

SAMB for “BCT”

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- Group: No. 139 D_{4h}^{17} $I4/mmm$ [tetragonal]
 - Associated point group: No. 15 D_{4h} $4/mmm$ [tetragonal]
 - Generation condition
 - model type: **tight_binding**
 - time-reversal type: **electric**
 - irrep: **[A1g]**
 - **spinful**
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- Unit cell:
 $a = 1.0$, $b = 1.0$, $c = 2.32$, $\alpha = 90.0$, $\beta = 90.0$, $\gamma = 90.0$
- Lattice vectors:
 $\mathbf{a}_1 = (1.0 \ 0 \ 0)$
 $\mathbf{a}_2 = (0 \ 1.0 \ 0)$
 $\mathbf{a}_3 = (0 \ 0 \ 2.32)$
- Plus sets:
 $+(0 \ 0 \ 0)$
 $+(\frac{1}{2} \ \frac{1}{2} \ \frac{1}{2})$

Table 1: High-symmetry line: Γ -X.

	symbol	position		symbol	position
	Γ	$(0 \ 0 \ 0)$		X	$(\frac{1}{2} \ 0 \ 0)$

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- Kets: dimension = 6

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	$(p_y, \downarrow)@A_1$								

- Sites in (primitive) unit cell:

Table 3: Site-clusters.

site	position	mapping
S ₁ A ₁	$\begin{pmatrix} 0 & 0 & 0 \end{pmatrix}$	[1,2,3,4,5,6,7,8,9,10,11,12,13,14,15,16]

- Bonds in (primitive) unit cell:

Table 4: Bond-clusters.

bond	tail	head	n	#	$\mathbf{b@c}$	mapping	
B ₁	b ₁	A ₁	A ₁	1	1	$\begin{pmatrix} 1 & 0 & 0 \end{pmatrix} @ \begin{pmatrix} \frac{1}{2} & 0 & 0 \end{pmatrix}$	[1,-2,3,-4,-9,10,-11,12]
	b ₂	A ₁	A ₁	1	1	$\begin{pmatrix} 0 & 1 & 0 \end{pmatrix} @ \begin{pmatrix} 0 & \frac{1}{2} & 0 \end{pmatrix}$	[5,-6,7,-8,-13,14,-15,16]
B ₂	b ₃	A ₁	A ₁	2	1	$\begin{pmatrix} \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \end{pmatrix} @ \begin{pmatrix} \frac{1}{4} & \frac{1}{4} & \frac{1}{4} \end{pmatrix}$	[1,-6,-9,14]
	b ₄	A ₁	A ₁	2	1	$\begin{pmatrix} \frac{1}{2} & \frac{1}{2} & -\frac{1}{2} \end{pmatrix} @ \begin{pmatrix} \frac{1}{4} & \frac{1}{4} & \frac{3}{4} \end{pmatrix}$	[-2,5,10,-13]
	b ₅	A ₁	A ₁	2	1	$\begin{pmatrix} -\frac{1}{2} & \frac{1}{2} & \frac{1}{2} \end{pmatrix} @ \begin{pmatrix} \frac{3}{4} & \frac{1}{4} & \frac{1}{4} \end{pmatrix}$	[-3,7,11,-15]
	b ₆	A ₁	A ₁	2	1	$\begin{pmatrix} \frac{1}{2} & -\frac{1}{2} & \frac{1}{2} \end{pmatrix} @ \begin{pmatrix} \frac{1}{4} & \frac{3}{4} & \frac{1}{4} \end{pmatrix}$	[-4,8,12,-16]
B ₃	b ₇	A ₁	A ₁	7	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]

- SAMB:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

$$\hat{\mathbb{Z}}_7 = \mathbb{X}_4[\mathbb{Q}_2^{(a,B_{1g})}] \otimes \mathbb{Y}_3[\mathbb{Q}_2^{(b,B_{1g})}]$$

$$\hat{\mathbb{Z}}_7(\mathbf{k}) = \mathbb{X}_4[\mathbb{Q}_2^{(a,B_{1g})}] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_{1g})}] \otimes \mathbb{F}_2[\mathbb{Q}_2^{(k,B_{1g})}]$$

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

$$\hat{\mathbb{Z}}_8 = \mathbb{X}_1[\mathbb{Q}_0^{(a,A_{1g})}] \otimes \mathbb{Y}_4[\mathbb{Q}_0^{(b,A_{1g})}]$$

$$\hat{\mathbb{Z}}_8(\mathbf{k}) = \mathbb{X}_1[\mathbb{Q}_0^{(a,A_{1g})}] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_{1g})}] \otimes \mathbb{F}_3[\mathbb{Q}_0^{(k,A_{1g})}]$$

$$\boxed{\text{No. 9}} \quad \hat{\mathbb{Q}}_0^{(A_{1g})} [\text{M}_3, \text{B}_2]$$

$$\hat{\mathbb{Z}}_9 = \mathbb{X}_2[\mathbb{Q}_0^{(a,A_{1g})}] \otimes \mathbb{Y}_4[\mathbb{Q}_0^{(b,A_{1g})}]$$

$$\hat{\mathbb{Z}}_9(\mathbf{k}) = \mathbb{X}_2[\mathbb{Q}_0^{(a,A_{1g})}] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_{1g})}] \otimes \mathbb{F}_3[\mathbb{Q}_0^{(k,A_{1g})}]$$

