SAMB for "CeCoSi"

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- Group: No. 129 D_{4h}^{7} $P4/nmm$ [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:
  $a = 4.057,\ b = 4.057,\ c = 6.987,\ \alpha = 90.0,\ \beta = 90.0,\ \gamma = 90.0$
- Lattice vectors:
  $\boldsymbol{a}_1 = \begin{pmatrix} 4.057 & 0 & 0 \end{pmatrix}$
  $\boldsymbol{a}_2 = \begin{pmatrix} 0 & 4.057 & 0 \end{pmatrix}$
  $\boldsymbol{a}_3 = \begin{pmatrix} 0 & 0 & 6.987 \end{pmatrix}$

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 = 36

Table 2: Hilbert space for full matrix.

No.	ket	No.	ket	No.	ket	No.	ket	No.	ket
1	$(p_x,\uparrow)$@Ce_1	2	$(p_x,\downarrow)$@Ce_1	3	$(p_y,\uparrow)$@Ce_1	4	$(p_y,\downarrow)$@Ce_1	5	$(p_z,\uparrow)$@Ce_1
6	$(p_z,\downarrow)$@Ce_1	7	$(p_x,\uparrow)$@Ce_2	8	$(p_x,\downarrow)$@Ce_2	9	$(p_y,\uparrow)$@Ce_2	10	$(p_y,\downarrow)$@Ce_2
11	$(p_z,\uparrow)$@Ce_2	12	$(p_z,\downarrow)$@Ce_2	13	$(p_x,\uparrow)$@Co_1	14	$(p_x,\downarrow)$@Co_1	15	$(p_y,\uparrow)$@Co_1
16	$(p_y,\downarrow)$@Co_1	17	$(p_z,\uparrow)$@Co_1	18	$(p_z,\downarrow)$@Co_1	19	$(p_x,\uparrow)$@Co_2	20	$(p_x,\downarrow)$@Co_2
21	$(p_y,\uparrow)$@Co_2	22	$(p_y,\downarrow)$@Co_2	23	$(p_z,\uparrow)$@Co_2	24	$(p_z,\downarrow)$@Co_2	25	$(p_x,\uparrow)$@Si_1
26	$(p_x,\downarrow)$@Si_1	27	$(p_y,\uparrow)$@Si_1	28	$(p_y,\downarrow)$@Si_1	29	$(p_z,\uparrow)$@Si_1	30	$(p_z,\downarrow)$@Si_1
31	$(p_x,\uparrow)$@Si_2	32	$(p_x,\downarrow)$@Si_2	33	$(p_y,\uparrow)$@Si_2	34	$(p_y,\downarrow)$@Si_2	35	$(p_z,\uparrow)$@Si_2
36	$(p_z,\downarrow)$@Si_2								

- Sites in (primitive) unit cell:

Table 3: Site-clusters.

	site	position	mapping
S_1 [2c: 4mm]	Ce_1	$\left(\frac{1}{4} \quad \frac{1}{4} \quad 0.678\right)$	[1,2,7,8,11,12,13,14]
	Ce_2	$\left(\frac{3}{4} \quad \frac{3}{4} \quad 0.322\right)$	[3,4,5,6,9,10,15,16]
S_2 [2a: -4m2]	Co_1	$\left(\frac{1}{4} \quad \frac{3}{4} \quad 0\right)$	[1,2,5,6,11,12,15,16]
	Co_2	$\left(\frac{3}{4} \quad \frac{1}{4} \quad 0\right)$	[3,4,7,8,9,10,13,14]
S_3 [2c: 4mm]	Si_1	$\left(\frac{1}{4} \quad \frac{1}{4} \quad 0.178\right)$	[1,2,7,8,11,12,13,14]
	Si_2	$\left(\frac{3}{4} \quad \frac{3}{4} \quad 0.822\right)$	[3,4,5,6,9,10,15,16]

- Bonds in (primitive) unit cell:

Table 4: Bond-clusters.

	bond	tail	head	n	#	$\boldsymbol{b}@\boldsymbol{c}$	mapping
B_1 [8i: .m.]	b_1	Co_1	Ce_1	1	1	$\left(0 \quad -\frac{1}{2} \quad 0.322\right)@\left(\frac{1}{4} \quad 0 \quad 0.839\right)$	[1,11]
	b_2	Co_1	Ce_1	1	1	$\left(0 \quad \frac{1}{2} \quad 0.322\right)@\left(\frac{1}{4} \quad \frac{1}{2} \quad 0.839\right)$	[2,12]
	b_3	Co_2	Ce_2	1	1	$\left(0 \quad \frac{1}{2} \quad -0.322\right)@\left(\frac{3}{4} \quad 0 \quad 0.161\right)$	[3,9]
	b_4	Co_2	Ce_2	1	1	$\left(0 \quad -\frac{1}{2} \quad -0.322\right)@\left(\frac{3}{4} \quad \frac{1}{2} \quad 0.161\right)$	[4,10]
	b_5	Co_1	Ce_2	1	1	$\left(-\frac{1}{2} \quad 0 \quad -0.322\right)@\left(\frac{1}{2} \quad \frac{3}{4} \quad 0.161\right)$	[5,15]
	b_6	Co_1	Ce_2	1	1	$\left(\frac{1}{2} \quad 0 \quad -0.322\right)@\left(0 \quad \frac{3}{4} \quad 0.161\right)$	[6,16]
	b_7	Co_2	Ce_1	1	1	$\left(\frac{1}{2} \quad 0 \quad 0.322\right)@\left(\frac{1}{2} \quad \frac{1}{4} \quad 0.839\right)$	[7,13]
	b_8	Co_2	Ce_1	1	1	$\left(-\frac{1}{2} \quad 0 \quad 0.322\right)@\left(0 \quad \frac{1}{4} \quad 0.839\right)$	[8,14]
B_2 [8j: ..m]	b_9	Si_2	Ce_1	1	1	$\left(-\frac{1}{2} \quad -\frac{1}{2} \quad 0.144\right)@\left(0 \quad 0 \quad \frac{3}{4}\right)$	[1,14]
	b_{10}	Si_2	Ce_1	1	1	$\left(\frac{1}{2} \quad \frac{1}{2} \quad 0.144\right)@\left(\frac{1}{2} \quad \frac{1}{2} \quad \frac{3}{4}\right)$	[2,13]
	b_{11}	Si_1	Ce_2	1	1	$\left(-\frac{1}{2} \quad \frac{1}{2} \quad -0.144\right)@\left(\frac{1}{2} \quad 0 \quad \frac{1}{4}\right)$	[3,15]
	b_{12}	Si_1	Ce_2	1	1	$\left(\frac{1}{2} \quad -\frac{1}{2} \quad -0.144\right)@\left(0 \quad \frac{1}{2} \quad \frac{1}{4}\right)$	[4,16]
	b_{13}	Si_1	Ce_2	1	1	$\left(-\frac{1}{2} \quad -\frac{1}{2} \quad -0.144\right)@\left(\frac{1}{2} \quad \frac{1}{2} \quad \frac{1}{4}\right)$	[5,10]
	b_{14}	Si_1	Ce_2	1	1	$\left(\frac{1}{2} \quad \frac{1}{2} \quad -0.144\right)@\left(0 \quad 0 \quad \frac{1}{4}\right)$	[6,9]
	b_{15}	Si_2	Ce_1	1	1	$\left(\frac{1}{2} \quad -\frac{1}{2} \quad 0.144\right)@\left(\frac{1}{2} \quad 0 \quad \frac{3}{4}\right)$	[7,11]
	b_{16}	Si_2	Ce_1	1	1	$\left(-\frac{1}{2} \quad \frac{1}{2} \quad 0.144\right)@\left(0 \quad \frac{1}{2} \quad \frac{3}{4}\right)$	[8,12]
B_3 [8i: .m.]	b_{17}	Si_1	Co_1	1	1	$\left(0 \quad \frac{1}{2} \quad 0.178\right)@\left(\frac{1}{4} \quad 0 \quad 0.089\right)$	[1,11]
	b_{18}	Si_1	Co_1	1	1	$\left(0 \quad -\frac{1}{2} \quad 0.178\right)@\left(\frac{1}{4} \quad \frac{1}{2} \quad 0.089\right)$	[2,12]
	b_{19}	Si_2	Co_2	1	1	$\left(0 \quad -\frac{1}{2} \quad -0.178\right)@\left(\frac{3}{4} \quad 0 \quad 0.911\right)$	[3,9]
	b_{20}	Si_2	Co_2	1	1	$\left(0 \quad \frac{1}{2} \quad -0.178\right)@\left(\frac{3}{4} \quad \frac{1}{2} \quad 0.911\right)$	[4,10]
	b_{21}	Si_2	Co_1	1	1	$\left(\frac{1}{2} \quad 0 \quad -0.178\right)@\left(\frac{1}{2} \quad \frac{3}{4} \quad 0.911\right)$	[5,15]
	b_{22}	Si_2	Co_1	1	1	$\left(-\frac{1}{2} \quad 0 \quad -0.178\right)@\left(0 \quad \frac{3}{4} \quad 0.911\right)$	[6,16]
	b_{23}	Si_1	Co_2	1	1	$\left(-\frac{1}{2} \quad 0 \quad 0.178\right)@\left(\frac{1}{2} \quad \frac{1}{4} \quad 0.089\right)$	[7,13]
	b_{24}	Si_1	Co_2	1	1	$\left(\frac{1}{2} \quad 0 \quad 0.178\right)@\left(0 \quad \frac{1}{4} \quad 0.089\right)$	[8,14]

- SAMB:

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

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

No. 2 $\hat{\mathbb{Q}}_2^{(A_{1g})}$ $[\mathrm{M}_1, \mathrm{S}_1]$

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

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

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

No. 4 $\hat{\mathbb{Q}}_2^{(A_{1g})}(1,-1)$ $[\mathrm{M}_1, \mathrm{S}_1]$

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

No. 5 $\hat{\mathbb{Q}}_0^{(A_{1g})}$ $[\mathrm{M}_1, \mathrm{S}_2]$

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

No. 6 $\hat{\mathbb{Q}}_2^{(A_{1g})}$ $[\mathrm{M}_1, \mathrm{S}_2]$

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

No. 7 $\hat{\mathbb{Q}}_0^{(A_{1g})}(1,1)$ $[\mathrm{M}_1, \mathrm{S}_2]$

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

No. 8 $\hat{\mathbb{Q}}_2^{(A_{1g})}(1,-1)$ $[\mathrm{M}_1, \mathrm{S}_2]$

$\hat{\mathbb{Z}}_8 = \mathbb{X}_4[\mathbb{Q}_2^{(a,A_{1g})}(1,-1)] \otimes \mathbb{Y}_2[\mathbb{Q}_0^{(s,A_{1g})}]$

No. 9 $\hat{\mathbb{Q}}_0^{(A_{1g})}$ $[\mathrm{M}_1, \mathrm{S}_3]$

$\hat{\mathbb{Z}}_9 = \mathbb{X}_1[\mathbb{Q}_0^{(a,A_{1g})}] \otimes \mathbb{Y}_3[\mathbb{Q}_0^{(s,A_{1g})}]$

No. 10 $\hat{\mathbb{Q}}_2^{(A_{1g})}$ $[\mathrm{M}_1, \mathrm{S}_3]$

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

No. 11 $\hat{\mathbb{Q}}_0^{(A_{1g})}(1,1)$ $[\mathrm{M}_1, \mathrm{S}_3]$

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

No. 12 $\hat{\mathbb{Q}}_2^{(A_{1g})}(1,-1)$ $[\mathrm{M}_1, \mathrm{S}_3]$

$\hat{\mathbb{Z}}_{12} = \mathbb{X}_4[\mathbb{Q}_2^{(a,A_{1g})}(1,-1)] \otimes \mathbb{Y}_3[\mathbb{Q}_0^{(s,A_{1g})}]$

