56}$ | $\frac{\sqrt{14}}{56}$ | $\frac{\sqrt{14}}{28}$ |
| | $-\frac{3\sqrt{14}}{56}$ | $\frac{\sqrt{14}}{56}$ | $-\frac{\sqrt{14}}{28}$ | $\frac{3\sqrt{14}}{56}$ | $-\frac{\sqrt{14}}{56}$ | $-\frac{\sqrt{14}}{56}$ | $\frac{\sqrt{14}}{56}$ | $\frac{\sqrt{14}}{56}$ | $-\frac{\sqrt{14}}{56}$ | $-\frac{3\sqrt{14}}{56}$ |

continued ...

[illegible]

15

[illegible]

continued ...

Table 18

[illegible]

continued ...

[illegible]

18

Table 18

[illegible]

continued ...

[illegible]

continued ...

| symbol | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
|---------------------------------|---------------------------|---------------------------|---------------------------|-------------------------|---------------------------|--------------------------|-------------------------|---------------------------|---------------------------|---------------------------|
| | $\frac{\sqrt{6}}{84}$ | $\frac{11\sqrt{6}}{168}$ | $-\frac{13\sqrt{6}}{168}$ | $\frac{\sqrt{6}}{84}$ | $\frac{\sqrt{6}}{84}$ | $\frac{\sqrt{6}}{84}$ | $\frac{\sqrt{6}}{84}$ | $\frac{\sqrt{6}}{84}$ | $-\frac{13\sqrt{6}}{168}$ | $-\frac{13\sqrt{6}}{168}$ |
| | $-\frac{13\sqrt{6}}{168}$ | $-\frac{13\sqrt{6}}{168}$ | $\frac{11\sqrt{6}}{168}$ | $\frac{\sqrt{6}}{84}$ | $-\frac{13\sqrt{6}}{168}$ | $\frac{11\sqrt{6}}{168}$ | $\frac{\sqrt{6}}{84}$ | $-\frac{13\sqrt{6}}{168}$ | | |
| $\mathbb{Q}_{7,1}^{(Eu)}$ | $\frac{5\sqrt{2}}{56}$ | $\frac{5\sqrt{2}}{56}$ | $\frac{5\sqrt{2}}{56}$ | $\frac{5\sqrt{2}}{56}$ | $-\frac{5\sqrt{2}}{56}$ | $-\frac{3\sqrt{2}}{56}$ | $\frac{\sqrt{2}}{7}$ | $-\frac{5\sqrt{2}}{56}$ | $-\frac{3\sqrt{2}}{56}$ | $\frac{\sqrt{2}}{7}$ |
| | $-\frac{\sqrt{2}}{7}$ | $-\frac{\sqrt{2}}{7}$ | $-\frac{\sqrt{2}}{7}$ | $-\frac{\sqrt{2}}{7}$ | $\frac{3\sqrt{2}}{56}$ | $\frac{3\sqrt{2}}{56}$ | $\frac{3\sqrt{2}}{56}$ | $\frac{3\sqrt{2}}{56}$ | $-\frac{5\sqrt{2}}{56}$ | $\frac{\sqrt{2}}{7}$ |
| | $-\frac{3\sqrt{2}}{56}$ | $-\frac{5\sqrt{2}}{56}$ | $\frac{\sqrt{2}}{7}$ | $-\frac{3\sqrt{2}}{56}$ | $-\frac{5\sqrt{2}}{56}$ | $-\frac{5\sqrt{2}}{56}$ | $-\frac{5\sqrt{2}}{56}$ | $-\frac{5\sqrt{2}}{56}$ | $\frac{5\sqrt{2}}{56}$ | $\frac{3\sqrt{2}}{56}$ |
| | $-\frac{\sqrt{2}}{7}$ | $\frac{5\sqrt{2}}{56}$ | $\frac{3\sqrt{2}}{56}$ | $-\frac{\sqrt{2}}{7}$ | $\frac{\sqrt{2}}{7}$ | $\frac{\sqrt{2}}{7}$ | $\frac{\sqrt{2}}{7}$ | $\frac{\sqrt{2}}{7}$ | $-\frac{3\sqrt{2}}{56}$ | $-\frac{3\sqrt{2}}{56}$ |
| | $-\frac{3\sqrt{2}}{56}$ | $-\frac{3\sqrt{2}}{56}$ | $\frac{5\sqrt{2}}{56}$ | $-\frac{\sqrt{2}}{7}$ | $\frac{3\sqrt{2}}{56}$ | $\frac{5\sqrt{2}}{56}$ | $-\frac{\sqrt{2}}{7}$ | $\frac{3\sqrt{2}}{56}$ | | |
| | | | | | | | | | | |
