SAMB for "D2h1"

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- Group: No. 47 D_{2h}^{1} $Pmmm$ [orthorhombic]
- Associated point group: No. 8 D_{2h} mmm [orthorhombic]

- Generation condition
  - model type: `tight_binding`
  - time-reversal type: `electric`
  - irrep: `[Ag]`
  - `spinful`

- Unit cell:
  $a = 1.0,\ b = 1.2,\ c = 1.5,\ \alpha = 90.0,\ \beta = 90.0,\ \gamma = 90.0$
- Lattice vectors:
  $\boldsymbol{a}_1 = \begin{pmatrix} 1.0 & 0 & 0 \end{pmatrix}$
  $\boldsymbol{a}_2 = \begin{pmatrix} 0 & 1.2 & 0 \end{pmatrix}$
  $\boldsymbol{a}_3 = \begin{pmatrix} 0 & 0 & 1.5 \end{pmatrix}$

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: mmm]	A_1	$\begin{pmatrix} 0 & 0 & 0 \end{pmatrix}$	[1,2,3,4,5,6,7,8]

- Bonds in (primitive) unit cell:

Table 4: Bond-clusters.

	bond	tail	head	n	#	$\boldsymbol{b}$@$\boldsymbol{c}$	mapping
B_1 [1b: mmm]	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,-3,4,-5,6,7,-8]
B_2 [1e: mmm]	b_2	A_1	A_1	2	1	$\begin{pmatrix} 0 & 1 & 0 \end{pmatrix}$ @ $\begin{pmatrix} 0 & \frac{1}{2} & 0 \end{pmatrix}$	[1,-2,3,-4,-5,6,-7,8]
B_3 [1c: mmm]	b_3	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]
B_4 [1f: mmm]	b_4	A_1	A_1	4	1	$\begin{pmatrix} 1 & 1 & 0 \end{pmatrix}$ @ $\begin{pmatrix} \frac{1}{2} & \frac{1}{2} & 0 \end{pmatrix}$	[1,-2,-5,6]
	b_5	A_1	A_1	4	1	$\begin{pmatrix} 1 & -1 & 0 \end{pmatrix}$ @ $\begin{pmatrix} \frac{1}{2} & \frac{1}{2} & 0 \end{pmatrix}$	[-3,4,7,-8]

- SAMB:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

$\boxed{\text{No. 9}}$ $\hat{\mathbb{Q}}_0^{(A_g)}$ $[\mathrm{M}_3, \mathrm{B}_1]$

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

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

$\boxed{\text{No. 10}}$ $\hat{\mathbb{Q}}_2^{(A_g,1)}$ $[\mathrm{M}_3, \mathrm{B}_1]$

$$\hat{\mathbb{Z}}_{10} = \mathbb{X}_3[\mathbb{Q}_2^{(a,A_g,1)}] \otimes \mathbb{Y}_2[\mathbb{Q}_0^{(b,A_g)}]$$

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

$\boxed{\text{No. 11}}$ $\hat{\mathbb{Q}}_2^{(A_g,2)}$ $[\mathrm{M}_3, \mathrm{B}_1]$

$$\hat{\mathbb{Z}}_{11} = \mathbb{X}_4[\mathbb{Q}_2^{(a,A_g,2)}] \otimes \mathbb{Y}_2[\mathbb{Q}_0^{(b,A_g)}]$$

$$\hat{\mathbb{Z}}_{11}(\boldsymbol{k}) = \mathbb{X}_4[\mathbb{Q}_2^{(a,A_g,2)}] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_g)}] \otimes \mathbb{F}_1[\mathbb{Q}_0^{(k,A_g)}]$$