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

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

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

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

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

$$\hat{\mathbb{Z}}_{15} = \frac{\sqrt{3}\mathbb{X}_5[\mathbb{Q}_2^{(a,B_{1g})}] \otimes \mathbb{Y}_5[\mathbb{Q}_2^{(b,B_{1g})}]}{3} + \frac{\sqrt{3}\mathbb{X}_7[\mathbb{Q}_{2,0}^{(a,E_g)}] \otimes \mathbb{Y}_6[\mathbb{Q}_{2,0}^{(b,E_g)}]}{3} + \frac{\sqrt{3}\mathbb{X}_8[\mathbb{Q}_{2,1}^{(a,E_g)}] \otimes \mathbb{Y}_7[\mathbb{Q}_{2,1}^{(b,E_g)}]}{3}$$

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

$$\hat{\mathbb{Z}}_{16} = -\frac{\sqrt{6}\mathbb{X}_5[\mathbb{Q}_2^{(a,B_{1g})}] \otimes \mathbb{Y}_5[\mathbb{Q}_2^{(b,B_{1g})}]}{3} + \frac{\sqrt{6}\mathbb{X}_7[\mathbb{Q}_{2,0}^{(a,E_g)}] \otimes \mathbb{Y}_6[\mathbb{Q}_{2,0}^{(b,E_g)}]}{6} + \frac{\sqrt{6}\mathbb{X}_8[\mathbb{Q}_{2,1}^{(a,E_g)}] \otimes \mathbb{Y}_7[\mathbb{Q}_{2,1}^{(b,E_g)}]}{6}$$

No. 17 $\hat{\mathbb{Q}}_0^{(A_{1g})}(1,1)$ $[\mathrm{M}_1, \mathrm{B}_1]$

$\hat{\mathbb{Z}}_{17} = \mathbb{X}_3[\mathbb{Q}_0^{(a,A_{1g})}(1,1)] \otimes \mathbb{Y}_4[\mathbb{Q}_0^{(b,A_{1g})}]$

No. 18 $\hat{\mathbb{Q}}_2^{(A_{1g})}(1,-1)$ $[\mathrm{M}_1, \mathrm{B}_1]$

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

No. 19 $\hat{\mathbb{Q}}_0^{(A_{1g})}(1,-1)$ $[\mathrm{M}_1,\mathrm{B}_1]$

$$\hat{\mathbb{Z}}_{19}=\frac{\sqrt{3}\mathbb{X}_{11}[\mathbb{Q}_{2,0}^{(a,E_g)}(1,-1)]\otimes\mathbb{Y}_6[\mathbb{Q}_{2,0}^{(b,E_g)}]}{3}+\frac{\sqrt{3}\mathbb{X}_{12}[\mathbb{Q}_{2,1}^{(a,E_g)}(1,-1)]\otimes\mathbb{Y}_7[\mathbb{Q}_{2,1}^{(b,E_g)}]}{3}+\frac{\sqrt{3}\mathbb{X}_9[\mathbb{Q}_2^{(a,B_{1g})}(1,-1)]\otimes\mathbb{Y}_5[\mathbb{Q}_2^{(b,B_{1g})}]}{3}$$

No. 20 $\hat{\mathbb{Q}}_2^{(A_{1g})}(1,-1)$ $[\mathrm{M}_1,\mathrm{B}_1]$

$$\hat{\mathbb{Z}}_{20}=\frac{\sqrt{6}\mathbb{X}_{11}[\mathbb{Q}_{2,0}^{(a,E_g)}(1,-1)]\otimes\mathbb{Y}_6[\mathbb{Q}_{2,0}^{(b,E_g)}]}{6}+\frac{\sqrt{6}\mathbb{X}_{12}[\mathbb{Q}_{2,1}^{(a,E_g)}(1,-1)]\otimes\mathbb{Y}_7[\mathbb{Q}_{2,1}^{(b,E_g)}]}{6}-\frac{\sqrt{6}\mathbb{X}_9[\mathbb{Q}_2^{(a,B_{1g})}(1,-1)]\otimes\mathbb{Y}_5[\mathbb{Q}_2^{(b,B_{1g})}]}{3}$$

No. 21 $\hat{\mathbb{Q}}_2^{(A_{1g})}(1,0)$ $[\mathrm{M}_1,\mathrm{B}_1]$

$$\hat{\mathbb{Z}}_{21}=\frac{\sqrt{2}\mathbb{X}_{13}[\mathbb{G}_{1,0}^{(a,E_g)}(1,0)]\otimes\mathbb{Y}_6[\mathbb{Q}_{2,0}^{(b,E_g)}]}{2}-\frac{\sqrt{2}\mathbb{X}_{14}[\mathbb{G}_{1,1}^{(a,E_g)}(1,0)]\otimes\mathbb{Y}_7[\mathbb{Q}_{2,1}^{(b,E_g)}]}{2}$$

No. 22 $\hat{\mathbb{Q}}_2^{(A_{1g})}$ $[\mathrm{M}_1,\mathrm{B}_1]$

$$\hat{\mathbb{Z}}_{22}=\frac{\sqrt{2}\mathbb{X}_{15}[\mathbb{M}_{1,0}^{(a,E_g)}]\otimes\mathbb{Y}_{10}[\mathbb{T}_{2,0}^{(b,E_g)}]}{2}-\frac{\sqrt{2}\mathbb{X}_{16}[\mathbb{M}_{1,1}^{(a,E_g)}]\otimes\mathbb{Y}_{11}[\mathbb{T}_{2,1}^{(b,E_g)}]}{2}$$

No. 23 $\hat{\mathbb{Q}}_2^{(A_{1g})}(1,1)$ $[\mathrm{M}_1,\mathrm{B}_1]$

$$\hat{\mathbb{Z}}_{23}=\frac{\sqrt{2}\mathbb{X}_{17}[\mathbb{M}_{1,0}^{(a,E_g)}(1,1)]\otimes\mathbb{Y}_{10}[\mathbb{T}_{2,0}^{(b,E_g)}]}{2}-\frac{\sqrt{2}\mathbb{X}_{18}[\mathbb{M}_{1,1}^{(a,E_g)}(1,1)]\otimes\mathbb{Y}_{11}[\mathbb{T}_{2,1}^{(b,E_g)}]}{2}$$

No. 24 $\hat{\mathbb{Q}}_2^{(A_{1g})}(1,-1)$ $[\mathrm{M}_1,\mathrm{B}_1]$

$$\hat{\mathbb{Z}}_{24}=\frac{\sqrt{2}\mathbb{X}_{19}[\mathbb{M}_{1,0}^{(a,E_g)}(1,-1)]\otimes\mathbb{Y}_{10}[\mathbb{T}_{2,0}^{(b,E_g)}]}{2}-\frac{\sqrt{2}\mathbb{X}_{20}[\mathbb{M}_{1,1}^{(a,E_g)}(1,-1)]\otimes\mathbb{Y}_{11}[\mathbb{T}_{2,1}^{(b,E_g)}]}{2}$$

No. 25 $\hat{\mathbb{Q}}_2^{(A_{1g})}(1,-1)$ $[\mathrm{M}_1,\mathrm{B}_1]$

$$\begin{aligned}\hat{\mathbb{Z}}_{25}=&-\frac{\sqrt{3}\mathbb{X}_{21}[\mathbb{M}_{3,0}^{(a,E_g,1)}(1,-1)]\otimes\mathbb{Y}_{10}[\mathbb{T}_{2,0}^{(b,E_g)}]}{6}+\frac{\sqrt{3}\mathbb{X}_{22}[\mathbb{M}_{3,1}^{(a,E_g,1)}(1,-1)]\otimes\mathbb{Y}_{11}[\mathbb{T}_{2,1}^{(b,E_g)}]}{6}-\frac{\sqrt{5}\mathbb{X}_{23}[\mathbb{M}_{3,0}^{(a,E_g,2)}(1,-1)]\otimes\mathbb{Y}_{10}[\mathbb{T}_{2,0}^{(b,E_g)}]}{6}\\&+\frac{\sqrt{5}\mathbb{X}_{24}[\mathbb{M}_{3,1}^{(a,E_g,2)}(1,-1)]\otimes\mathbb{Y}_{11}[\mathbb{T}_{2,1}^{(b,E_g)}]}{6}-\frac{\sqrt{5}\mathbb{X}_{27}[\mathbb{M}_3^{(a,B_{1g})}(1,-1)]\otimes\mathbb{Y}_9[\mathbb{T}_2^{(b,B_{1g})}]}{3}\end{aligned}$$

No. 26 $\hat{\mathbb{Q}}_4^{(A_{1g},1)}(1,-1)$ $[\mathrm{M}_1,\mathrm{B}_1]$

$$\hat{\mathbb{Z}}_{26} = \frac{\sqrt{195}\mathbb{X}_{21}[\mathbb{M}_{3,0}^{(a,E_g,1)}(1,-1)]\otimes\mathbb{Y}_{10}[\mathbb{T}_{2,0}^{(b,E_g)}]}{78} - \frac{\sqrt{195}\mathbb{X}_{22}[\mathbb{M}_{3,1}^{(a,E_g,1)}(1,-1)]\otimes\mathbb{Y}_{11}[\mathbb{T}_{2,1}^{(b,E_g)}]}{78} - \frac{\sqrt{13}\mathbb{X}_{23}[\mathbb{M}_{3,0}^{(a,E_g,2)}(1,-1)]\otimes\mathbb{Y}_{10}[\mathbb{T}_{2,0}^{(b,E_g)}]}{6}$$
$$+ \frac{\sqrt{13}\mathbb{X}_{24}[\mathbb{M}_{3,1}^{(a,E_g,2)}(1,-1)]\otimes\mathbb{Y}_{11}[\mathbb{T}_{2,1}^{(b,E_g)}]}{6} + \frac{5\sqrt{13}\mathbb{X}_{27}[\mathbb{M}_{3}^{(a,B_{1g})}(1,-1)]\otimes\mathbb{Y}_{9}[\mathbb{T}_{2}^{(b,B_{1g})}]}{39}$$

No. 27 $\hat{\mathbb{Q}}_4^{(A_{1g},2)}(1,-1)$ $[\mathrm{M}_1,\mathrm{B}_1]$

$$\hat{\mathbb{Z}}_{27} = -\frac{\sqrt{65}\mathbb{X}_{21}[\mathbb{M}_{3,0}^{(a,E_g,1)}(1,-1)]\otimes\mathbb{Y}_{10}[\mathbb{T}_{2,0}^{(b,E_g)}]}{13} + \frac{\sqrt{65}\mathbb{X}_{22}[\mathbb{M}_{3,1}^{(a,E_g,1)}(1,-1)]\otimes\mathbb{Y}_{11}[\mathbb{T}_{2,1}^{(b,E_g)}]}{13} + \frac{\sqrt{39}\mathbb{X}_{27}[\mathbb{M}_{3}^{(a,B_{1g})}(1,-1)]\otimes\mathbb{Y}_{9}[\mathbb{T}_{2}^{(b,B_{1g})}]}{13}$$

No. 28 $\hat{\mathbb{Q}}_2^{(A_{1g})}(1,0)$ $[\mathrm{M}_1,\mathrm{B}_1]$

$$\hat{\mathbb{Z}}_{28} = \mathbb{X}_{31}[\mathbb{T}_{2}^{(a,A_{1g})}(1,0)]\otimes\mathbb{Y}_{8}[\mathbb{T}_{0}^{(b,A_{1g})}]$$

