SAMB for "BCT"

- 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`

- Unit cell:
    $a = 1.0,\ b = 1.0,\ c = 2.32,\ \alpha = 90.0,\ \beta = 90.0,\ \gamma = 90.0$
- Lattice vectors:
    $\boldsymbol{a}_1 = \begin{pmatrix} 1.0 & 0 & 0 \end{pmatrix}$
    $\boldsymbol{a}_2 = \begin{pmatrix} 0 & 1.0 & 0 \end{pmatrix}$
    $\boldsymbol{a}_3 = \begin{pmatrix} 0 & 0 & 2.32 \end{pmatrix}$
- Plus sets:
    $+ \begin{pmatrix} 0 & 0 & 0 \end{pmatrix}$
    $+ \begin{pmatrix} \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \end{pmatrix}$

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 = 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 [2a: 4/mmm]	A_1	$\begin{pmatrix} 0 & 0 & 0 \end{pmatrix}$	[1,2,3,4,5,6,7,8,9,10,11,12,13,14,15,16]

- Bonds in (primitive) unit cell:

Table 4: Bond-clusters.

	bond	tail	head	n	#	$b@c$	mapping
B_1 [4c: 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,-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 [8f: ..2/m]	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 [2b: 4/mmm]	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:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

No. 13 $\hat{\mathbb{Q}}_0^{(A_{1g})}$ [$\mathrm{M_1, B_3}$]

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

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

No. 14 $\hat{\mathbb{Q}}_0^{(A_{1g})}$ [$\mathrm{M_3, B_3}$]

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

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

No. 15 $\hat{\mathbb{Q}}_0^{(A_{1g})}(1,1)$ [$\mathrm{M_3, B_3}$]

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

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

Table 5: Atomic SAMB group.

group	bra	ket
$\mathrm{M_1}$	$(s,\uparrow),(s,\downarrow)$	$(s,\uparrow),(s,\downarrow)$
$\mathrm{M_2}$	$(s,\uparrow),(s,\downarrow)$	$(p_x,\uparrow),(p_x,\downarrow),(p_y,\uparrow),(p_y,\downarrow)$
$\mathrm{M_3}$	$(p_x,\uparrow),(p_x,\downarrow),(p_y,\uparrow),(p_y,\downarrow)$	$(p_x,\uparrow),(p_x,\downarrow),(p_y,\uparrow),(p_y,\downarrow)$

Table 6: Atomic SAMB.

symbol	type	group	form
$\mathbb{X}_1$	$\mathbb{Q}_0^{(a,A_{1g})}$	M_1	$\begin{pmatrix} \frac{\sqrt{2}}{2} & 0 \\ 0 & \frac{\sqrt{2}}{2} \end{pmatrix}$
$\mathbb{X}_2$	$\mathbb{Q}_0^{(a,A_{1g})}$	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$_1$	$\left(\begin{matrix} \frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2} \end{matrix}\right)$
$\mathbb{Y}_3$	$\mathbb{Q}_2^{(b,B_{1g})}$	B$_1$	$\left(\begin{matrix} \frac{\sqrt{2}}{2} & -\frac{\sqrt{2}}{2} \end{matrix}\right)$
$\mathbb{Y}_4$	$\mathbb{Q}_0^{(b,A_{1g})}$	B$_2$	$\left(\begin{matrix} \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \end{matrix}\right)$
$\mathbb{Y}_5$	$\mathbb{Q}_2^{(b,B_{2g})}$	B$_2$	$\left(\begin{matrix} \frac{1}{2} & \frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} \end{matrix}\right)$
$\mathbb{Y}_6$	$\mathbb{Q}_{2,0}^{(b,E_g)}$	B$_2$	$\left(\begin{matrix} \frac{1}{2} & -\frac{1}{2} & \frac{1}{2} & -\frac{1}{2} \end{matrix}\right)$
$\mathbb{Y}_7$	$\mathbb{Q}_{2,1}^{(b,E_g)}$	B$_2$	$\left(\begin{matrix} \frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} & \frac{1}{2} \end{matrix}\right)$
$\mathbb{Y}_8$	$\mathbb{Q}_0^{(b,A_{1g})}$	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	$\sqrt{2}c_{007}$

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
$\{m_{110}|0\}$	$\{m_{110}|0\}$, $\{m_{1-10}|0\}$
$\{-4^{+}_{001}|0\}$	$\{-4^{+}_{001}|0\}$, $\{-4^{-}_{001}|0\}$

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	$\{m_{001}|0\}$
11	$\{m_{100}|0\}$	12	$\{m_{010}|0\}$	13	$\{m_{110}|0\}$	14	$\{m_{1-10}|0\}$	15	$\{-4^{+}_{001}|0\}$
16	$\{-4^{-}_{001}|0\}$								

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

	1	2_{001}	2_{100}	2_{110}	4^{+}_{001}	-1	m_{001}	m_{100}	m_{110}	-4^{+}_{001}
A_{1g}	1	1	1	1	1	1	1	1	1	1
A_{2g}	1	1	-1	-1	1	1	1	-1	-1	1
B_{1g}	1	1	1	-1	-1	1	1	1	-1	-1
B_{2g}	1	1	-1	1	-1	1	1	-1	1	-1
E_g	2	-2	0	0	0	2	-2	0	0	0
A_{1u}	1	1	1	1	1	-1	-1	-1	-1	-1
A_{2u}	1	1	-1	-1	1	-1	-1	1	1	-1
B_{1u}	1	1	1	-1	-1	-1	-1	-1	1	1
B_{2u}	1	1	-1	1	-1	-1	-1	1	-1	1
E_u	2	-2	0	0	0	-2	2	0	0	0

Table 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	$(2 \quad 1 \quad 1)$	2	$(-2 \quad -1 \quad 1)$	3	$(2 \quad -1 \quad -1)$	4	$(-2 \quad 1 \quad -1)$
5	$(1 \quad 2 \quad -1)$	6	$(-1 \quad -2 \quad -1)$	7	$(-1 \quad 2 \quad 1)$	8	$(1 \quad -2 \quad 1)$
9	$(-2 \quad -1 \quad -1)$	10	$(2 \quad 1 \quad -1)$	11	$(-2 \quad 1 \quad 1)$	12	$(2 \quad -1 \quad 1)$
13	$(-1 \quad -2 \quad 1)$	14	$(1 \quad 2 \quad 1)$	15	$(1 \quad -2 \quad -1)$	16	$(-1 \quad 2 \quad -1)$

Table 18: Virtual-cluster basis.

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

continued ...

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Table 18

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