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

$$\hat{\mathbb{Z}}_{10} = \mathbb{X}_3[\mathbb{Q}_0^{(a,A_{1g})}(1,1)] \otimes \mathbb{Y}_4[\mathbb{Q}_0^{(b,A_{1g})}]$$

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

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

$$\hat{\mathbb{Z}}_{11} = \mathbb{X}_5[\mathbb{Q}_2^{(a,B_{2g})}] \otimes \mathbb{Y}_5[\mathbb{Q}_2^{(b,B_{2g})}]$$

$$\hat{\mathbb{Z}}_{11}(\mathbf{k}) = \mathbb{X}_5[\mathbb{Q}_2^{(a,B_{2g})}] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_{1g})}] \otimes \mathbb{F}_4[\mathbb{Q}_2^{(k,B_{2g})}]$$

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

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

$$\hat{Z}_{12}(\mathbf{k}) = \frac{\sqrt{2}\mathbb{X}_6[\mathbb{Q}_{2,0}^{(a,E_g)}(1,-1)] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_{1g})}] \otimes \mathbb{F}_5[\mathbb{Q}_{2,0}^{(k,E_g)}]}{2} + \frac{\sqrt{2}\mathbb{X}_7[\mathbb{Q}_{2,1}^{(a,E_g)}(1,-1)] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_{1g})}] \otimes \mathbb{F}_6[\mathbb{Q}_{2,1}^{(k,E_g)}]}{2}$$

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

$$\hat{Z}_{13} = \mathbb{X}_1[\mathbb{Q}_0^{(a,A_{1g})}] \otimes \mathbb{Y}_8[\mathbb{Q}_0^{(b,A_{1g})}]$$

$$\hat{Z}_{13}(\mathbf{k}) = \mathbb{X}_1[\mathbb{Q}_0^{(a,A_{1g})}] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_{1g})}] \otimes \mathbb{F}_7[\mathbb{Q}_0^{(k,A_{1g})}]$$

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

$$\hat{Z}_{14} = \mathbb{X}_2[\mathbb{Q}_0^{(a,A_{1g})}] \otimes \mathbb{Y}_8[\mathbb{Q}_0^{(b,A_{1g})}]$$

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

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

$$\hat{Z}_{15} = \mathbb{X}_3[\mathbb{Q}_0^{(a,A_{1g})}(1,1)] \otimes \mathbb{Y}_8[\mathbb{Q}_0^{(b,A_{1g})}]$$

$$\hat{Z}_{15}(\mathbf{k}) = \mathbb{X}_3[\mathbb{Q}_0^{(a,A_{1g})}(1,1)] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_{1g})}] \otimes \mathbb{F}_7[\mathbb{Q}_0^{(k,A_{1g})}]$$

Table 5: Atomic SAMB group.

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

Table 6: Atomic SAMB.

symbol	type	group	form
\mathbb{X}_1	$\mathbb{Q}_0^{(a,A_{1g})}$	M_1	$\begin{pmatrix} \frac{\sqrt{2}}{2} & 0 \\ 0 & \frac{\sqrt{2}}{2} \end{pmatrix}$
\mathbb{X}_2	$\mathbb{Q}_0^{(a,A_{1g})}$	M_3	$\begin{pmatrix} \frac{1}{2} & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 \\ 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & \frac{1}{2} \end{pmatrix}$
\mathbb{X}_3	$\mathbb{Q}_0^{(a,A_{1g})}(1,1)$	M_3	$\begin{pmatrix} 0 & 0 & -\frac{i}{2} & 0 \\ 0 & 0 & 0 & \frac{i}{2} \\ \frac{i}{2} & 0 & 0 & 0 \\ 0 & -\frac{i}{2} & 0 & 0 \end{pmatrix}$
\mathbb{X}_4	$\mathbb{Q}_2^{(a,B_{1g})}$	M_3	$\begin{pmatrix} \frac{1}{2} & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 \\ 0 & 0 & -\frac{1}{2} & 0 \\ 0 & 0 & 0 & -\frac{1}{2} \end{pmatrix}$
\mathbb{X}_5	$\mathbb{Q}_2^{(a,B_{2g})}$	M_3	$\begin{pmatrix} 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & \frac{1}{2} \\ \frac{1}{2} & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 \end{pmatrix}$
\mathbb{X}_6	$\mathbb{Q}_{2,0}^{(a,E_g)}(1,-1)$	M_3	$\begin{pmatrix} 0 & 0 & 0 & -\frac{1}{2} \\ 0 & 0 & \frac{1}{2} & 0 \\ 0 & \frac{1}{2} & 0 & 0 \\ -\frac{1}{2} & 0 & 0 & 0 \end{pmatrix}$
\mathbb{X}_7	$\mathbb{Q}_{2,1}^{(a,E_g)}(1,-1)$	M_3	$\begin{pmatrix} 0 & 0 & 0 & -\frac{i}{2} \\ 0 & 0 & -\frac{i}{2} & 0 \\ 0 & \frac{i}{2} & 0 & 0 \\ \frac{i}{2} & 0 & 0 & 0 \end{pmatrix}$