No. 29 $\hat{\mathbb{Q}}_0^{(A_{1g})}(1,0)$ $[\mathrm{M}_1,\mathrm{B}_1]$

$$\hat{\mathbb{Z}}_{29} = \frac{\sqrt{3}\mathbb{X}_{25}[\mathbb{T}_{2,0}^{(a,E_g)}(1,0)]\otimes\mathbb{Y}_{10}[\mathbb{T}_{2,0}^{(b,E_g)}]}{3} + \frac{\sqrt{3}\mathbb{X}_{26}[\mathbb{T}_{2,1}^{(a,E_g)}(1,0)]\otimes\mathbb{Y}_{11}[\mathbb{T}_{2,1}^{(b,E_g)}]}{3} + \frac{\sqrt{3}\mathbb{X}_{28}[\mathbb{T}_{2}^{(a,B_{1g})}(1,0)]\otimes\mathbb{Y}_{9}[\mathbb{T}_{2}^{(b,B_{1g})}]}{3}$$

No. 30 $\hat{\mathbb{Q}}_2^{(A_{1g})}(1,0)$ $[\mathrm{M}_1,\mathrm{B}_1]$

$$\hat{\mathbb{Z}}_{30} = \frac{\sqrt{6}\mathbb{X}_{25}[\mathbb{T}_{2,0}^{(a,E_g)}(1,0)]\otimes\mathbb{Y}_{10}[\mathbb{T}_{2,0}^{(b,E_g)}]}{6} + \frac{\sqrt{6}\mathbb{X}_{26}[\mathbb{T}_{2,1}^{(a,E_g)}(1,0)]\otimes\mathbb{Y}_{11}[\mathbb{T}_{2,1}^{(b,E_g)}]}{6} - \frac{\sqrt{6}\mathbb{X}_{28}[\mathbb{T}_{2}^{(a,B_{1g})}(1,0)]\otimes\mathbb{Y}_{9}[\mathbb{T}_{2}^{(b,B_{1g})}]}{3}$$

No. 31 $\hat{\mathbb{Q}}_0^{(A_{1g})}$ $[\mathrm{M}_1,\mathrm{B}_2]$

$$\hat{\mathbb{Z}}_{31} = \mathbb{X}_{1}[\mathbb{Q}_{0}^{(a,A_{1g})}]\otimes\mathbb{Y}_{12}[\mathbb{Q}_{0}^{(b,A_{1g})}]$$

No. 32 $\hat{\mathbb{Q}}_2^{(A_{1g})}$ $[\mathrm{M}_1,\mathrm{B}_2]$

$$\hat{\mathbb{Z}}_{32} = \mathbb{X}_{2}[\mathbb{Q}_{2}^{(a,A_{1g})}]\otimes\mathbb{Y}_{12}[\mathbb{Q}_{0}^{(b,A_{1g})}]$$

No. 33 $\hat{\mathbb{Q}}_0^{(A_{1g})}$ $[\mathrm{M}_1,\mathrm{B}_2]$

$$\hat{\mathbb{Z}}_{33} = \frac{\sqrt{3}\mathbb{X}_{6}[\mathbb{Q}_{2}^{(a,B_{2g})}]\otimes\mathbb{Y}_{13}[\mathbb{Q}_{2}^{(b,B_{2g})}]}{3} + \frac{\sqrt{3}\mathbb{X}_{7}[\mathbb{Q}_{2,0}^{(a,E_g)}]\otimes\mathbb{Y}_{14}[\mathbb{Q}_{2,0}^{(b,E_g)}]}{3} + \frac{\sqrt{3}\mathbb{X}_{8}[\mathbb{Q}_{2,1}^{(a,E_g)}]\otimes\mathbb{Y}_{15}[\mathbb{Q}_{2,1}^{(b,E_g)}]}{3}$$

No. 34 $\hat{\mathbb{Q}}_2^{(A_{1g})}$ $[\mathrm{M}_1, \mathrm{B}_2]$

$$\hat{\mathbb{Z}}_{34} = -\frac{\sqrt{6}\mathbb{X}_6[\mathbb{Q}_2^{(a,B_{2g})}] \otimes \mathbb{Y}_{13}[\mathbb{Q}_2^{(b,B_{2g})}]}{3} + \frac{\sqrt{6}\mathbb{X}_7[\mathbb{Q}_{2,0}^{(a,E_g)}] \otimes \mathbb{Y}_{14}[\mathbb{Q}_{2,0}^{(b,E_g)}]}{6} + \frac{\sqrt{6}\mathbb{X}_8[\mathbb{Q}_{2,1}^{(a,E_g)}] \otimes \mathbb{Y}_{15}[\mathbb{Q}_{2,1}^{(b,E_g)}]}{6}$$

No. 35 $\hat{\mathbb{Q}}_0^{(A_{1g})}(1,1)$ $[\mathrm{M}_1, \mathrm{B}_2]$

$$\hat{\mathbb{Z}}_{35} = \mathbb{X}_3[\mathbb{Q}_0^{(a,A_{1g})}(1,1)] \otimes \mathbb{Y}_{12}[\mathbb{Q}_0^{(b,A_{1g})}]$$

No. 36 $\hat{\mathbb{Q}}_2^{(A_{1g})}(1,-1)$ $[\mathrm{M}_1, \mathrm{B}_2]$

$$\hat{\mathbb{Z}}_{36} = \mathbb{X}_4[\mathbb{Q}_2^{(a,A_{1g})}(1,-1)] \otimes \mathbb{Y}_{12}[\mathbb{Q}_0^{(b,A_{1g})}]$$

No. 37 $\hat{\mathbb{Q}}_0^{(A_{1g})}(1,-1)$ $[\mathrm{M}_1, \mathrm{B}_2]$

$$\hat{\mathbb{Z}}_{37} = \frac{\sqrt{3}\mathbb{X}_{10}[\mathbb{Q}_2^{(a,B_{2g})}(1,-1)] \otimes \mathbb{Y}_{13}[\mathbb{Q}_2^{(b,B_{2g})}]}{3} + \frac{\sqrt{3}\mathbb{X}_{11}[\mathbb{Q}_{2,0}^{(a,E_g)}(1,-1)] \otimes \mathbb{Y}_{14}[\mathbb{Q}_{2,0}^{(b,E_g)}]}{3} + \frac{\sqrt{3}\mathbb{X}_{12}[\mathbb{Q}_{2,1}^{(a,E_g)}(1,-1)] \otimes \mathbb{Y}_{15}[\mathbb{Q}_{2,1}^{(b,E_g)}]}{3}$$

No. 38 $\hat{\mathbb{Q}}_2^{(A_{1g})}(1,-1)$ $[\mathrm{M}_1, \mathrm{B}_2]$

$$\hat{\mathbb{Z}}_{38} = -\frac{\sqrt{6}\mathbb{X}_{10}[\mathbb{Q}_2^{(a,B_{2g})}(1,-1)] \otimes \mathbb{Y}_{13}[\mathbb{Q}_2^{(b,B_{2g})}]}{3} + \frac{\sqrt{6}\mathbb{X}_{11}[\mathbb{Q}_{2,0}^{(a,E_g)}(1,-1)] \otimes \mathbb{Y}_{14}[\mathbb{Q}_{2,0}^{(b,E_g)}]}{6} + \frac{\sqrt{6}\mathbb{X}_{12}[\mathbb{Q}_{2,1}^{(a,E_g)}(1,-1)] \otimes \mathbb{Y}_{15}[\mathbb{Q}_{2,1}^{(b,E_g)}]}{6}$$

No. 39 $\hat{\mathbb{Q}}_2^{(A_{1g})}(1,0)$ $[\mathrm{M}_1, \mathrm{B}_2]$

$$\hat{\mathbb{Z}}_{39} = \frac{\sqrt{2}\mathbb{X}_{13}[\mathbb{G}_{1,0}^{(a,E_g)}(1,0)] \otimes \mathbb{Y}_{14}[\mathbb{Q}_{2,0}^{(b,E_g)}]}{2} - \frac{\sqrt{2}\mathbb{X}_{14}[\mathbb{G}_{1,1}^{(a,E_g)}(1,0)] \otimes \mathbb{Y}_{15}[\mathbb{Q}_{2,1}^{(b,E_g)}]}{2}$$

No. 40 $\hat{\mathbb{Q}}_2^{(A_{1g})}$ $[\mathrm{M}_1, \mathrm{B}_2]$

$$\hat{\mathbb{Z}}_{40} = \frac{\sqrt{2}\mathbb{X}_{15}[\mathbb{M}_{1,0}^{(a,E_g)}] \otimes \mathbb{Y}_{18}[\mathbb{T}_{2,0}^{(b,E_g)}]}{2} - \frac{\sqrt{2}\mathbb{X}_{16}[\mathbb{M}_{1,1}^{(a,E_g)}] \otimes \mathbb{Y}_{19}[\mathbb{T}_{2,1}^{(b,E_g)}]}{2}$$

No. 41 $\hat{\mathbb{Q}}_2^{(A_{1g})}(1,1)$ $[\mathrm{M}_1, \mathrm{B}_2]$

$$\hat{\mathbb{Z}}_{41} = \frac{\sqrt{2}\mathbb{X}_{17}[\mathbb{M}_{1,0}^{(a,E_g)}(1,1)] \otimes \mathbb{Y}_{18}[\mathbb{T}_{2,0}^{(b,E_g)}]}{2} - \frac{\sqrt{2}\mathbb{X}_{18}[\mathbb{M}_{1,1}^{(a,E_g)}(1,1)] \otimes \mathbb{Y}_{19}[\mathbb{T}_{2,1}^{(b,E_g)}]}{2}$$

No. 42 $\hat{\mathbb{Q}}_2^{(A_{1g})}(1,-1)$ $[\mathrm{M}_1,\mathrm{B}_2]$

$$\hat{\mathbb{Z}}_{42} = \frac{\sqrt{2}\mathbb{X}_{19}[\mathbb{M}_{1,0}^{(a,E_g)}(1,-1)]\otimes\mathbb{Y}_{18}[\mathbb{T}_{2,0}^{(b,E_g)}]}{2} - \frac{\sqrt{2}\mathbb{X}_{20}[\mathbb{M}_{1,1}^{(a,E_g)}(1,-1)]\otimes\mathbb{Y}_{19}[\mathbb{T}_{2,1}^{(b,E_g)}]}{2}$$

No. 43 $\hat{\mathbb{Q}}_2^{(A_{1g})}(1,-1)$ $[\mathrm{M}_1,\mathrm{B}_2]$

$$\begin{aligned}\hat{\mathbb{Z}}_{43} = &-\frac{\sqrt{3}\mathbb{X}_{21}[\mathbb{M}_{3,0}^{(a,E_g,1)}(1,-1)]\otimes\mathbb{Y}_{18}[\mathbb{T}_{2,0}^{(b,E_g)}]}{6} + \frac{\sqrt{3}\mathbb{X}_{22}[\mathbb{M}_{3,1}^{(a,E_g,1)}(1,-1)]\otimes\mathbb{Y}_{19}[\mathbb{T}_{2,1}^{(b,E_g)}]}{6} - \frac{\sqrt{5}\mathbb{X}_{23}[\mathbb{M}_{3,0}^{(a,E_g,2)}(1,-1)]\otimes\mathbb{Y}_{18}[\mathbb{T}_{2,0}^{(b,E_g)}]}{6}\\ &+ \frac{\sqrt{5}\mathbb{X}_{24}[\mathbb{M}_{3,1}^{(a,E_g,2)}(1,-1)]\otimes\mathbb{Y}_{19}[\mathbb{T}_{2,1}^{(b,E_g)}]}{6} + \frac{\sqrt{5}\mathbb{X}_{29}[\mathbb{M}_{3}^{(a,B_{2g})}(1,-1)]\otimes\mathbb{Y}_{17}[\mathbb{T}_{2}^{(b,B_{2g})}]}{3}\end{aligned}$$