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

$$\hat{\mathbb{Z}}_{12} = \mathbb{X}_5[\mathbb{Q}_0^{(a,A_g)}(1,1)] \otimes \mathbb{Y}_2[\mathbb{Q}_0^{(b,A_g)}]$$

$$\hat{\mathbb{Z}}_{12}(\boldsymbol{k}) = \mathbb{X}_5[\mathbb{Q}_0^{(a,A_g)}(1,1)] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_g)}] \otimes \mathbb{F}_1[\mathbb{Q}_0^{(k,A_g)}]$$

$\boxed{\text{No. 13}}$ $\hat{\mathbb{Q}}_2^{(A_g,1)}(1,-1)$ $[\mathrm{M}_3, \mathrm{B}_1]$

$$\hat{\mathbb{Z}}_{13} = \mathbb{X}_6[\mathbb{Q}_2^{(a,A_g,1)}(1,-1)] \otimes \mathbb{Y}_2[\mathbb{Q}_0^{(b,A_g)}]$$

$$\hat{\mathbb{Z}}_{13}(\boldsymbol{k}) = \mathbb{X}_6[\mathbb{Q}_2^{(a,A_g,1)}(1,-1)] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_g)}] \otimes \mathbb{F}_1[\mathbb{Q}_0^{(k,A_g)}]$$

$\boxed{\text{No. 14}}$ $\hat{\mathbb{Q}}_2^{(A_g,2)}(1,-1)$ $[\mathrm{M}_3, \mathrm{B}_1]$

$$\hat{\mathbb{Z}}_{14} = \mathbb{X}_7[\mathbb{Q}_2^{(a,A_g,2)}(1,-1)] \otimes \mathbb{Y}_2[\mathbb{Q}_0^{(b,A_g)}]$$

$$\hat{\mathbb{Z}}_{14}(\boldsymbol{k}) = \mathbb{X}_7[\mathbb{Q}_2^{(a,A_g,2)}(1,-1)] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_g)}] \otimes \mathbb{F}_1[\mathbb{Q}_0^{(k,A_g)}]$$

$\boxed{\text{No. 15}}$ $\hat{\mathbb{Q}}_0^{(A_g)}$ $[\mathrm{M}_1, \mathrm{B}_2]$

$$\hat{\mathbb{Z}}_{15} = \mathbb{X}_1[\mathbb{Q}_0^{(a,A_g)}] \otimes \mathbb{Y}_3[\mathbb{Q}_0^{(b,A_g)}]$$

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

$\boxed{\text{No. 16}}$ $\hat{\mathbb{Q}}_0^{(A_g)}$ $[\mathrm{M}_3, \mathrm{B}_2]$

$$\hat{\mathbb{Z}}_{16} = \mathbb{X}_2[\mathbb{Q}_0^{(a,A_g)}] \otimes \mathbb{Y}_3[\mathbb{Q}_0^{(b,A_g)}]$$

$$\hat{\mathbb{Z}}_{16}(\boldsymbol{k}) = \mathbb{X}_2[\mathbb{Q}_0^{(a,A_g)}] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_g)}] \otimes \mathbb{F}_2[\mathbb{Q}_0^{(k,A_g)}]$$

$\boxed{\text{No. 17}}$ $\hat{\mathbb{Q}}_2^{(A_g,1)}$ $[\mathrm{M}_3, \mathrm{B}_2]$

$$\hat{\mathbb{Z}}_{17} = \mathbb{X}_3[\mathbb{Q}_2^{(a,A_g,1)}] \otimes \mathbb{Y}_3[\mathbb{Q}_0^{(b,A_g)}]$$

$$\hat{\mathbb{Z}}_{17}(\boldsymbol{k}) = \mathbb{X}_3[\mathbb{Q}_2^{(a,A_g,1)}] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_g)}] \otimes \mathbb{F}_2[\mathbb{Q}_0^{(k,A_g)}]$$