| $\mathbb{Q}_{7,0}^{(T_{2u},1)}$ | $-\frac{1}{14}$ | $\frac{1}{14}$ | $-\frac{1}{14}$ | $\frac{1}{14}$ | $\frac{3}{28}$ | $\frac{3}{14}$ | $-\frac{1}{14}$ | $-\frac{3}{28}$ | $-\frac{3}{14}$ | $-\frac{1}{14}$ |
| | $-\frac{3}{14}$ | $\frac{3}{14}$ | $-\frac{3}{14}$ | $\frac{3}{14}$ | $-\frac{3}{28}$ | $\frac{3}{28}$ | $\frac{3}{28}$ | $-\frac{3}{28}$ | $-\frac{3}{28}$ | $\frac{1}{14}$ |
| | $\frac{3}{14}$ | $\frac{3}{28}$ | $\frac{1}{14}$ | $-\frac{3}{14}$ | $\frac{1}{14}$ | $-\frac{1}{14}$ | $\frac{1}{14}$ | $-\frac{1}{14}$ | $-\frac{3}{28}$ | $-\frac{3}{14}$ |
| | $\frac{1}{14}$ | $\frac{3}{28}$ | $\frac{3}{14}$ | $\frac{1}{14}$ | $\frac{3}{14}$ | $-\frac{3}{14}$ | $\frac{3}{14}$ | $-\frac{3}{14}$ | $\frac{3}{28}$ | $-\frac{3}{28}$ |
| | $-\frac{3}{28}$ | $\frac{3}{28}$ | $\frac{3}{28}$ | $-\frac{1}{14}$ | $-\frac{3}{14}$ | $-\frac{3}{28}$ | $-\frac{1}{14}$ | $\frac{3}{14}$ | | |
| | | | | | | | | | | |
| $\mathbb{Q}_{7,1}^{(T_{2u},1)}$ | $-\frac{3}{28}$ | $\frac{3}{28}$ | $\frac{3}{28}$ | $-\frac{3}{28}$ | $\frac{1}{14}$ | $-\frac{3}{28}$ | $\frac{3}{14}$ | $-\frac{1}{14}$ | $-\frac{3}{28}$ | $-\frac{3}{14}$ |
| | $-\frac{1}{14}$ | $\frac{1}{14}$ | $\frac{1}{14}$ | $-\frac{1}{14}$ | $-\frac{3}{14}$ | $-\frac{3}{14}$ | $\frac{3}{14}$ | $\frac{3}{14}$ | $\frac{1}{14}$ | $-\frac{3}{14}$ |
| | $\frac{3}{28}$ | $-\frac{1}{14}$ | $\frac{3}{14}$ | $\frac{3}{28}$ | $\frac{3}{28}$ | $-\frac{3}{28}$ | $-\frac{3}{28}$ | $\frac{3}{28}$ | $-\frac{1}{14}$ | $\frac{3}{28}$ |
| | $-\frac{3}{14}$ | $\frac{1}{14}$ | $\frac{3}{28}$ | $\frac{3}{14}$ | $\frac{1}{14}$ | $-\frac{1}{14}$ | $-\frac{1}{14}$ | $\frac{1}{14}$ | $\frac{3}{14}$ | $\frac{3}{14}$ |
| | $-\frac{3}{14}$ | $-\frac{3}{14}$ | $-\frac{1}{14}$ | $\frac{3}{14}$ | $-\frac{3}{28}$ | $\frac{1}{14}$ | $-\frac{3}{14}$ | $-\frac{3}{28}$ | | |
| | | | | | | | | | | |
| $\mathbb{Q}_{7,2}^{(T_{2u},1)}$ | $-\frac{3}{14}$ | $-\frac{3}{14}$ | $\frac{3}{14}$ | $\frac{3}{14}$ | $-\frac{3}{14}$ | $\frac{1}{14}$ | $\frac{3}{28}$ | $-\frac{3}{14}$ | $-\frac{1}{14}$ | $-\frac{3}{28}$ |
| | $-\frac{3}{28}$ | $-\frac{3}{28}$ | $\frac{3}{28}$ | $\frac{3}{28}$ | $-\frac{1}{14}$ | $\frac{1}{14}$ | $-\frac{1}{14}$ | $\frac{1}{14}$ | $\frac{3}{14}$ | $\frac{3}{28}$ |
| | $-\frac{1}{14}$ | $\frac{3}{14}$ | $-\frac{3}{28}$ | $\frac{1}{14}$ | $\frac{3}{14}$ | $\frac{3}{14}$ | $-\frac{3}{14}$ | $-\frac{3}{14}$ | $\frac{3}{14}$ | $-\frac{1}{14}$ |
| | $-\frac{3}{28}$ | $\frac{3}{14}$ | $\frac{1}{14}$ | $\frac{3}{28}$ | $\frac{3}{28}$ | $\frac{3}{28}$ | $-\frac{3}{28}$ | $-\frac{3}{28}$ | $\frac{1}{14}$ | $-\frac{1}{14}$ |
| | | | | | | | | | | |