No. 44 $\hat{\mathbb{Q}}_4^{(A_{1g},1)}(1,-1)$ $[\mathrm{M}_1,\mathrm{B}_2]$

$$\hat{\mathbb{Z}}_{44} = -\frac{\sqrt{3}\mathbb{X}_{23}[\mathbb{M}_{3,0}^{(a,E_g,2)}(1,-1)]\otimes\mathbb{Y}_{18}[\mathbb{T}_{2,0}^{(b,E_g)}]}{3} + \frac{\sqrt{3}\mathbb{X}_{24}[\mathbb{M}_{3,1}^{(a,E_g,2)}(1,-1)]\otimes\mathbb{Y}_{19}[\mathbb{T}_{2,1}^{(b,E_g)}]}{3} - \frac{\sqrt{3}\mathbb{X}_{29}[\mathbb{M}_{3}^{(a,B_{2g})}(1,-1)]\otimes\mathbb{Y}_{17}[\mathbb{T}_{2}^{(b,B_{2g})}]}{3}$$

No. 45 $\hat{\mathbb{Q}}_4^{(A_{1g},2)}(1,-1)$ $[\mathrm{M}_1,\mathrm{B}_2]$

$$\begin{aligned}\hat{\mathbb{Z}}_{45} = &-\frac{\sqrt{15}\mathbb{X}_{21}[\mathbb{M}_{3,0}^{(a,E_g,1)}(1,-1)]\otimes\mathbb{Y}_{18}[\mathbb{T}_{2,0}^{(b,E_g)}]}{6} + \frac{\sqrt{15}\mathbb{X}_{22}[\mathbb{M}_{3,1}^{(a,E_g,1)}(1,-1)]\otimes\mathbb{Y}_{19}[\mathbb{T}_{2,1}^{(b,E_g)}]}{6}\\ &+ \frac{\mathbb{X}_{23}[\mathbb{M}_{3,0}^{(a,E_g,2)}(1,-1)]\otimes\mathbb{Y}_{18}[\mathbb{T}_{2,0}^{(b,E_g)}]}{6} - \frac{\mathbb{X}_{24}[\mathbb{M}_{3,1}^{(a,E_g,2)}(1,-1)]\otimes\mathbb{Y}_{19}[\mathbb{T}_{2,1}^{(b,E_g)}]}{6} - \frac{\mathbb{X}_{29}[\mathbb{M}_{3}^{(a,B_{2g})}(1,-1)]\otimes\mathbb{Y}_{17}[\mathbb{T}_{2}^{(b,B_{2g})}]}{3}\end{aligned}$$

No. 46 $\hat{\mathbb{Q}}_2^{(A_{1g})}(1,0)$ $[\mathrm{M}_1,\mathrm{B}_2]$

$$\hat{\mathbb{Z}}_{46} = \mathbb{X}_{31}[\mathbb{T}_{2}^{(a,A_{1g})}(1,0)]\otimes\mathbb{Y}_{16}[\mathbb{T}_{0}^{(b,A_{1g})}]$$

No. 47 $\hat{\mathbb{Q}}_0^{(A_{1g})}(1,0)$ $[\mathrm{M}_1,\mathrm{B}_2]$

$$\hat{\mathbb{Z}}_{47} = \frac{\sqrt{3}\mathbb{X}_{25}[\mathbb{T}_{2,0}^{(a,E_g)}(1,0)]\otimes\mathbb{Y}_{18}[\mathbb{T}_{2,0}^{(b,E_g)}]}{3} + \frac{\sqrt{3}\mathbb{X}_{26}[\mathbb{T}_{2,1}^{(a,E_g)}(1,0)]\otimes\mathbb{Y}_{19}[\mathbb{T}_{2,1}^{(b,E_g)}]}{3} + \frac{\sqrt{3}\mathbb{X}_{30}[\mathbb{T}_{2}^{(a,B_{2g})}(1,0)]\otimes\mathbb{Y}_{17}[\mathbb{T}_{2}^{(b,B_{2g})}]}{3}$$

No. 48 $\hat{\mathbb{Q}}_2^{(A_{1g})}(1,0)$ $[\mathrm{M}_1,\mathrm{B}_2]$

$$\hat{\mathbb{Z}}_{48} = \frac{\sqrt{6}\mathbb{X}_{25}[\mathbb{T}_{2,0}^{(a,E_g)}(1,0)]\otimes\mathbb{Y}_{18}[\mathbb{T}_{2,0}^{(b,E_g)}]}{6} + \frac{\sqrt{6}\mathbb{X}_{26}[\mathbb{T}_{2,1}^{(a,E_g)}(1,0)]\otimes\mathbb{Y}_{19}[\mathbb{T}_{2,1}^{(b,E_g)}]}{6} - \frac{\sqrt{6}\mathbb{X}_{30}[\mathbb{T}_{2}^{(a,B_{2g})}(1,0)]\otimes\mathbb{Y}_{17}[\mathbb{T}_{2}^{(b,B_{2g})}]}{3}$$

No. 49 $\hat{\mathbb{Q}}_0^{(A_{1g})}$ $[\mathrm{M}_1, \mathrm{B}_3]$

$$\hat{\mathbb{Z}}_{49} = \mathbb{X}_1[\mathbb{Q}_0^{(a,A_{1g})}] \otimes \mathbb{Y}_{20}[\mathbb{Q}_0^{(b,A_{1g})}]$$

No. 50 $\hat{\mathbb{Q}}_2^{(A_{1g})}$ $[\mathrm{M}_1, \mathrm{B}_3]$

$$\hat{\mathbb{Z}}_{50} = \mathbb{X}_2[\mathbb{Q}_2^{(a,A_{1g})}] \otimes \mathbb{Y}_{20}[\mathbb{Q}_0^{(b,A_{1g})}]$$

No. 51 $\hat{\mathbb{Q}}_0^{(A_{1g})}$ $[\mathrm{M}_1, \mathrm{B}_3]$

$$\hat{\mathbb{Z}}_{51} = \frac{\sqrt{3}\mathbb{X}_5[\mathbb{Q}_2^{(a,B_{1g})}] \otimes \mathbb{Y}_{21}[\mathbb{Q}_2^{(b,B_{1g})}]}{3} + \frac{\sqrt{3}\mathbb{X}_7[\mathbb{Q}_{2,0}^{(a,E_g)}] \otimes \mathbb{Y}_{22}[\mathbb{Q}_{2,0}^{(b,E_g)}]}{3} + \frac{\sqrt{3}\mathbb{X}_8[\mathbb{Q}_{2,1}^{(a,E_g)}] \otimes \mathbb{Y}_{23}[\mathbb{Q}_{2,1}^{(b,E_g)}]}{3}$$

No. 52 $\hat{\mathbb{Q}}_2^{(A_{1g})}$ $[\mathrm{M}_1, \mathrm{B}_3]$

$$\hat{\mathbb{Z}}_{52} = -\frac{\sqrt{6}\mathbb{X}_5[\mathbb{Q}_2^{(a,B_{1g})}] \otimes \mathbb{Y}_{21}[\mathbb{Q}_2^{(b,B_{1g})}]}{3} + \frac{\sqrt{6}\mathbb{X}_7[\mathbb{Q}_{2,0}^{(a,E_g)}] \otimes \mathbb{Y}_{22}[\mathbb{Q}_{2,0}^{(b,E_g)}]}{6} + \frac{\sqrt{6}\mathbb{X}_8[\mathbb{Q}_{2,1}^{(a,E_g)}] \otimes \mathbb{Y}_{23}[\mathbb{Q}_{2,1}^{(b,E_g)}]}{6}$$

No. 53 $\hat{\mathbb{Q}}_0^{(A_{1g})}(1,1)$ $[\mathrm{M}_1, \mathrm{B}_3]$

$$\hat{\mathbb{Z}}_{53} = \mathbb{X}_3[\mathbb{Q}_0^{(a,A_{1g})}(1,1)] \otimes \mathbb{Y}_{20}[\mathbb{Q}_0^{(b,A_{1g})}]$$

No. 54 $\hat{\mathbb{Q}}_2^{(A_{1g})}(1,-1)$ $[\mathrm{M}_1, \mathrm{B}_3]$

$$\hat{\mathbb{Z}}_{54} = \mathbb{X}_4[\mathbb{Q}_2^{(a,A_{1g})}(1,-1)] \otimes \mathbb{Y}_{20}[\mathbb{Q}_0^{(b,A_{1g})}]$$

No. 55 $\hat{\mathbb{Q}}_0^{(A_{1g})}(1,-1)$ $[\mathrm{M}_1, \mathrm{B}_3]$

$$\hat{\mathbb{Z}}_{55} = \frac{\sqrt{3}\mathbb{X}_{11}[\mathbb{Q}_{2,0}^{(a,E_g)}(1,-1)] \otimes \mathbb{Y}_{22}[\mathbb{Q}_{2,0}^{(b,E_g)}]}{3} + \frac{\sqrt{3}\mathbb{X}_{12}[\mathbb{Q}_{2,1}^{(a,E_g)}(1,-1)] \otimes \mathbb{Y}_{23}[\mathbb{Q}_{2,1}^{(b,E_g)}]}{3} + \frac{\sqrt{3}\mathbb{X}_9[\mathbb{Q}_2^{(a,B_{1g})}(1,-1)] \otimes \mathbb{Y}_{21}[\mathbb{Q}_2^{(b,B_{1g})}]}{3}$$

No. 56 $\hat{\mathbb{Q}}_2^{(A_{1g})}(1,-1)$ $[\mathrm{M}_1, \mathrm{B}_3]$

$$\hat{\mathbb{Z}}_{56} = \frac{\sqrt{6}\mathbb{X}_{11}[\mathbb{Q}_{2,0}^{(a,E_g)}(1,-1)] \otimes \mathbb{Y}_{22}[\mathbb{Q}_{2,0}^{(b,E_g)}]}{6} + \frac{\sqrt{6}\mathbb{X}_{12}[\mathbb{Q}_{2,1}^{(a,E_g)}(1,-1)] \otimes \mathbb{Y}_{23}[\mathbb{Q}_{2,1}^{(b,E_g)}]}{6} - \frac{\sqrt{6}\mathbb{X}_9[\mathbb{Q}_2^{(a,B_{1g})}(1,-1)] \otimes \mathbb{Y}_{21}[\mathbb{Q}_2^{(b,B_{1g})}]}{3}$$

No. 57 $\hat{\mathbb{Q}}_2^{(A_{1g})}(1,0)$ $[\mathrm{M}_1, \mathrm{B}_3]$

$$\hat{\mathbb{Z}}_{57} = \frac{\sqrt{2}\mathbb{X}_{13}[\mathbb{G}_{1,0}^{(a,E_g)}(1,0)] \otimes \mathbb{Y}_{22}[\mathbb{Q}_{2,0}^{(b,E_g)}]}{2} - \frac{\sqrt{2}\mathbb{X}_{14}[\mathbb{G}_{1,1}^{(a,E_g)}(1,0)] \otimes \mathbb{Y}_{23}[\mathbb{Q}_{2,1}^{(b,E_g)}]}{2}$$

No. 58 $\hat{\mathbb{Q}}_2^{(A_{1g})}$ $[\mathrm{M}_1, \mathrm{B}_3]$

$$\hat{\mathbb{Z}}_{58} = \frac{\sqrt{2}\mathbb{X}_{15}[\mathbb{M}_{1,0}^{(a,E_g)}] \otimes \mathbb{Y}_{26}[\mathbb{T}_{2,0}^{(b,E_g)}]}{2} - \frac{\sqrt{2}\mathbb{X}_{16}[\mathbb{M}_{1,1}^{(a,E_g)}] \otimes \mathbb{Y}_{27}[\mathbb{T}_{2,1}^{(b,E_g)}]}{2}$$