$\boxed{\text{No. 18}}$ $\hat{\mathbb{Q}}_2^{(A_g,2)}$ $[\mathrm{M}_3, \mathrm{B}_2]$

$$\hat{\mathbb{Z}}_{18} = \mathbb{X}_4[\mathbb{Q}_2^{(a,A_g,2)}] \otimes \mathbb{Y}_3[\mathbb{Q}_0^{(b,A_g)}]$$

$$\hat{\mathbb{Z}}_{18}(\boldsymbol{k}) = \mathbb{X}_4[\mathbb{Q}_2^{(a,A_g,2)}] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_g)}] \otimes \mathbb{F}_2[\mathbb{Q}_0^{(k,A_g)}]$$

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

$$\hat{\mathbb{Z}}_{19} = \mathbb{X}_5[\mathbb{Q}_0^{(a,A_g)}(1,1)] \otimes \mathbb{Y}_3[\mathbb{Q}_0^{(b,A_g)}]$$

$\hat{\mathbb{Z}}_{19}(\boldsymbol{k}) = \mathbb{X}_5[\mathbb{Q}_0^{(a,A_g)}(1,1)] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_g)}] \otimes \mathbb{F}_2[\mathbb{Q}_0^{(k,A_g)}]$

$\boxed{\text{No. 20}}$ $\hat{\mathbb{Q}}_2^{(A_g,1)}(1,-1)$ $[\mathrm{M}_3, \mathrm{B}_2]$

$\hat{\mathbb{Z}}_{20} = \mathbb{X}_6[\mathbb{Q}_2^{(a,A_g,1)}(1,-1)] \otimes \mathbb{Y}_3[\mathbb{Q}_0^{(b,A_g)}]$

$\hat{\mathbb{Z}}_{20}(\boldsymbol{k}) = \mathbb{X}_6[\mathbb{Q}_2^{(a,A_g,1)}(1,-1)] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_g)}] \otimes \mathbb{F}_2[\mathbb{Q}_0^{(k,A_g)}]$

$\boxed{\text{No. 21}}$ $\hat{\mathbb{Q}}_2^{(A_g,2)}(1,-1)$ $[\mathrm{M}_3, \mathrm{B}_2]$

$\hat{\mathbb{Z}}_{21} = \mathbb{X}_7[\mathbb{Q}_2^{(a,A_g,2)}(1,-1)] \otimes \mathbb{Y}_3[\mathbb{Q}_0^{(b,A_g)}]$

$\hat{\mathbb{Z}}_{21}(\boldsymbol{k}) = \mathbb{X}_7[\mathbb{Q}_2^{(a,A_g,2)}(1,-1)] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_g)}] \otimes \mathbb{F}_2[\mathbb{Q}_0^{(k,A_g)}]$

$\boxed{\text{No. 22}}$ $\hat{\mathbb{Q}}_0^{(A_g)}$ $[\mathrm{M}_1, \mathrm{B}_3]$

$\hat{\mathbb{Z}}_{22} = \mathbb{X}_1[\mathbb{Q}_0^{(a,A_g)}] \otimes \mathbb{Y}_4[\mathbb{Q}_0^{(b,A_g)}]$

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

$\boxed{\text{No. 23}}$ $\hat{\mathbb{Q}}_0^{(A_g)}$ $[\mathrm{M}_3, \mathrm{B}_3]$

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

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

$\boxed{\text{No. 24}}$ $\hat{\mathbb{Q}}_2^{(A_g,1)}$ $[\mathrm{M}_3, \mathrm{B}_3]$

$\hat{\mathbb{Z}}_{24} = \mathbb{X}_3[\mathbb{Q}_2^{(a,A_g,1)}] \otimes \mathbb{Y}_4[\mathbb{Q}_0^{(b,A_g)}]$

$\hat{\mathbb{Z}}_{24}(\boldsymbol{k}) = \mathbb{X}_3[\mathbb{Q}_2^{(a,A_g,1)}] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_g)}] \otimes \mathbb{F}_3[\mathbb{Q}_0^{(k,A_g)}]$

