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`

- 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	#	$\boldsymbol{b}$@$\boldsymbol{c}$	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:

$\boxed{\text{No. 1}}$ $\hat{\mathbb{Q}}_{0}^{(A_{1g})}$ $[\mathrm{M}_1, \mathrm{S}_1]$

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

$\boxed{\text{No. 2}}$ $\hat{\mathbb{Q}}_{0}^{(A_{1g})}$ $[\mathrm{M}_3, \mathrm{S}_1]$

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

$\boxed{\text{No. 3}}$ $\hat{\mathbb{Q}}_{0}^{(A_{1g})}(1,1)$ $[\mathrm{M}_3, \mathrm{S}_1]$

$$\hat{\mathbb{Z}}_{3} = \mathbb{X}_{9}[\mathbb{Q}_{0}^{(a,A_{1g})}(1,1)] \otimes \mathbb{Y}_{1}[\mathbb{Q}_{0}^{(s,A_{1g})}]$$

$\boxed{\text{No. 4}}$ $\hat{\mathbb{Q}}_{0}^{(A_{1g})}$ $[\mathrm{M}_1, \mathrm{B}_1]$

$$\hat{\mathbb{Z}}_{4} = \mathbb{X}_{1}[\mathbb{Q}_{0}^{(a,A_{1g})}] \otimes \mathbb{Y}_{2}[\mathbb{Q}_{0}^{(b,A_{1g})}]$$

$\boxed{\text{No. 5}}$ $\hat{\mathbb{Q}}_{2}^{(A_{1g})}(1,-1)$ $[\mathrm{M}_2, \mathrm{B}_1]$

$$\hat{\mathbb{Z}}_{5} = -\frac{\sqrt{2}\mathbb{X}_{3}[\mathbb{M}_{2,0}^{(a,E_{u})}(1,-1)] \otimes \mathbb{Y}_{4}[\mathbb{T}_{1,0}^{(b,E_{u})}]}{2} + \frac{\sqrt{2}\mathbb{X}_{4}[\mathbb{M}_{2,1}^{(a,E_{u})}(1,-1)] \otimes \mathbb{Y}_{5}[\mathbb{T}_{1,1}^{(b,E_{u})}]}{2}$$

$\boxed{\text{No. 6}}$ $\hat{\mathbb{Q}}_{0}^{(A_{1g})}$ $[\mathrm{M}_2, \mathrm{B}_1]$

$$\hat{\mathbb{Z}}_{6} = \frac{\sqrt{2}\mathbb{X}_{5}[\mathbb{T}_{1,0}^{(a,E_{u})}] \otimes \mathbb{Y}_{4}[\mathbb{T}_{1,0}^{(b,E_{u})}]}{2} + \frac{\sqrt{2}\mathbb{X}_{6}[\mathbb{T}_{1,1}^{(a,E_{u})}] \otimes \mathbb{Y}_{5}[\mathbb{T}_{1,1}^{(b,E_{u})}]}{2}$$

$\boxed{\text{No. 7}}$ $\hat{\mathbb{Q}}_{0}^{(A_{1g})}$ $[\mathrm{M}_3, \mathrm{B}_1]$

$$\hat{\mathbb{Z}}_{7} = \mathbb{X}_{8}[\mathbb{Q}_{0}^{(a,A_{1g})}] \otimes \mathbb{Y}_{2}[\mathbb{Q}_{0}^{(b,A_{1g})}]$$

$\boxed{\text{No. 8}}$ $\hat{\mathbb{Q}}_{0}^{(A_{1g})}(1,1)$ $[\mathrm{M}_3, \mathrm{B}_1]$

$$\hat{\mathbb{Z}}_{8} = \mathbb{X}_{9}[\mathbb{Q}_{0}^{(a,A_{1g})}(1,1)] \otimes \mathbb{Y}_{2}[\mathbb{Q}_{0}^{(b,A_{1g})}]$$

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

$$\hat{\mathbb{Z}}_9 = \mathbb{X}_{10}[\mathbb{Q}_2^{(a,B_{1g})}] \otimes \mathbb{Y}_3[\mathbb{Q}_2^{(b,B_{1g})}]$$

$\boxed{\text{No. 10}}$ $\hat{\mathbb{Q}}_0^{(A_{1g})}$ $[\mathrm{M}_1, \mathrm{B}_2]$

$$\hat{\mathbb{Z}}_{10} = \mathbb{X}_1[\mathbb{Q}_0^{(a,A_{1g})}] \otimes \mathbb{Y}_6[\mathbb{Q}_0^{(b,A_{1g})}]$$