No. 59 $\hat{\mathbb{Q}}_2^{(A_{1g})}(1,1)$ $[\mathrm{M}_1, \mathrm{B}_3]$

$$\hat{\mathbb{Z}}_{59} = \frac{\sqrt{2}\mathbb{X}_{17}[\mathbb{M}_{1,0}^{(a,E_g)}(1,1)] \otimes \mathbb{Y}_{26}[\mathbb{T}_{2,0}^{(b,E_g)}]}{2} - \frac{\sqrt{2}\mathbb{X}_{18}[\mathbb{M}_{1,1}^{(a,E_g)}(1,1)] \otimes \mathbb{Y}_{27}[\mathbb{T}_{2,1}^{(b,E_g)}]}{2}$$

No. 60 $\hat{\mathbb{Q}}_2^{(A_{1g})}(1,-1)$ $[\mathrm{M}_1, \mathrm{B}_3]$

$$\hat{\mathbb{Z}}_{60} = \frac{\sqrt{2}\mathbb{X}_{19}[\mathbb{M}_{1,0}^{(a,E_g)}(1,-1)] \otimes \mathbb{Y}_{26}[\mathbb{T}_{2,0}^{(b,E_g)}]}{2} - \frac{\sqrt{2}\mathbb{X}_{20}[\mathbb{M}_{1,1}^{(a,E_g)}(1,-1)] \otimes \mathbb{Y}_{27}[\mathbb{T}_{2,1}^{(b,E_g)}]}{2}$$

No. 61 $\hat{\mathbb{Q}}_2^{(A_{1g})}(1,-1)$ $[\mathrm{M}_1, \mathrm{B}_3]$

$$\begin{aligned}\hat{\mathbb{Z}}_{61} = &-\frac{\sqrt{3}\mathbb{X}_{21}[\mathbb{M}_{3,0}^{(a,E_g,1)}(1,-1)] \otimes \mathbb{Y}_{26}[\mathbb{T}_{2,0}^{(b,E_g)}]}{6} + \frac{\sqrt{3}\mathbb{X}_{22}[\mathbb{M}_{3,1}^{(a,E_g,1)}(1,-1)] \otimes \mathbb{Y}_{27}[\mathbb{T}_{2,1}^{(b,E_g)}]}{6} - \frac{\sqrt{5}\mathbb{X}_{23}[\mathbb{M}_{3,0}^{(a,E_g,2)}(1,-1)] \otimes \mathbb{Y}_{26}[\mathbb{T}_{2,0}^{(b,E_g)}]}{6} \\ &+ \frac{\sqrt{5}\mathbb{X}_{24}[\mathbb{M}_{3,1}^{(a,E_g,2)}(1,-1)] \otimes \mathbb{Y}_{27}[\mathbb{T}_{2,1}^{(b,E_g)}]}{6} - \frac{\sqrt{5}\mathbb{X}_{27}[\mathbb{M}_{3}^{(a,B_{1g})}(1,-1)] \otimes \mathbb{Y}_{25}[\mathbb{T}_{2}^{(b,B_{1g})}]}{3}\end{aligned}$$

No. 62 $\hat{\mathbb{Q}}_4^{(A_{1g},1)}(1,-1)$ $[\mathrm{M}_1, \mathrm{B}_3]$

$$\begin{aligned}\hat{\mathbb{Z}}_{62} = &\frac{\sqrt{195}\mathbb{X}_{21}[\mathbb{M}_{3,0}^{(a,E_g,1)}(1,-1)] \otimes \mathbb{Y}_{26}[\mathbb{T}_{2,0}^{(b,E_g)}]}{78} - \frac{\sqrt{195}\mathbb{X}_{22}[\mathbb{M}_{3,1}^{(a,E_g,1)}(1,-1)] \otimes \mathbb{Y}_{27}[\mathbb{T}_{2,1}^{(b,E_g)}]}{78} - \frac{\sqrt{13}\mathbb{X}_{23}[\mathbb{M}_{3,0}^{(a,E_g,2)}(1,-1)] \otimes \mathbb{Y}_{26}[\mathbb{T}_{2,0}^{(b,E_g)}]}{6} \\ &+ \frac{\sqrt{13}\mathbb{X}_{24}[\mathbb{M}_{3,1}^{(a,E_g,2)}(1,-1)] \otimes \mathbb{Y}_{27}[\mathbb{T}_{2,1}^{(b,E_g)}]}{6} + \frac{5\sqrt{13}\mathbb{X}_{27}[\mathbb{M}_{3}^{(a,B_{1g})}(1,-1)] \otimes \mathbb{Y}_{25}[\mathbb{T}_{2}^{(b,B_{1g})}]}{39}\end{aligned}$$

No. 63 $\hat{\mathbb{Q}}_4^{(A_{1g},2)}(1,-1)$ $[\mathrm{M}_1, \mathrm{B}_3]$

$$\hat{\mathbb{Z}}_{63} = -\frac{\sqrt{65}\mathbb{X}_{21}[\mathbb{M}_{3,0}^{(a,E_g,1)}(1,-1)] \otimes \mathbb{Y}_{26}[\mathbb{T}_{2,0}^{(b,E_g)}]}{13} + \frac{\sqrt{65}\mathbb{X}_{22}[\mathbb{M}_{3,1}^{(a,E_g,1)}(1,-1)] \otimes \mathbb{Y}_{27}[\mathbb{T}_{2,1}^{(b,E_g)}]}{13} + \frac{\sqrt{39}\mathbb{X}_{27}[\mathbb{M}_{3}^{(a,B_{1g})}(1,-1)] \otimes \mathbb{Y}_{25}[\mathbb{T}_{2}^{(b,B_{1g})}]}{13}$$

No. 64 $\hat{\mathbb{Q}}_2^{(A_{1g})}(1,0)$ $[\mathrm{M}_1, \mathrm{B}_3]$

$$\hat{\mathbb{Z}}_{64} = \mathbb{X}_{31}[\mathbb{T}_2^{(a,A_{1g})}(1,0)] \otimes \mathbb{Y}_{24}[\mathbb{T}_0^{(b,A_{1g})}]$$

No. 65 $\hat{\mathbb{Q}}_0^{(A_{1g})}(1,0)$ $[\mathrm{M}_1, \mathrm{B}_3]$

$$\hat{\mathbb{Z}}_{65} = \frac{\sqrt{3}\mathbb{X}_{25}[\mathbb{T}_{2,0}^{(a,E_g)}(1,0)] \otimes \mathbb{Y}_{26}[\mathbb{T}_{2,0}^{(b,E_g)}]}{3} + \frac{\sqrt{3}\mathbb{X}_{26}[\mathbb{T}_{2,1}^{(a,E_g)}(1,0)] \otimes \mathbb{Y}_{27}[\mathbb{T}_{2,1}^{(b,E_g)}]}{3} + \frac{\sqrt{3}\mathbb{X}_{28}[\mathbb{T}_2^{(a,B_{1g})}(1,0)] \otimes \mathbb{Y}_{25}[\mathbb{T}_2^{(b,B_{1g})}]}{3}$$

No. 66 $\hat{\mathbb{Q}}_2^{(A_{1g})}(1,0)$ $[\mathrm{M}_1, \mathrm{B}_3]$

$$\hat{\mathbb{Z}}_{66} = \frac{\sqrt{6}\mathbb{X}_{25}[\mathbb{T}_{2,0}^{(a,E_g)}(1,0)] \otimes \mathbb{Y}_{26}[\mathbb{T}_{2,0}^{(b,E_g)}]}{6} + \frac{\sqrt{6}\mathbb{X}_{26}[\mathbb{T}_{2,1}^{(a,E_g)}(1,0)] \otimes \mathbb{Y}_{27}[\mathbb{T}_{2,1}^{(b,E_g)}]}{6} - \frac{\sqrt{6}\mathbb{X}_{28}[\mathbb{T}_2^{(a,B_{1g})}(1,0)] \otimes \mathbb{Y}_{25}[\mathbb{T}_2^{(b,B_{1g})}]}{3}$$

Table 5: Atomic SAMB group.

group	bra	ket
M_1	$(p_x,\uparrow),(p_x,\downarrow),(p_y,\uparrow),(p_y,\downarrow),(p_z,\uparrow),(p_z,\downarrow)$	$(p_x,\uparrow),(p_x,\downarrow),(p_y,\uparrow),(p_y,\downarrow),(p_z,\uparrow),(p_z,\downarrow)$

Table 6: Atomic SAMB.

symbol	type	group	form
$\mathbb{X}_1$	$\mathbb{Q}_0^{(a,A_{1g})}$	M_1	$\begin{pmatrix} \frac{\sqrt{6}}{6} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{6}}{6} & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{6}}{6} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{6}}{6} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{6}}{6} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{6}}{6} \end{pmatrix}$

continued ...

Table 6

symbol	type	group	form
$\mathbb{X}_2$	$\mathbb{Q}_2^{(a,A_{1g})}$	M_1	$\begin{pmatrix} -\frac{\sqrt{3}}{6} & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{3}}{6} & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{3}}{6} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{3}}{6} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{3}}{3} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{3}}{3} \end{pmatrix}$
$\mathbb{X}_3$	$\mathbb{Q}_0^{(a,A_{1g})}(1,1)$	M_1	$\begin{pmatrix} 0 & 0 & -\frac{\sqrt{3}i}{6} & 0 & 0 & \frac{\sqrt{3}}{6} \\ 0 & 0 & 0 & \frac{\sqrt{3}i}{6} & -\frac{\sqrt{3}}{6} & 0 \\ \frac{\sqrt{3}i}{6} & 0 & 0 & 0 & 0 & -\frac{\sqrt{3}i}{6} \\ 0 & -\frac{\sqrt{3}i}{6} & 0 & 0 & -\frac{\sqrt{3}i}{6} & 0 \\ 0 & -\frac{\sqrt{3}}{6} & 0 & \frac{\sqrt{3}i}{6} & 0 & 0 \\ \frac{\sqrt{3}}{6} & 0 & \frac{\sqrt{3}i}{6} & 0 & 0 & 0 \end{pmatrix}$
$\mathbb{X}_4$	$\mathbb{Q}_2^{(a,A_{1g})}(1,-1)$	M_1	$\begin{pmatrix} 0 & 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 & -\frac{\sqrt{6}}{12} \\ 0 & 0 & 0 & \frac{\sqrt{6}i}{6} & \frac{\sqrt{6}}{12} & 0 \\ \frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 & \frac{\sqrt{6}i}{12} \\ 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 & \frac{\sqrt{6}i}{12} & 0 \\ 0 & \frac{\sqrt{6}}{12} & 0 & -\frac{\sqrt{6}i}{12} & 0 & 0 \\ -\frac{\sqrt{6}}{12} & 0 & -\frac{\sqrt{6}i}{12} & 0 & 0 & 0 \end{pmatrix}$
$\mathbb{X}_5$	$\mathbb{Q}_2^{(a,B_{1g})}$	M_1	$\begin{pmatrix} \frac{1}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{1}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$
$\mathbb{X}_6$	$\mathbb{Q}_2^{(a,B_{2g})}$	M_1	$\begin{pmatrix} 0 & 0 & \frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2} & 0 & 0 \\ \frac{1}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$

continued ...