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

$\hat{\mathbb{Z}}_{25} = \mathbb{X}_4[\mathbb{Q}_2^{(a,A_g,2)}] \otimes \mathbb{Y}_4[\mathbb{Q}_0^{(b,A_g)}]$

$$\hat{\mathbb{Z}}_{25}(\boldsymbol{k}) = \mathbb{X}_4[\mathbb{Q}_2^{(a,A_g,2)}] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_g)}] \otimes \mathbb{F}_3[\mathbb{Q}_0^{(k,A_g)}]$$

$\boxed{\text{No. 26}}$ $\hat{\mathbb{Q}}_0^{(A_g)}(1,1)$ $[\mathrm{M}_3, \mathrm{B}_3]$

$$\hat{\mathbb{Z}}_{26} = \mathbb{X}_5[\mathbb{Q}_0^{(a,A_g)}(1,1)] \otimes \mathbb{Y}_4[\mathbb{Q}_0^{(b,A_g)}]$$

$$\hat{\mathbb{Z}}_{26}(\boldsymbol{k}) = \mathbb{X}_5[\mathbb{Q}_0^{(a,A_g)}(1,1)] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_g)}] \otimes \mathbb{F}_3[\mathbb{Q}_0^{(k,A_g)}]$$

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

$$\hat{\mathbb{Z}}_{27} = \mathbb{X}_6[\mathbb{Q}_2^{(a,A_g,1)}(1,-1)] \otimes \mathbb{Y}_4[\mathbb{Q}_0^{(b,A_g)}]$$

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

$\boxed{\text{No. 28}}$ $\hat{\mathbb{Q}}_2^{(A_g,2)}(1,-1)$ $[\mathrm{M}_3, \mathrm{B}_3]$

$$\hat{\mathbb{Z}}_{28} = \mathbb{X}_7[\mathbb{Q}_2^{(a,A_g,2)}(1,-1)] \otimes \mathbb{Y}_4[\mathbb{Q}_0^{(b,A_g)}]$$

$$\hat{\mathbb{Z}}_{28}(\boldsymbol{k}) = \mathbb{X}_7[\mathbb{Q}_2^{(a,A_g,2)}(1,-1)] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_g)}] \otimes \mathbb{F}_3[\mathbb{Q}_0^{(k,A_g)}]$$

$\boxed{\text{No. 29}}$ $\hat{\mathbb{Q}}_0^{(A_g)}$ $[\mathrm{M}_1, \mathrm{B}_4]$

$$\hat{\mathbb{Z}}_{29} = \mathbb{X}_1[\mathbb{Q}_0^{(a,A_g)}] \otimes \mathbb{Y}_5[\mathbb{Q}_0^{(b,A_g)}]$$

$$\hat{\mathbb{Z}}_{29}(\boldsymbol{k}) = \mathbb{X}_1[\mathbb{Q}_0^{(a,A_g)}] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_g)}] \otimes \mathbb{F}_4[\mathbb{Q}_0^{(k,A_g)}]$$

$\boxed{\text{No. 30}}$ $\hat{\mathbb{Q}}_0^{(A_g)}$ $[\mathrm{M}_3, \mathrm{B}_4]$

$$\hat{\mathbb{Z}}_{30} = \mathbb{X}_2[\mathbb{Q}_0^{(a,A_g)}] \otimes \mathbb{Y}_5[\mathbb{Q}_0^{(b,A_g)}]$$

$$\hat{\mathbb{Z}}_{30}(\boldsymbol{k}) = \mathbb{X}_2[\mathbb{Q}_0^{(a,A_g)}] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_g)}] \otimes \mathbb{F}_4[\mathbb{Q}_0^{(k,A_g)}]$$

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

$$\hat{\mathbb{Z}}_{31} = \mathbb{X}_3[\mathbb{Q}_2^{(a,A_g,1)}] \otimes \mathbb{Y}_5[\mathbb{Q}_0^{(b,A_g)}]$$

$$\hat{\mathbb{Z}}_{31}(\boldsymbol{k}) = \mathbb{X}_3[\mathbb{Q}_2^{(a,A_g,1)}] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_g)}] \otimes \mathbb{F}_4[\mathbb{Q}_0^{(k,A_g)}]$$