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	$\mathbb{Q}_0^{(b, A_{1g})}$	B_2	$\begin{pmatrix} \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \end{pmatrix}$
\mathbb{Y}_5	$\mathbb{Q}_2^{(b, B_{2g})}$	B_2	$\begin{pmatrix} \frac{1}{2} & \frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} \end{pmatrix}$
\mathbb{Y}_6	$\mathbb{Q}_{2,0}^{(b, E_g)}$	B_2	$\begin{pmatrix} \frac{1}{2} & -\frac{1}{2} & \frac{1}{2} & -\frac{1}{2} \end{pmatrix}$
\mathbb{Y}_7	$\mathbb{Q}_{2,1}^{(b, E_g)}$	B_2	$\begin{pmatrix} \frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} & \frac{1}{2} \end{pmatrix}$
\mathbb{Y}_8	$\mathbb{Q}_0^{(b, A_{1g})}$	B_3	$\begin{pmatrix} 1 \end{pmatrix}$

Table 8: Uniform SAMB.

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

Table 9: Structure SAMB.

symbol	type	cluster	form
\mathbb{F}_1	$\mathbb{Q}_0^{(k, A_{1g})}$	B_1	$c_{001} + c_{002}$
\mathbb{F}_2	$\mathbb{Q}_2^{(k, B_{1g})}$	B_1	$c_{001} - c_{002}$
\mathbb{F}_3	$\mathbb{Q}_0^{(k, A_{1g})}$	B_2	$\frac{\sqrt{2}c_{003}}{2} + \frac{\sqrt{2}c_{004}}{2} + \frac{\sqrt{2}c_{005}}{2} + \frac{\sqrt{2}c_{006}}{2}$
\mathbb{F}_4	$\mathbb{Q}_2^{(k, B_{2g})}$	B_2	$\frac{\sqrt{2}c_{003}}{2} + \frac{\sqrt{2}c_{004}}{2} - \frac{\sqrt{2}c_{005}}{2} - \frac{\sqrt{2}c_{006}}{2}$
\mathbb{F}_5	$\mathbb{Q}_{2,0}^{(k, E_g)}$	B_2	$\frac{\sqrt{2}c_{003}}{2} - \frac{\sqrt{2}c_{004}}{2} + \frac{\sqrt{2}c_{005}}{2} - \frac{\sqrt{2}c_{006}}{2}$
\mathbb{F}_6	$\mathbb{Q}_{2,1}^{(k, E_g)}$	B_2	$\frac{\sqrt{2}c_{003}}{2} - \frac{\sqrt{2}c_{004}}{2} - \frac{\sqrt{2}c_{005}}{2} + \frac{\sqrt{2}c_{006}}{2}$

\mathbb{F}_7	$\mathbb{Q}_0^{(k, A_{1g})}$	B_3	$\sqrt{2}c_{007}$
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Table 10: Polar harmonics.

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

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

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

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

continued ...

Table 11

rep. SO	symmetry operations
$\{\mathbf{m}_{110} 0\}$	$\{\mathbf{m}_{110} 0\}, \{\mathbf{m}_{1-10} 0\}$
$\{-4_{001}^+ 0\}$	$\{-4_{001}^+ 0\}, \{-4_{001}^- 0\}$

Table 12: Symmetry operations.

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

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

	1	2 ₀₀₁	2 ₁₀₀	2 ₁₁₀	4 ₀₀₁ ⁺	-1	m ₀₀₁	m ₁₀₀	m ₁₁₀	-4 ₀₀₁ ⁺
<i>A</i> _{1g}	1	1	1	1	1	1	1	1	1	1
<i>A</i> _{2g}	1	1	-1	-1	1	1	1	-1	-1	1
<i>B</i> _{1g}	1	1	1	-1	-1	1	1	1	-1	-1
<i>B</i> _{2g}	1	1	-1	1	-1	1	1	-1	1	-1
<i>E</i> _g	2	-2	0	0	0	2	-2	0	0	0
<i>A</i> _{1u}	1	1	1	1	1	-1	-1	-1	-1	-1
<i>A</i> _{2u}	1	1	-1	-1	1	-1	-1	1	1	-1
<i>B</i> _{1u}	1	1	1	-1	-1	-1	-1	-1	1	1
<i>B</i> _{2u}	1	1	-1	1	-1	-1	-1	1	-1	1
<i>E</i> _u	2	-2	0	0	0	-2	2	0	0	0

Table 14: 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 15: 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 16: 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 17: 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 18: Virtual-cluster basis.

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

continued ...

Table 18

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