Table 6

symbol	type	group	form
$\mathbb{X}_7$	$\mathbb{Q}_{2,0}^{(a,E_g)}$	M_1	$\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{2} \\ 0 & 0 & \frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2} & 0 & 0 \end{pmatrix}$
$\mathbb{X}_8$	$\mathbb{Q}_{2,1}^{(a,E_g)}$	M_1	$\begin{pmatrix} 0 & 0 & 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{2} \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{1}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 & 0 & 0 \end{pmatrix}$
$\mathbb{X}_9$	$\mathbb{Q}_2^{(a,B_{1g})}(1,-1)$	M_1	$\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{2}}{4} \\ 0 & 0 & 0 & 0 & \frac{\sqrt{2}}{4} & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{2}i}{4} \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{2}i}{4} & 0 \\ 0 & \frac{\sqrt{2}}{4} & 0 & \frac{\sqrt{2}i}{4} & 0 & 0 \\ -\frac{\sqrt{2}}{4} & 0 & \frac{\sqrt{2}i}{4} & 0 & 0 & 0 \end{pmatrix}$
$\mathbb{X}_{10}$	$\mathbb{Q}_2^{(a,B_{2g})}(1,-1)$	M_1	$\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{2}i}{4} \\ 0 & 0 & 0 & 0 & \frac{\sqrt{2}i}{4} & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{2}}{4} \\ 0 & 0 & 0 & 0 & \frac{\sqrt{2}}{4} & 0 \\ 0 & -\frac{\sqrt{2}i}{4} & 0 & \frac{\sqrt{2}}{4} & 0 & 0 \\ -\frac{\sqrt{2}i}{4} & 0 & -\frac{\sqrt{2}}{4} & 0 & 0 & 0 \end{pmatrix}$
$\mathbb{X}_{11}$	$\mathbb{Q}_{2,0}^{(a,E_g)}(1,-1)$	M_1	$\begin{pmatrix} 0 & 0 & 0 & -\frac{\sqrt{2}}{4} & \frac{\sqrt{2}i}{4} & 0 \\ 0 & 0 & \frac{\sqrt{2}}{4} & 0 & 0 & -\frac{\sqrt{2}i}{4} \\ 0 & \frac{\sqrt{2}}{4} & 0 & 0 & 0 & 0 \\ -\frac{\sqrt{2}}{4} & 0 & 0 & 0 & 0 & 0 \\ -\frac{\sqrt{2}i}{4} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{2}i}{4} & 0 & 0 & 0 & 0 \end{pmatrix}$

continued ...

Table 6

symbol	type	group	form
$\mathbb{X}_{12}$	$\mathbb{Q}_{2,1}^{(a,E_g)}(1,-1)$	M_1	$\begin{pmatrix} 0 & 0 & 0 & -\frac{\sqrt{2}i}{4} & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{2}i}{4} & 0 & 0 & 0 \\ 0 & \frac{\sqrt{2}i}{4} & 0 & 0 & -\frac{\sqrt{2}i}{4} & 0 \\ \frac{\sqrt{2}i}{4} & 0 & 0 & 0 & 0 & \frac{\sqrt{2}i}{4} \\ 0 & 0 & \frac{\sqrt{2}i}{4} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{2}i}{4} & 0 & 0 \end{pmatrix}$
$\mathbb{X}_{13}$	$\mathbb{G}_{1,0}^{(a,E_g)}(1,0)$	M_1	$\begin{pmatrix} 0 & 0 & 0 & -\frac{\sqrt{2}}{4} & -\frac{\sqrt{2}i}{4} & 0 \\ 0 & 0 & \frac{\sqrt{2}}{4} & 0 & 0 & \frac{\sqrt{2}i}{4} \\ 0 & \frac{\sqrt{2}}{4} & 0 & 0 & 0 & 0 \\ -\frac{\sqrt{2}}{4} & 0 & 0 & 0 & 0 & 0 \\ \frac{\sqrt{2}i}{4} & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{2}i}{4} & 0 & 0 & 0 & 0 \end{pmatrix}$
$\mathbb{X}_{14}$	$\mathbb{G}_{1,1}^{(a,E_g)}(1,0)$	M_1	$\begin{pmatrix} 0 & 0 & 0 & \frac{\sqrt{2}i}{4} & 0 & 0 \\ 0 & 0 & \frac{\sqrt{2}i}{4} & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{2}i}{4} & 0 & 0 & -\frac{\sqrt{2}i}{4} & 0 \\ -\frac{\sqrt{2}i}{4} & 0 & 0 & 0 & 0 & \frac{\sqrt{2}i}{4} \\ 0 & 0 & \frac{\sqrt{2}i}{4} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{2}i}{4} & 0 & 0 \end{pmatrix}$
$\mathbb{X}_{15}$	$\mathbb{M}_{1,0}^{(a,E_g)}$	M_1	$\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{i}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{i}{2} \\ 0 & 0 & \frac{i}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{i}{2} & 0 & 0 \end{pmatrix}$
$\mathbb{X}_{16}$	$\mathbb{M}_{1,1}^{(a,E_g)}$	M_1	$\begin{pmatrix} 0 & 0 & 0 & 0 & \frac{i}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{i}{2} \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ -\frac{i}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{i}{2} & 0 & 0 & 0 & 0 \end{pmatrix}$

continued ...

Table 6

symbol	type	group	form
$\mathbb{X}_{17}$	$\mathbb{M}_{1,0}^{(a,E_g)}(1,1)$	M_1	$\begin{pmatrix} 0 & \frac{\sqrt{30}}{15} & 0 & -\frac{\sqrt{30}i}{20} & \frac{\sqrt{30}}{20} & 0 \\ \frac{\sqrt{30}}{15} & 0 & \frac{\sqrt{30}i}{20} & 0 & 0 & -\frac{\sqrt{30}}{20} \\ 0 & -\frac{\sqrt{30}i}{20} & 0 & -\frac{\sqrt{30}}{30} & 0 & 0 \\ \frac{\sqrt{30}i}{20} & 0 & -\frac{\sqrt{30}}{30} & 0 & 0 & 0 \\ \frac{\sqrt{30}}{20} & 0 & 0 & 0 & 0 & -\frac{\sqrt{30}}{30} \\ 0 & -\frac{\sqrt{30}}{20} & 0 & 0 & -\frac{\sqrt{30}}{30} & 0 \end{pmatrix}$
$\mathbb{X}_{18}$	$\mathbb{M}_{1,1}^{(a,E_g)}(1,1)$	M_1	$\begin{pmatrix} 0 & \frac{\sqrt{30}i}{30} & 0 & \frac{\sqrt{30}}{20} & 0 & 0 \\ -\frac{\sqrt{30}i}{30} & 0 & \frac{\sqrt{30}}{20} & 0 & 0 & 0 \\ 0 & \frac{\sqrt{30}}{20} & 0 & -\frac{\sqrt{30}i}{15} & \frac{\sqrt{30}}{20} & 0 \\ \frac{\sqrt{30}}{20} & 0 & \frac{\sqrt{30}i}{15} & 0 & 0 & -\frac{\sqrt{30}}{20} \\ 0 & 0 & \frac{\sqrt{30}}{20} & 0 & 0 & \frac{\sqrt{30}i}{30} \\ 0 & 0 & 0 & -\frac{\sqrt{30}}{20} & -\frac{\sqrt{30}i}{30} & 0 \end{pmatrix}$
$\mathbb{X}_{19}$	$\mathbb{M}_{1,0}^{(a,E_g)}(1,-1)$	M_1	$\begin{pmatrix} 0 & \frac{\sqrt{6}}{6} & 0 & 0 & 0 & 0 \\ \frac{\sqrt{6}}{6} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{6}}{6} & 0 & 0 \\ 0 & 0 & \frac{\sqrt{6}}{6} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{6}}{6} \\ 0 & 0 & 0 & 0 & \frac{\sqrt{6}}{6} & 0 \end{pmatrix}$
$\mathbb{X}_{20}$	$\mathbb{M}_{1,1}^{(a,E_g)}(1,-1)$	M_1	$\begin{pmatrix} 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 \\ \frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 \\ 0 & 0 & \frac{\sqrt{6}i}{6} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{6}i}{6} \\ 0 & 0 & 0 & 0 & \frac{\sqrt{6}i}{6} & 0 \end{pmatrix}$
$\mathbb{X}_{21}$	$\mathbb{M}_{3,0}^{(a,E_g,1)}(1,-1)$	M_1	$\begin{pmatrix} 0 & \frac{\sqrt{5}}{5} & 0 & \frac{\sqrt{5}i}{10} & -\frac{\sqrt{5}}{10} & 0 \\ \frac{\sqrt{5}}{5} & 0 & -\frac{\sqrt{5}i}{10} & 0 & 0 & \frac{\sqrt{5}}{10} \\ 0 & \frac{\sqrt{5}i}{10} & 0 & -\frac{\sqrt{5}}{10} & 0 & 0 \\ -\frac{\sqrt{5}i}{10} & 0 & -\frac{\sqrt{5}}{10} & 0 & 0 & 0 \\ -\frac{\sqrt{5}}{10} & 0 & 0 & 0 & 0 & -\frac{\sqrt{5}}{10} \\ 0 & \frac{\sqrt{5}}{10} & 0 & 0 & -\frac{\sqrt{5}}{10} & 0 \end{pmatrix}$

continued ...

Table 6

symbol	type	group	form
$\mathbb{X}_{22}$	$\mathbb{M}_{3,1}^{(a,E_g,1)}(1,-1)$	M_1	$\begin{pmatrix} 0 & \frac{\sqrt{5}i}{10} & 0 & -\frac{\sqrt{5}}{10} & 0 & 0 \\ -\frac{\sqrt{5}i}{10} & 0 & -\frac{\sqrt{5}}{10} & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{5}}{10} & 0 & -\frac{\sqrt{5}i}{5} & -\frac{\sqrt{5}}{10} & 0 \\ -\frac{\sqrt{5}}{10} & 0 & \frac{\sqrt{5}i}{5} & 0 & 0 & \frac{\sqrt{5}}{10} \\ 0 & 0 & -\frac{\sqrt{5}}{10} & 0 & 0 & \frac{\sqrt{5}i}{10} \\ 0 & 0 & 0 & \frac{\sqrt{5}}{10} & -\frac{\sqrt{5}i}{10} & 0 \end{pmatrix}$
$\mathbb{X}_{23}$	$\mathbb{M}_{3,0}^{(a,E_g,2)}(1,-1)$	M_1	$\begin{pmatrix} 0 & 0 & 0 & -\frac{\sqrt{3}i}{6} & -\frac{\sqrt{3}}{6} & 0 \\ 0 & 0 & \frac{\sqrt{3}i}{6} & 0 & 0 & \frac{\sqrt{3}}{6} \\ 0 & -\frac{\sqrt{3}i}{6} & 0 & \frac{\sqrt{3}}{6} & 0 & 0 \\ \frac{\sqrt{3}i}{6} & 0 & \frac{\sqrt{3}}{6} & 0 & 0 & 0 \\ -\frac{\sqrt{3}}{6} & 0 & 0 & 0 & 0 & -\frac{\sqrt{3}}{6} \\ 0 & \frac{\sqrt{3}}{6} & 0 & 0 & -\frac{\sqrt{3}}{6} & 0 \end{pmatrix}$
$\mathbb{X}_{24}$	$\mathbb{M}_{3,1}^{(a,E_g,2)}(1,-1)$	M_1	$\begin{pmatrix} 0 & -\frac{\sqrt{3}i}{6} & 0 & \frac{\sqrt{3}}{6} & 0 & 0 \\ \frac{\sqrt{3}i}{6} & 0 & \frac{\sqrt{3}}{6} & 0 & 0 & 0 \\ 0 & \frac{\sqrt{3}}{6} & 0 & 0 & -\frac{\sqrt{3}}{6} & 0 \\ \frac{\sqrt{3}}{6} & 0 & 0 & 0 & 0 & \frac{\sqrt{3}}{6} \\ 0 & 0 & -\frac{\sqrt{3}}{6} & 0 & 0 & \frac{\sqrt{3}i}{6} \\ 0 & 0 & 0 & \frac{\sqrt{3}}{6} & -\frac{\sqrt{3}i}{6} & 0 \end{pmatrix}$
$\mathbb{X}_{25}$	$\mathbb{T}_{2,0}^{(a,E_g)}(1,0)$	M_1	$\begin{pmatrix} 0 & 0 & 0 & \frac{\sqrt{6}i}{12} & \frac{\sqrt{6}}{12} & 0 \\ 0 & 0 & -\frac{\sqrt{6}i}{12} & 0 & 0 & -\frac{\sqrt{6}}{12} \\ 0 & \frac{\sqrt{6}i}{12} & 0 & \frac{\sqrt{6}}{6} & 0 & 0 \\ -\frac{\sqrt{6}i}{12} & 0 & \frac{\sqrt{6}}{6} & 0 & 0 & 0 \\ \frac{\sqrt{6}}{12} & 0 & 0 & 0 & 0 & -\frac{\sqrt{6}}{6} \\ 0 & -\frac{\sqrt{6}}{12} & 0 & 0 & -\frac{\sqrt{6}}{6} & 0 \end{pmatrix}$
$\mathbb{X}_{26}$	$\mathbb{T}_{2,1}^{(a,E_g)}(1,0)$	M_1	$\begin{pmatrix} 0 & \frac{\sqrt{6}i}{6} & 0 & \frac{\sqrt{6}}{12} & 0 & 0 \\ -\frac{\sqrt{6}i}{6} & 0 & \frac{\sqrt{6}}{12} & 0 & 0 & 0 \\ 0 & \frac{\sqrt{6}}{12} & 0 & 0 & -\frac{\sqrt{6}}{12} & 0 \\ \frac{\sqrt{6}}{12} & 0 & 0 & 0 & 0 & \frac{\sqrt{6}}{12} \\ 0 & 0 & -\frac{\sqrt{6}}{12} & 0 & 0 & -\frac{\sqrt{6}i}{6} \\ 0 & 0 & 0 & \frac{\sqrt{6}}{12} & \frac{\sqrt{6}i}{6} & 0 \end{pmatrix}$

continued ...