$\boxed{\text{No. 32}}$ $\hat{\mathbb{Q}}_2^{(A_g,2)}$ $[\mathrm{M}_3, \mathrm{B}_4]$

$$\hat{\mathbb{Z}}_{32} = \mathbb{X}_4[\mathbb{Q}_2^{(a,A_g,2)}] \otimes \mathbb{Y}_5[\mathbb{Q}_0^{(b,A_g)}]$$

$$\hat{\mathbb{Z}}_{32}(\boldsymbol{k}) = \mathbb{X}_4[\mathbb{Q}_2^{(a,A_g,2)}] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_g)}] \otimes \mathbb{F}_4[\mathbb{Q}_0^{(k,A_g)}]$$

$\boxed{\text{No. 33}}$ $\hat{\mathbb{Q}}_0^{(A_g)}$ $[\mathrm{M}_3, \mathrm{B}_4]$

$$\hat{\mathbb{Z}}_{33} = \mathbb{X}_8[\mathbb{Q}_2^{(a,B_{1g})}] \otimes \mathbb{Y}_6[\mathbb{Q}_2^{(b,B_{1g})}]$$

$$\hat{\mathbb{Z}}_{33}(\boldsymbol{k}) = \mathbb{X}_8[\mathbb{Q}_2^{(a,B_{1g})}] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_g)}] \otimes \mathbb{F}_5[\mathbb{Q}_2^{(k,B_{1g})}]$$

$\boxed{\text{No. 34}}$ $\hat{\mathbb{Q}}_0^{(A_g)}(1,1)$ $[\mathrm{M}_3, \mathrm{B}_4]$

$$\hat{\mathbb{Z}}_{34} = \mathbb{X}_5[\mathbb{Q}_0^{(a,A_g)}(1,1)] \otimes \mathbb{Y}_5[\mathbb{Q}_0^{(b,A_g)}]$$

$$\hat{\mathbb{Z}}_{34}(\boldsymbol{k}) = \mathbb{X}_5[\mathbb{Q}_0^{(a,A_g)}(1,1)] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_g)}] \otimes \mathbb{F}_4[\mathbb{Q}_0^{(k,A_g)}]$$

$\boxed{\text{No. 35}}$ $\hat{\mathbb{Q}}_2^{(A_g,1)}(1,-1)$ $[\mathrm{M}_3, \mathrm{B}_4]$

$$\hat{\mathbb{Z}}_{35} = \mathbb{X}_6[\mathbb{Q}_2^{(a,A_g,1)}(1,-1)] \otimes \mathbb{Y}_5[\mathbb{Q}_0^{(b,A_g)}]$$

$$\hat{\mathbb{Z}}_{35}(\boldsymbol{k}) = \mathbb{X}_6[\mathbb{Q}_2^{(a,A_g,1)}(1,-1)] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_g)}] \otimes \mathbb{F}_4[\mathbb{Q}_0^{(k,A_g)}]$$

$\boxed{\text{No. 36}}$ $\hat{\mathbb{Q}}_2^{(A_g,2)}(1,-1)$ $[\mathrm{M}_3, \mathrm{B}_4]$

$$\hat{\mathbb{Z}}_{36} = \mathbb{X}_7[\mathbb{Q}_2^{(a,A_g,2)}(1,-1)] \otimes \mathbb{Y}_5[\mathbb{Q}_0^{(b,A_g)}]$$

$$\hat{\mathbb{Z}}_{36}(\boldsymbol{k}) = \mathbb{X}_7[\mathbb{Q}_2^{(a,A_g,2)}(1,-1)] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_g)}] \otimes \mathbb{F}_4[\mathbb{Q}_0^{(k,A_g)}]$$

