SAMB for "D4h1"

- 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`

- Unit cell:
    $a = 1.0,\ b = 1.0,\ c = 1.5,\ \alpha = 90.0,\ \beta = 90.0,\ \gamma = 90.0$
- Lattice vectors:
    $\boldsymbol{a}_1 = \begin{pmatrix} 1.0 & 0 & 0 \end{pmatrix}$
    $\boldsymbol{a}_2 = \begin{pmatrix} 0 & 1.0 & 0 \end{pmatrix}$
    $\boldsymbol{a}_3 = \begin{pmatrix} 0 & 0 & 1.5 \end{pmatrix}$

Table 1: High-symmetry line: Γ-X.

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

- 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 [1a: 4/mmm]	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	#	$\boldsymbol{b}@\boldsymbol{c}$	mapping
B_1 [2f: mmm.]	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 [1c: 4/mmm]	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 [1b: 4/mmm]	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 [2e: mmm.]	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:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Table 5: Atomic SAMB group.

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

continued ...

Table 6

symbol	type	group	form
$\mathbb{X}_{13}$	$\mathbb{Q}_0^{(a,A_{1g})}(1,1)$	M$_3$	$\begin{pmatrix} 0 & 0 & -\frac{\sqrt{3}i}{6} & 0 & 0 & \frac{\sqrt{3}}{6} \\ 0 & 0 & 0 & \frac{\sqrt{3}i}{6} & -\frac{\sqrt{3}}{6} & 0 \\ \frac{\sqrt{3}i}{6} & 0 & 0 & 0 & 0 & -\frac{\sqrt{3}i}{6} \\ 0 & -\frac{\sqrt{3}i}{6} & 0 & 0 & -\frac{\sqrt{3}i}{6} & 0 \\ 0 & -\frac{\sqrt{3}}{6} & 0 & \frac{\sqrt{3}i}{6} & 0 & 0 \\ \frac{\sqrt{3}}{6} & 0 & \frac{\sqrt{3}i}{6} & 0 & 0 & 0 \end{pmatrix}$
$\mathbb{X}_{14}$	$\mathbb{Q}_2^{(a,A_{1g})}(1,-1)$	M$_3$	$\begin{pmatrix} 0 & 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 & -\frac{\sqrt{6}}{12} \\ 0 & 0 & 0 & \frac{\sqrt{6}i}{6} & \frac{\sqrt{6}}{12} & 0 \\ \frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 & \frac{\sqrt{6}i}{12} \\ 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 & \frac{\sqrt{6}i}{12} & 0 \\ 0 & \frac{\sqrt{6}}{12} & 0 & -\frac{\sqrt{6}i}{12} & 0 & 0 \\ -\frac{\sqrt{6}}{12} & 0 & -\frac{\sqrt{6}i}{12} & 0 & 0 & 0 \end{pmatrix}$
$\mathbb{X}_{15}$	$\mathbb{Q}_2^{(a,B_{1g})}$	M$_3$	$\begin{pmatrix} \frac{1}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{1}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$
$\mathbb{X}_{16}$	$\mathbb{Q}_2^{(a,B_{2g})}$	M$_3$	$\begin{pmatrix} 0 & 0 & \frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2} & 0 & 0 \\ \frac{1}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$
$\mathbb{X}_{17}$	$\mathbb{Q}_{2,0}^{(a,E_g)}$	M$_3$	$\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{2} \\ 0 & 0 & \frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2} & 0 & 0 \end{pmatrix}$

Table 6

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

continued ...

Table 6

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

Table 7: Cluster SAMB.

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

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Table 7

symbol	type	cluster	form
$\mathbb{Y}_{12}$	$\mathbb{Q}_0^{(b,A_{1g})}$	B$_4$	$\left(\begin{array}{cccc}\frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2}\end{array}\right)$
$\mathbb{Y}_{13}$	$\mathbb{Q}_2^{(b,B_{1g})}$	B$_4$	$\left(\begin{array}{cccc}\frac{1}{2} & \frac{1}{2} & -\frac{1}{2} & -\frac{1}{2}\end{array}\right)$
$\mathbb{Y}_{14}$	$\mathbb{Q}_{2,0}^{(b,E_g)}$	B$_4$	$\left(\begin{array}{cccc}\frac{\sqrt{2}}{2} & -\frac{\sqrt{2}}{2} & 0 & 0\end{array}\right)$
$\mathbb{Y}_{15}$	$\mathbb{Q}_{2,1}^{(b,E_g)}$	B$_4$	$\left(\begin{array}{cccc}0 & 0 & -\frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2}\end{array}\right)$
$\mathbb{Y}_{16}$	$\mathbb{T}_1^{(b,A_{2u})}$	B$_4$	$\left(\begin{array}{cccc}\frac{i}{2} & -\frac{i}{2} & -\frac{i}{2} & \frac{i}{2}\end{array}\right)$
$\mathbb{Y}_{17}$	$\mathbb{T}_{1,0}^{(b,E_u)}$	B$_4$	$\left(\begin{array}{cccc}0 & 0 & \frac{\sqrt{2}i}{2} & \frac{\sqrt{2}i}{2}\end{array}\right)$
$\mathbb{Y}_{18}$	$\mathbb{T}_{1,1}^{(b,E_u)}$	B$_4$	$\left(\begin{array}{cccc}\frac{\sqrt{2}i}{2} & \frac{\sqrt{2}i}{2} & 0 & 0\end{array}\right)$
$\mathbb{Y}_{19}$	$\mathbb{T}_3^{(b,B_{2u})}$	B$_4$	$\left(\begin{array}{cccc}\frac{i}{2} & -\frac{i}{2} & \frac{i}{2} & -\frac{i}{2}\end{array}\right)$

Table 8: Polar harmonics.

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

Table 9: Axial harmonics.

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

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

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

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

Table 11: Symmetry operations.

No.	SO	No.	SO	No.	SO	No.	SO	No.	SO
1	$\{1\|0\}$	2	$\{2_{001}\|0\}$	3	$\{2_{100}\|0\}$	4	$\{2_{010}\|0\}$	5	$\{2_{110}\|0\}$
6	$\{2_{1-10}\|0\}$	7	$\{4^{+}_{001}\|0\}$	8	$\{4^{-}_{001}\|0\}$	9	$\{-1\|0\}$	10	$\{m_{001}\|0\}$
11	$\{m_{100}\|0\}$	12	$\{m_{010}\|0\}$	13	$\{m_{110}\|0\}$	14	$\{m_{1-10}\|0\}$	15	$\{-4^{+}_{001}\|0\}$
16	$\{-4^{-}_{001}\|0\}$								

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

	1	2_{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 13: Parity conversion.

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

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

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

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

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

Table 16: Virtual-cluster sites.

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

Table 17: Virtual-cluster basis.

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

Table 17

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