Table 6

symbol	type	group	form
$\mathbb{X}_{27}$	$\mathbb{M}_3^{(a,B_{1g})}(1,-1)$	M_1	$\begin{pmatrix} 0 & 0 & \frac{\sqrt{3}}{6} & 0 & 0 & -\frac{\sqrt{3}i}{6} \\ 0 & 0 & 0 & -\frac{\sqrt{3}}{6} & \frac{\sqrt{3}i}{6} & 0 \\ \frac{\sqrt{3}}{6} & 0 & 0 & 0 & 0 & \frac{\sqrt{3}}{6} \\ 0 & -\frac{\sqrt{3}}{6} & 0 & 0 & \frac{\sqrt{3}}{6} & 0 \\ 0 & -\frac{\sqrt{3}i}{6} & 0 & \frac{\sqrt{3}}{6} & 0 & 0 \\ \frac{\sqrt{3}i}{6} & 0 & \frac{\sqrt{3}}{6} & 0 & 0 & 0 \end{pmatrix}$
$\mathbb{X}_{28}$	$\mathbb{T}_2^{(a,B_{1g})}(1,0)$	M_1	$\begin{pmatrix} 0 & 0 & -\frac{\sqrt{6}}{6} & 0 & 0 & -\frac{\sqrt{6}i}{12} \\ 0 & 0 & 0 & \frac{\sqrt{6}}{6} & \frac{\sqrt{6}i}{12} & 0 \\ -\frac{\sqrt{6}}{6} & 0 & 0 & 0 & 0 & \frac{\sqrt{6}}{12} \\ 0 & \frac{\sqrt{6}}{6} & 0 & 0 & \frac{\sqrt{6}}{12} & 0 \\ 0 & -\frac{\sqrt{6}i}{12} & 0 & \frac{\sqrt{6}}{12} & 0 & 0 \\ \frac{\sqrt{6}i}{12} & 0 & \frac{\sqrt{6}}{12} & 0 & 0 & 0 \end{pmatrix}$
$\mathbb{X}_{29}$	$\mathbb{M}_3^{(a,B_{2g})}(1,-1)$	M_1	$\begin{pmatrix} \frac{\sqrt{3}}{6} & 0 & 0 & 0 & 0 & \frac{\sqrt{3}}{6} \\ 0 & -\frac{\sqrt{3}}{6} & 0 & 0 & \frac{\sqrt{3}}{6} & 0 \\ 0 & 0 & -\frac{\sqrt{3}}{6} & 0 & 0 & \frac{\sqrt{3}i}{6} \\ 0 & 0 & 0 & \frac{\sqrt{3}}{6} & -\frac{\sqrt{3}i}{6} & 0 \\ 0 & \frac{\sqrt{3}}{6} & 0 & \frac{\sqrt{3}i}{6} & 0 & 0 \\ \frac{\sqrt{3}}{6} & 0 & -\frac{\sqrt{3}i}{6} & 0 & 0 & 0 \end{pmatrix}$
$\mathbb{X}_{30}$	$\mathbb{T}_2^{(a,B_{2g})}(1,0)$	M_1	$\begin{pmatrix} \frac{\sqrt{6}}{6} & 0 & 0 & 0 & 0 & -\frac{\sqrt{6}}{12} \\ 0 & -\frac{\sqrt{6}}{6} & 0 & 0 & -\frac{\sqrt{6}}{12} & 0 \\ 0 & 0 & -\frac{\sqrt{6}}{6} & 0 & 0 & -\frac{\sqrt{6}i}{12} \\ 0 & 0 & 0 & \frac{\sqrt{6}}{6} & \frac{\sqrt{6}i}{12} & 0 \\ 0 & -\frac{\sqrt{6}}{12} & 0 & -\frac{\sqrt{6}i}{12} & 0 & 0 \\ -\frac{\sqrt{6}}{12} & 0 & \frac{\sqrt{6}i}{12} & 0 & 0 & 0 \end{pmatrix}$
$\mathbb{X}_{31}$	$\mathbb{T}_2^{(a,A_{1g})}(1,0)$	M_1	$\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{2}i}{4} \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{2}i}{4} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{2}}{4} \\ 0 & 0 & 0 & 0 & \frac{\sqrt{2}}{4} & 0 \\ 0 & \frac{\sqrt{2}i}{4} & 0 & \frac{\sqrt{2}}{4} & 0 & 0 \\ -\frac{\sqrt{2}i}{4} & 0 & \frac{\sqrt{2}}{4} & 0 & 0 & 0 \end{pmatrix}$

Table 7: Cluster SAMB.

symbol	type	cluster	form
$\mathbb{Y}_1$	$\mathbb{Q}_0^{(s,A_{1g})}$	S_1	$\begin{pmatrix} \frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2} \end{pmatrix}$
$\mathbb{Y}_2$	$\mathbb{Q}_0^{(s,A_{1g})}$	S_2	$\begin{pmatrix} \frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2} \end{pmatrix}$
$\mathbb{Y}_3$	$\mathbb{Q}_0^{(s,A_{1g})}$	S_3	$\begin{pmatrix} \frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2} \end{pmatrix}$
$\mathbb{Y}_4$	$\mathbb{Q}_0^{(b,A_{1g})}$	B_1	$\begin{pmatrix} \frac{\sqrt{2}}{4} & \frac{\sqrt{2}}{4} & \frac{\sqrt{2}}{4} & \frac{\sqrt{2}}{4} & \frac{\sqrt{2}}{4} & \frac{\sqrt{2}}{4} & \frac{\sqrt{2}}{4} & \frac{\sqrt{2}}{4} \end{pmatrix}$
$\mathbb{Y}_5$	$\mathbb{Q}_2^{(b,B_{1g})}$	B_1	$\begin{pmatrix} \frac{\sqrt{2}}{4} & \frac{\sqrt{2}}{4} & \frac{\sqrt{2}}{4} & \frac{\sqrt{2}}{4} & -\frac{\sqrt{2}}{4} & -\frac{\sqrt{2}}{4} & -\frac{\sqrt{2}}{4} & -\frac{\sqrt{2}}{4} \end{pmatrix}$
$\mathbb{Y}_6$	$\mathbb{Q}_{2,0}^{(b,E_g)}$	B_1	$\begin{pmatrix} \frac{1}{2} & -\frac{1}{2} & \frac{1}{2} & -\frac{1}{2} & 0 & 0 & 0 & 0 \end{pmatrix}$
$\mathbb{Y}_7$	$\mathbb{Q}_{2,1}^{(b,E_g)}$	B_1	$\begin{pmatrix} 0 & 0 & 0 & 0 & -\frac{1}{2} & \frac{1}{2} & -\frac{1}{2} & \frac{1}{2} \end{pmatrix}$
$\mathbb{Y}_8$	$\mathbb{T}_0^{(b,A_{1g})}$	B_1	$\begin{pmatrix} \frac{\sqrt{2}i}{4} & \frac{\sqrt{2}i}{4} & \frac{\sqrt{2}i}{4} & \frac{\sqrt{2}i}{4} & \frac{\sqrt{2}i}{4} & \frac{\sqrt{2}i}{4} & \frac{\sqrt{2}i}{4} & \frac{\sqrt{2}i}{4} \end{pmatrix}$
$\mathbb{Y}_9$	$\mathbb{T}_2^{(b,B_{1g})}$	B_1	$\begin{pmatrix} \frac{\sqrt{2}i}{4} & \frac{\sqrt{2}i}{4} & \frac{\sqrt{2}i}{4} & \frac{\sqrt{2}i}{4} & -\frac{\sqrt{2}i}{4} & -\frac{\sqrt{2}i}{4} & -\frac{\sqrt{2}i}{4} & -\frac{\sqrt{2}i}{4} \end{pmatrix}$
$\mathbb{Y}_{10}$	$\mathbb{T}_{2,0}^{(b,E_g)}$	B_1	$\begin{pmatrix} \frac{i}{2} & -\frac{i}{2} & \frac{i}{2} & -\frac{i}{2} & 0 & 0 & 0 & 0 \end{pmatrix}$
$\mathbb{Y}_{11}$	$\mathbb{T}_{2,1}^{(b,E_g)}$	B_1	$\begin{pmatrix} 0 & 0 & 0 & 0 & -\frac{i}{2} & \frac{i}{2} & -\frac{i}{2} & \frac{i}{2} \end{pmatrix}$
$\mathbb{Y}_{12}$	$\mathbb{Q}_0^{(b,A_{1g})}$	B_2	$\begin{pmatrix} \frac{\sqrt{2}}{4} & \frac{\sqrt{2}}{4} & \frac{\sqrt{2}}{4} & \frac{\sqrt{2}}{4} & \frac{\sqrt{2}}{4} & \frac{\sqrt{2}}{4} & \frac{\sqrt{2}}{4} & \frac{\sqrt{2}}{4} \end{pmatrix}$
$\mathbb{Y}_{13}$	$\mathbb{Q}_2^{(b,B_{2g})}$	B_2	$\begin{pmatrix} \frac{\sqrt{2}}{4} & \frac{\sqrt{2}}{4} & -\frac{\sqrt{2}}{4} & -\frac{\sqrt{2}}{4} & \frac{\sqrt{2}}{4} & \frac{\sqrt{2}}{4} & -\frac{\sqrt{2}}{4} & -\frac{\sqrt{2}}{4} \end{pmatrix}$
$\mathbb{Y}_{14}$	$\mathbb{Q}_{2,0}^{(b,E_g)}$	B_2	$\begin{pmatrix} \frac{\sqrt{2}}{4} & -\frac{\sqrt{2}}{4} & \frac{\sqrt{2}}{4} & -\frac{\sqrt{2}}{4} & -\frac{\sqrt{2}}{4} & \frac{\sqrt{2}}{4} & \frac{\sqrt{2}}{4} & -\frac{\sqrt{2}}{4} \end{pmatrix}$
$\mathbb{Y}_{15}$	$\mathbb{Q}_{2,1}^{(b,E_g)}$	B_2	$\begin{pmatrix} \frac{\sqrt{2}}{4} & -\frac{\sqrt{2}}{4} & -\frac{\sqrt{2}}{4} & \frac{\sqrt{2}}{4} & -\frac{\sqrt{2}}{4} & \frac{\sqrt{2}}{4} & -\frac{\sqrt{2}}{4} & \frac{\sqrt{2}}{4} \end{pmatrix}$
$\mathbb{Y}_{16}$	$\mathbb{T}_0^{(b,A_{1g})}$	B_2	$\begin{pmatrix} \frac{\sqrt{2}i}{4} & \frac{\sqrt{2}i}{4} & \frac{\sqrt{2}i}{4} & \frac{\sqrt{2}i}{4} & \frac{\sqrt{2}i}{4} & \frac{\sqrt{2}i}{4} & \frac{\sqrt{2}i}{4} & \frac{\sqrt{2}i}{4} \end{pmatrix}$
$\mathbb{Y}_{17}$	$\mathbb{T}_2^{(b,B_{2g})}$	B_2	$\begin{pmatrix} \frac{\sqrt{2}i}{4} & \frac{\sqrt{2}i}{4} & -\frac{\sqrt{2}i}{4} & -\frac{\sqrt{2}i}{4} & \frac{\sqrt{2}i}{4} & \frac{\sqrt{2}i}{4} & -\frac{\sqrt{2}i}{4} & -\frac{\sqrt{2}i}{4} \end{pmatrix}$
$\mathbb{Y}_{18}$	$\mathbb{T}_{2,0}^{(b,E_g)}$	B_2	$\begin{pmatrix} \frac{\sqrt{2}i}{4} & -\frac{\sqrt{2}i}{4} & \frac{\sqrt{2}i}{4} & -\frac{\sqrt{2}i}{4} & -\frac{\sqrt{2}i}{4} & \frac{\sqrt{2}i}{4} & \frac{\sqrt{2}i}{4} & -\frac{\sqrt{2}i}{4} \end{pmatrix}$
$\mathbb{Y}_{19}$	$\mathbb{T}_{2,1}^{(b,E_g)}$	B_2	$\begin{pmatrix} \frac{\sqrt{2}i}{4} & -\frac{\sqrt{2}i}{4} & -\frac{\sqrt{2}i}{4} & \frac{\sqrt{2}i}{4} & -\frac{\sqrt{2}i}{4} & \frac{\sqrt{2}i}{4} & -\frac{\sqrt{2}i}{4} & \frac{\sqrt{2}i}{4} \end{pmatrix}$
$\mathbb{Y}_{20}$	$\mathbb{Q}_0^{(b,A_{1g})}$	B_3	$\begin{pmatrix} \frac{\sqrt{2}}{4} & \frac{\sqrt{2}}{4} & \frac{\sqrt{2}}{4} & \frac{\sqrt{2}}{4} & \frac{\sqrt{2}}{4} & \frac{\sqrt{2}}{4} & \frac{\sqrt{2}}{4} & \frac{\sqrt{2}}{4} \end{pmatrix}$
$\mathbb{Y}_{21}$	$\mathbb{Q}_2^{(b,B_{1g})}$	B_3	$\begin{pmatrix} \frac{\sqrt{2}}{4} & \frac{\sqrt{2}}{4} & \frac{\sqrt{2}}{4} & \frac{\sqrt{2}}{4} & -\frac{\sqrt{2}}{4} & -\frac{\sqrt{2}}{4} & -\frac{\sqrt{2}}{4} & -\frac{\sqrt{2}}{4} \end{pmatrix}$
$\mathbb{Y}_{22}$	$\mathbb{Q}_{2,0}^{(b,E_g)}$	B_3	$\begin{pmatrix} \frac{1}{2} & -\frac{1}{2} & \frac{1}{2} & -\frac{1}{2} & 0 & 0 & 0 & 0 \end{pmatrix}$
$\mathbb{Y}_{23}$	$\mathbb{Q}_{2,1}^{(b,E_g)}$	B_3	$\begin{pmatrix} 0 & 0 & 0 & 0 & -\frac{1}{2} & \frac{1}{2} & -\frac{1}{2} & \frac{1}{2} \end{pmatrix}$
$\mathbb{Y}_{24}$	$\mathbb{T}_0^{(b,A_{1g})}$	B_3	$\begin{pmatrix} \frac{\sqrt{2}i}{4} & \frac{\sqrt{2}i}{4} & \frac{\sqrt{2}i}{4} & \frac{\sqrt{2}i}{4} & \frac{\sqrt{2}i}{4} & \frac{\sqrt{2}i}{4} & \frac{\sqrt{2}i}{4} & \frac{\sqrt{2}i}{4} \end{pmatrix}$
$\mathbb{Y}_{25}$	$\mathbb{T}_2^{(b,B_{1g})}$	B_3	$\begin{pmatrix} \frac{\sqrt{2}i}{4} & \frac{\sqrt{2}i}{4} & \frac{\sqrt{2}i}{4} & \frac{\sqrt{2}i}{4} & -\frac{\sqrt{2}i}{4} & -\frac{\sqrt{2}i}{4} & -\frac{\sqrt{2}i}{4} & -\frac{\sqrt{2}i}{4} \end{pmatrix}$
$\mathbb{Y}_{26}$	$\mathbb{T}_{2,0}^{(b,E_g)}$	B_3	$\begin{pmatrix} \frac{i}{2} & -\frac{i}{2} & \frac{i}{2} & -\frac{i}{2} & 0 & 0 & 0 & 0 \end{pmatrix}$
$\mathbb{Y}_{27}$	$\mathbb{T}_{2,1}^{(b,E_g)}$	B_3	$\begin{pmatrix} 0 & 0 & 0 & 0 & -\frac{i}{2} & \frac{i}{2} & -\frac{i}{2} & \frac{i}{2} \end{pmatrix}$