$\boxed{\text{No. 37}}$ $\hat{\mathbb{Q}}_0^{(A_g)}(1,-1)$ $[\mathrm{M}_3, \mathrm{B}_4]$

$$\hat{\mathbb{Z}}_{37} = \mathbb{X}_9[\mathbb{Q}_2^{(a,B_{1g})}(1,-1)] \otimes \mathbb{Y}_6[\mathbb{Q}_2^{(b,B_{1g})}]$$

$$\hat{\mathbb{Z}}_{37}(\boldsymbol{k}) = \mathbb{X}_9[\mathbb{Q}_2^{(a,B_{1g})}(1,-1)] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_g)}] \otimes \mathbb{F}_5[\mathbb{Q}_2^{(k,B_{1g})}]$$

$\boxed{\text{No. 38}}$ $\hat{\mathbb{Q}}_2^{(A_g,2)}(1,0)$ $[\mathrm{M}_3, \mathrm{B}_4]$

$$\hat{\mathbb{Z}}_{38} = -\mathbb{X}_{10}[\mathbb{G}_1^{(a,B_{1g})}(1,0)] \otimes \mathbb{Y}_6[\mathbb{Q}_2^{(b,B_{1g})}]$$

$$\hat{\mathbb{Z}}_{38}(\boldsymbol{k}) = -\mathbb{X}_{10}[\mathbb{G}_1^{(a,B_{1g})}(1,0)] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_g)}] \otimes \mathbb{F}_5[\mathbb{Q}_2^{(k,B_{1g})}]$$

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
$\mathbb{X}_1$	$\mathbb{Q}_0^{(a,A_g)}$	M_1	$\begin{pmatrix} \frac{\sqrt{2}}{2} & 0 \\ 0 & \frac{\sqrt{2}}{2} \end{pmatrix}$
$\mathbb{X}_2$	$\mathbb{Q}_0^{(a,A_g)}$	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
$\mathbb{X}_3$	$\mathbb{Q}_2^{(a,A_g,1)}$	M_3	$\begin{pmatrix} -\frac{\sqrt{3}}{6} & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{3}}{6} & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{3}}{6} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{3}}{6} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{3}}{3} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{3}}{3} \end{pmatrix}$
$\mathbb{X}_4$	$\mathbb{Q}_2^{(a,A_g,2)}$	M_3	$\begin{pmatrix} \frac{1}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{1}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$
$\mathbb{X}_5$	$\mathbb{Q}_0^{(a,A_g)}(1,1)$	M_3	$\begin{pmatrix} 0 & 0 & -\frac{\sqrt{3}i}{6} & 0 & 0 & \frac{\sqrt{3}}{6} \\ 0 & 0 & 0 & \frac{\sqrt{3}i}{6} & -\frac{\sqrt{3}}{6} & 0 \\ \frac{\sqrt{3}i}{6} & 0 & 0 & 0 & 0 & -\frac{\sqrt{3}i}{6} \\ 0 & -\frac{\sqrt{3}i}{6} & 0 & 0 & -\frac{\sqrt{3}i}{6} & 0 \\ 0 & -\frac{\sqrt{3}}{6} & 0 & \frac{\sqrt{3}i}{6} & 0 & 0 \\ \frac{\sqrt{3}}{6} & 0 & \frac{\sqrt{3}i}{6} & 0 & 0 & 0 \end{pmatrix}$
$\mathbb{X}_6$	$\mathbb{Q}_2^{(a,A_g,1)}(1,-1)$	M_3	$\begin{pmatrix} 0 & 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 & -\frac{\sqrt{6}}{12} \\ 0 & 0 & 0 & \frac{\sqrt{6}i}{6} & \frac{\sqrt{6}}{12} & 0 \\ \frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 & \frac{\sqrt{6}i}{12} \\ 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 & \frac{\sqrt{6}i}{12} & 0 \\ 0 & \frac{\sqrt{6}}{12} & 0 & -\frac{\sqrt{6}i}{12} & 0 & 0 \\ -\frac{\sqrt{6}}{12} & 0 & -\frac{\sqrt{6}i}{12} & 0 & 0 & 0 \end{pmatrix}$
$\mathbb{X}_7$	$\mathbb{Q}_2^{(a,A_g,2)}(1,-1)$	M_3	$\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{2}}{4} \\ 0 & 0 & 0 & 0 & \frac{\sqrt{2}}{4} & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{2}i}{4} \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{2}i}{4} & 0 \\ 0 & \frac{\sqrt{2}}{4} & 0 & \frac{\sqrt{2}i}{4} & 0 & 0 \\ -\frac{\sqrt{2}}{4} & 0 & \frac{\sqrt{2}i}{4} & 0 & 0 & 0 \end{pmatrix}$