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Table 18

| symbol | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
|---------------------------------|--------------------------|-------------------------|--------------------------|--------------------------|--------------------------|--------------------------|--------------------------|--------------------------|--------------------------|--------------------------|
| $\mathbb{Q}_{8,2}^{(T_{1g},1)}$ | $-\frac{\sqrt{14}}{56}$ | $\frac{3\sqrt{14}}{56}$ | $\frac{\sqrt{14}}{28}$ | $\frac{\sqrt{14}}{56}$ | $-\frac{3\sqrt{14}}{56}$ | $\frac{3\sqrt{14}}{56}$ | $\frac{3\sqrt{14}}{56}$ | $-\frac{3\sqrt{14}}{56}$ | $-\frac{\sqrt{14}}{56}$ | $-\frac{\sqrt{14}}{56}$ |
| | $\frac{\sqrt{14}}{56}$ | $\frac{\sqrt{14}}{56}$ | $-\frac{3\sqrt{14}}{56}$ | $\frac{\sqrt{14}}{56}$ | $-\frac{\sqrt{14}}{28}$ | $\frac{3\sqrt{14}}{56}$ | $-\frac{\sqrt{14}}{56}$ | $-\frac{\sqrt{14}}{28}$ | | |
| | $-\frac{\sqrt{14}}{56}$ | $-\frac{\sqrt{14}}{56}$ | $\frac{\sqrt{14}}{56}$ | $\frac{\sqrt{14}}{56}$ | $\frac{\sqrt{14}}{56}$ | $-\frac{3\sqrt{14}}{56}$ | $-\frac{\sqrt{14}}{28}$ | $\frac{\sqrt{14}}{56}$ | $\frac{3\sqrt{14}}{56}$ | $\frac{\sqrt{14}}{28}$ |
| | $-\frac{\sqrt{14}}{28}$ | $-\frac{\sqrt{14}}{28}$ | $\frac{\sqrt{14}}{28}$ | $\frac{\sqrt{14}}{28}$ | $-\frac{3\sqrt{14}}{56}$ | $\frac{3\sqrt{14}}{56}$ | $-\frac{3\sqrt{14}}{56}$ | $\frac{3\sqrt{14}}{56}$ | $-\frac{\sqrt{14}}{56}$ | $-\frac{\sqrt{14}}{28}$ |
| | $\frac{3\sqrt{14}}{56}$ | $-\frac{\sqrt{14}}{56}$ | $\frac{\sqrt{14}}{28}$ | $-\frac{3\sqrt{14}}{56}$ | $-\frac{\sqrt{14}}{56}$ | $-\frac{\sqrt{14}}{56}$ | $\frac{\sqrt{14}}{56}$ | $\frac{\sqrt{14}}{56}$ | $\frac{\sqrt{14}}{56}$ | $-\frac{3\sqrt{14}}{56}$ |