Table 8: Polar harmonics.

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

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	$\mathbb{G}_3^{(B_{1g})}$	3	B_{1g}	–	–	$\sqrt{15}XYZ$
4	$\mathbb{G}_3^{(B_{2g})}$	3	B_{2g}	–	–	$\frac{\sqrt{15}Z(X-Y)(X+Y)}{2}$
5	$\mathbb{G}_{3,0}^{(E_g,1)}$	3	E_g	1	0	$\frac{X\left(2X^2-3Y^2-3Z^2\right)}{2}$
6	$\mathbb{G}_{3,1}^{(E_g,1)}$	3	E_g	1	1	$-\frac{Y\left(3X^2-2Y^2+3Z^2\right)}{2}$
7	$\mathbb{G}_{3,0}^{(E_g,2)}$	3	E_g	2	0	$\frac{\sqrt{15}X(Y-Z)(Y+Z)}{2}$
8	$\mathbb{G}_{3,1}^{(E_g,2)}$	3	E_g	2	1	$\frac{\sqrt{15}Y(X-Z)(X+Z)}{2}$

- Group info.: Generator = $\{2_{001}|\frac{1}{2}\frac{1}{2}0\}$, $\{4^+_{001}|\frac{1}{2}00\}$, $\{2_{010}|0\frac{1}{2}0\}$, $\{-1|0\}$

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

rep. SO	symmetry operations
$\{1\|0\}$	$\{1\|0\}$
$\{2_{001}\|\frac{1}{2}\frac{1}{2}0\}$	$\{2_{001}\|\frac{1}{2}\frac{1}{2}0\}$
$\{2_{100}\|\frac{1}{2}00\}$	$\{2_{100}\|\frac{1}{2}00\},\ \{2_{010}\|0\frac{1}{2}0\}$
$\{2_{110}\|\frac{1}{2}\frac{1}{2}0\}$	$\{2_{110}\|\frac{1}{2}\frac{1}{2}0\},\ \{2_{1-10}\|0\}$
$\{4^{+}_{001}\|\frac{1}{2}00\}$	$\{4^{+}_{001}\|\frac{1}{2}00\},\ \{4^{-}_{001}\|0\frac{1}{2}0\}$
$\{-1\|0\}$	$\{-1\|0\}$
$\{\mathrm{m}_{001}\|\frac{1}{2}\frac{1}{2}0\}$	$\{\mathrm{m}_{001}\|\frac{1}{2}\frac{1}{2}0\}$
$\{\mathrm{m}_{100}\|\frac{1}{2}00\}$	$\{\mathrm{m}_{100}\|\frac{1}{2}00\},\ \{\mathrm{m}_{010}\|0\frac{1}{2}0\}$
$\{\mathrm{m}_{110}\|\frac{1}{2}\frac{1}{2}0\}$	$\{\mathrm{m}_{110}\|\frac{1}{2}\frac{1}{2}0\},\ \{\mathrm{m}_{1-10}\|0\}$
$\{-4^{+}_{001}\|\frac{1}{2}00\}$	$\{-4^{+}_{001}\|\frac{1}{2}00\},\ \{-4^{-}_{001}\|0\frac{1}{2}0\}$

Table 11: Symmetry operations.

No.	SO	No.	SO	No.	SO	No.	SO	No.	SO
1	$\{1\|0\}$	2	$\{2_{001}\|\frac{1}{2}\frac{1}{2}0\}$	3	$\{2_{100}\|\frac{1}{2}00\}$	4	$\{2_{010}\|0\frac{1}{2}0\}$	5	$\{2_{110}\|\frac{1}{2}\frac{1}{2}0\}$
6	$\{2_{1-10}\|0\}$	7	$\{4^{+}_{001}\|\frac{1}{2}00\}$	8	$\{4^{-}_{001}\|0\frac{1}{2}0\}$	9	$\{-1\|0\}$	10	$\{\mathrm{m}_{001}\|\frac{1}{2}\frac{1}{2}0\}$
11	$\{\mathrm{m}_{100}\|\frac{1}{2}00\}$	12	$\{\mathrm{m}_{010}\|0\frac{1}{2}0\}$	13	$\{\mathrm{m}_{110}\|\frac{1}{2}\frac{1}{2}0\}$	14	$\{\mathrm{m}_{1-10}\|0\}$	15	$\{-4^{+}_{001}\|\frac{1}{2}00\}$
16	$\{-4^{-}_{001}\|0\frac{1}{2}0\}$								

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

continued ...

Table 12

	1	2_{001}	2_{100}	2_{110}	4^+_{001}	-1	m_{001}	m_{100}	m_{110}	-4^+_{001}
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
$\mathbb{Q}_0^{(A_{1g})}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$
	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$				
$\mathbb{Q}_1^{(A_{2u})}$	$\frac{1}{4}$	$\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$
	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$				
$\mathbb{Q}_{1,0}^{(E_u)}$	$\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{10}$
	$-\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{20}$				
$\mathbb{Q}_{1,1}^{(E_u)}$	$\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{20}$
	$\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{10}$				
$\mathbb{Q}_2^{(B_{1g})}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$
	$\frac{1}{4}$	$\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$				

continued ...

Table 17

symbol	1	2	3	4	5	6	7	8	9	10
$\mathbb{Q}_2^{(B_{2g})}$	$\frac{1}{4}$	$\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$
	$-\frac{1}{4}$	$-\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$				
$\mathbb{Q}_{2,0}^{(E_g)}$	$\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{20}$
	$\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{10}$				
$\mathbb{Q}_{2,1}^{(E_g)}$	$\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{10}$
	$-\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{20}$				
$\mathbb{Q}_3^{(B_{1u})}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$
	$-\frac{1}{4}$	$-\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$				
$\mathbb{Q}_3^{(B_{2u})}$	$\frac{1}{4}$	$\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$
	$\frac{1}{4}$	$\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$				
$\mathbb{Q}_{3,0}^{(E_u,1)}$	$\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{20}$
	$-\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{10}$				
$\mathbb{Q}_{3,1}^{(E_u,1)}$	$-\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{10}$
	$-\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{20}$				
$\mathbb{Q}_4^{(A_{2g})}$	$\frac{1}{4}$	$\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$
	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$				
$\mathbb{Q}_{4,0}^{(E_g,1)}$	$-\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{10}$
	$-\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{20}$				
$\mathbb{Q}_{4,1}^{(E_g,1)}$	$\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{20}$
	$-\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{10}$				
$\mathbb{Q}_5^{(A_{1u})}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$
	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$				