continued ...

Table 6

symbol	type	group	form
$\mathbb{X}_8$	$\mathbb{Q}_2^{(a,B_{1g})}$	M_3	$\begin{pmatrix} 0 & 0 & \frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2} & 0 & 0 \\ \frac{1}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$
$\mathbb{X}_9$	$\mathbb{Q}_2^{(a,B_{1g})}(1,-1)$	M_3	$\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{2}i}{4} \\ 0 & 0 & 0 & 0 & \frac{\sqrt{2}i}{4} & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{2}}{4} \\ 0 & 0 & 0 & 0 & \frac{\sqrt{2}}{4} & 0 \\ 0 & -\frac{\sqrt{2}i}{4} & 0 & \frac{\sqrt{2}}{4} & 0 & 0 \\ -\frac{\sqrt{2}i}{4} & 0 & -\frac{\sqrt{2}}{4} & 0 & 0 & 0 \end{pmatrix}$
$\mathbb{X}_{10}$	$\mathbb{G}_1^{(a,B_{1g})}(1,0)$	M_3	$\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{2}i}{4} \\ 0 & 0 & 0 & 0 & \frac{\sqrt{2}i}{4} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{2}}{4} \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{2}}{4} & 0 \\ 0 & -\frac{\sqrt{2}i}{4} & 0 & -\frac{\sqrt{2}}{4} & 0 & 0 \\ -\frac{\sqrt{2}i}{4} & 0 & \frac{\sqrt{2}}{4} & 0 & 0 & 0 \end{pmatrix}$

Table 7: Cluster SAMB.

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

Table 8: Uniform SAMB.

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

Table 9: Structure SAMB.

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

Table 10: Polar harmonics.

No.	symbol	rank	irrep.	mul.	comp.	form
1	$\mathbb{Q}_0^{(A_g)}$	0	A_g	–	–	1
2	$\mathbb{Q}_2^{(A_g,1)}$	2	A_g	1	–	$-\frac{x^2}{2} - \frac{y^2}{2} + z^2$
3	$\mathbb{Q}_2^{(A_g,2)}$	2	A_g	2	–	$\frac{\sqrt{3}(x-y)(x+y)}{2}$
4	$\mathbb{Q}_2^{(B_{1g})}$	2	B_{1g}	–	–	$\sqrt{3}xy$

Table 11: Axial harmonics.

No.	symbol	rank	irrep.	mul.	comp.	form
1	$\mathbb{G}_1^{(B_{1g})}$	1	B_{1g}	–	–	Z

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

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

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

Table 13: Symmetry operations.

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

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

	1	2_{001}	2_{010}	2_{100}	-1	m_{001}	m_{010}	m_{100}
A_g	1	1	1	1	1	1	1	1
B_{1g}	1	1	-1	-1	1	1	-1	-1
B_{2g}	1	-1	1	-1	1	-1	1	-1
B_{3g}	1	-1	-1	1	1	-1	-1	1
A_u	1	1	1	1	-1	-1	-1	-1
B_{1u}	1	1	-1	-1	-1	-1	1	1
B_{2u}	1	-1	1	-1	-1	1	-1	1
B_{3u}	1	-1	-1	1	-1	1	1	-1

Table 15: Parity conversion.