| | $-\frac{\sqrt{14}}{28}$ | $\frac{\sqrt{14}}{56}$ | $\frac{3\sqrt{14}}{56}$ | $\frac{\sqrt{14}}{28}$ | $-\frac{\sqrt{14}}{28}$ | $-\frac{\sqrt{14}}{28}$ | $\frac{\sqrt{14}}{28}$ | $\frac{\sqrt{14}}{28}$ | $-\frac{3\sqrt{14}}{56}$ | $\frac{3\sqrt{14}}{56}$ |
| | $-\frac{3\sqrt{14}}{56}$ | $\frac{3\sqrt{14}}{56}$ | $-\frac{\sqrt{14}}{56}$ | $-\frac{\sqrt{14}}{28}$ | $\frac{3\sqrt{14}}{56}$ | $-\frac{\sqrt{14}}{56}$ | $\frac{\sqrt{14}}{28}$ | $-\frac{3\sqrt{14}}{56}$ | | |
| $\mathbb{Q}_9^{(A_{1u})}$ | $\frac{\sqrt{3}}{12}$ | $\frac{\sqrt{3}}{12}$ | $\frac{\sqrt{3}}{12}$ | $\frac{\sqrt{3}}{12}$ | $\frac{\sqrt{3}}{12}$ | $\frac{\sqrt{3}}{12}$ | $\frac{\sqrt{3}}{12}$ | $\frac{\sqrt{3}}{12}$ | $\frac{\sqrt{3}}{12}$ | $\frac{\sqrt{3}}{12}$ |
| | $\frac{\sqrt{3}}{12}$ | $\frac{\sqrt{3}}{12}$ | $\frac{\sqrt{3}}{12}$ | $\frac{\sqrt{3}}{12}$ | $\frac{\sqrt{3}}{12}$ | $\frac{\sqrt{3}}{12}$ | $\frac{\sqrt{3}}{12}$ | $\frac{\sqrt{3}}{12}$ | $\frac{\sqrt{3}}{12}$ | $\frac{\sqrt{3}}{12}$ |
| | $\frac{\sqrt{3}}{12}$ | $\frac{\sqrt{3}}{12}$ | $\frac{\sqrt{3}}{12}$ | $\frac{\sqrt{3}}{12}$ | $-\frac{\sqrt{3}}{12}$ | $-\frac{\sqrt{3}}{12}$ | $-\frac{\sqrt{3}}{12}$ | $-\frac{\sqrt{3}}{12}$ | $-\frac{\sqrt{3}}{12}$ | $-\frac{\sqrt{3}}{12}$ |
| | $-\frac{\sqrt{3}}{12}$ | $-\frac{\sqrt{3}}{12}$ | $-\frac{\sqrt{3}}{12}$ | $-\frac{\sqrt{3}}{12}$ | $-\frac{\sqrt{3}}{12}$ | $-\frac{\sqrt{3}}{12}$ | $-\frac{\sqrt{3}}{12}$ | $-\frac{\sqrt{3}}{12}$ | $-\frac{\sqrt{3}}{12}$ | $-\frac{\sqrt{3}}{12}$ |
| | $-\frac{\sqrt{3}}{12}$ | $-\frac{\sqrt{3}}{12}$ | $-\frac{\sqrt{3}}{12}$ | $-\frac{\sqrt{3}}{12}$ | $-\frac{\sqrt{3}}{12}$ | $-\frac{\sqrt{3}}{12}$ | $-\frac{\sqrt{3}}{12}$ | $-\frac{\sqrt{3}}{12}$ | | |