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

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

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

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

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

Table 18: Virtual-cluster sites.

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

Table 19: Virtual-cluster basis.

symbol	1	2	3	4	5	6	7	8
$\mathbb{Q}_0^{(A_g)}$	$\frac{\sqrt{2}}{4}$	$\frac{\sqrt{2}}{4}$	$\frac{\sqrt{2}}{4}$	$\frac{\sqrt{2}}{4}$	$\frac{\sqrt{2}}{4}$	$\frac{\sqrt{2}}{4}$	$\frac{\sqrt{2}}{4}$	$\frac{\sqrt{2}}{4}$
$\mathbb{Q}_1^{(B_{1u})}$	$\frac{\sqrt{2}}{4}$	$\frac{\sqrt{2}}{4}$	$-\frac{\sqrt{2}}{4}$	$-\frac{\sqrt{2}}{4}$	$-\frac{\sqrt{2}}{4}$	$-\frac{\sqrt{2}}{4}$	$\frac{\sqrt{2}}{4}$	$\frac{\sqrt{2}}{4}$
$\mathbb{Q}_1^{(B_{2u})}$	$\frac{\sqrt{2}}{4}$	$-\frac{\sqrt{2}}{4}$	$\frac{\sqrt{2}}{4}$	$-\frac{\sqrt{2}}{4}$	$-\frac{\sqrt{2}}{4}$	$\frac{\sqrt{2}}{4}$	$-\frac{\sqrt{2}}{4}$	$\frac{\sqrt{2}}{4}$
$\mathbb{Q}_1^{(B_{3u})}$	$\frac{\sqrt{2}}{4}$	$-\frac{\sqrt{2}}{4}$	$-\frac{\sqrt{2}}{4}$	$\frac{\sqrt{2}}{4}$	$-\frac{\sqrt{2}}{4}$	$\frac{\sqrt{2}}{4}$	$\frac{\sqrt{2}}{4}$	$-\frac{\sqrt{2}}{4}$
$\mathbb{Q}_2^{(B_{1g})}$	$\frac{\sqrt{2}}{4}$	$\frac{\sqrt{2}}{4}$	$-\frac{\sqrt{2}}{4}$	$-\frac{\sqrt{2}}{4}$	$\frac{\sqrt{2}}{4}$	$\frac{\sqrt{2}}{4}$	$-\frac{\sqrt{2}}{4}$	$-\frac{\sqrt{2}}{4}$
$\mathbb{Q}_2^{(B_{2g})}$	$\frac{\sqrt{2}}{4}$	$-\frac{\sqrt{2}}{4}$	$\frac{\sqrt{2}}{4}$	$-\frac{\sqrt{2}}{4}$	$\frac{\sqrt{2}}{4}$	$-\frac{\sqrt{2}}{4}$	$\frac{\sqrt{2}}{4}$	$-\frac{\sqrt{2}}{4}$
$\mathbb{Q}_2^{(B_{3g})}$	$\frac{\sqrt{2}}{4}$	$-\frac{\sqrt{2}}{4}$	$-\frac{\sqrt{2}}{4}$	$\frac{\sqrt{2}}{4}$	$\frac{\sqrt{2}}{4}$	$-\frac{\sqrt{2}}{4}$	$-\frac{\sqrt{2}}{4}$	$\frac{\sqrt{2}}{4}$
$\mathbb{Q}_3^{(A_u)}$	$\frac{\sqrt{2}}{4}$	$\frac{\sqrt{2}}{4}$	$\frac{\sqrt{2}}{4}$	$\frac{\sqrt{2}}{4}$	$-\frac{\sqrt{2}}{4}$	$-\frac{\sqrt{2}}{4}$	$-\frac{\sqrt{2}}{4}$	$-\frac{\sqrt{2}}{4}$