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

$$\hat{\mathbb{Z}}_{11} = -\frac{\sqrt{2}\mathbb{X}_3[\mathbb{M}_{2,0}^{(a,E_u)}(1,-1)] \otimes \mathbb{Y}_{11}[\mathbb{T}_{1,0}^{(b,E_u)}]}{2} + \frac{\sqrt{2}\mathbb{X}_4[\mathbb{M}_{2,1}^{(a,E_u)}(1,-1)] \otimes \mathbb{Y}_{12}[\mathbb{T}_{1,1}^{(b,E_u)}]}{2}$$

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

$$\hat{\mathbb{Z}}_{12} = \mathbb{X}_2[\mathbb{M}_2^{(a,B_{1u})}(1,-1)] \otimes \mathbb{Y}_{13}[\mathbb{T}_3^{(b,B_{1u})}]$$

$\boxed{\text{No. 13}}$ $\hat{\mathbb{Q}}_0^{(A_{1g})}$ $[\mathrm{M}_2, \mathrm{B}_2]$

$$\hat{\mathbb{Z}}_{13} = \frac{\sqrt{2}\mathbb{X}_5[\mathbb{T}_{1,0}^{(a,E_u)}] \otimes \mathbb{Y}_{11}[\mathbb{T}_{1,0}^{(b,E_u)}]}{2} + \frac{\sqrt{2}\mathbb{X}_6[\mathbb{T}_{1,1}^{(a,E_u)}] \otimes \mathbb{Y}_{12}[\mathbb{T}_{1,1}^{(b,E_u)}]}{2}$$

$\boxed{\text{No. 14}}$ $\hat{\mathbb{Q}}_0^{(A_{1g})}(1,0)$ $[\mathrm{M}_2, \mathrm{B}_2]$

$$\hat{\mathbb{Z}}_{14} = \mathbb{X}_7[\mathbb{T}_1^{(a,A_{2u})}(1,0)] \otimes \mathbb{Y}_{10}[\mathbb{T}_1^{(b,A_{2u})}]$$

$\boxed{\text{No. 15}}$ $\hat{\mathbb{Q}}_0^{(A_{1g})}$ $[\mathrm{M}_3, \mathrm{B}_2]$

$$\hat{\mathbb{Z}}_{15} = \mathbb{X}_8[\mathbb{Q}_0^{(a,A_{1g})}] \otimes \mathbb{Y}_6[\mathbb{Q}_0^{(b,A_{1g})}]$$

$\boxed{\text{No. 16}}$ $\hat{\mathbb{Q}}_0^{(A_{1g})}(1,1)$ $[\mathrm{M}_3, \mathrm{B}_2]$

$$\hat{\mathbb{Z}}_{16} = \mathbb{X}_9[\mathbb{Q}_0^{(a,A_{1g})}(1,1)] \otimes \mathbb{Y}_6[\mathbb{Q}_0^{(b,A_{1g})}]$$

$\boxed{\text{No. 17}}$ $\hat{\mathbb{Q}}_0^{(A_{1g})}$ $[\mathrm{M}_3, \mathrm{B}_2]$

$$\hat{\mathbb{Z}}_{17} = \mathbb{X}_{11}[\mathbb{Q}_2^{(a,B_{2g})}] \otimes \mathbb{Y}_7[\mathbb{Q}_2^{(b,B_{2g})}]$$

$\boxed{\text{No. 18}}$ $\hat{\mathbb{Q}}_0^{(A_{1g})}(1,-1)$ $[\mathrm{M}_3, \mathrm{B}_2]$

$$\hat{\mathbb{Z}}_{18} = \frac{\sqrt{2}\mathbb{X}_{12}[\mathbb{Q}_{2,0}^{(a,E_g)}(1,-1)] \otimes \mathbb{Y}_8[\mathbb{Q}_{2,0}^{(b,E_g)}]}{2} + \frac{\sqrt{2}\mathbb{X}_{13}[\mathbb{Q}_{2,1}^{(a,E_g)}(1,-1)] \otimes \mathbb{Y}_9[\mathbb{Q}_{2,1}^{(b,E_g)}]}{2}$$

$\boxed{\text{No. 19}}$ $\hat{\mathbb{Q}}_0^{(A_{1g})}$ $[\mathrm{M}_1, \mathrm{B}_3]$

$$\hat{\mathbb{Z}}_{19} = \mathbb{X}_1[\mathbb{Q}_0^{(a,A_{1g})}] \otimes \mathbb{Y}_{14}[\mathbb{Q}_0^{(b,A_{1g})}]$$

$\boxed{\text{No. 20}}$ $\hat{\mathbb{Q}}_0^{(A_{1g})}(1,0)$ $[\mathrm{M}_2, \mathrm{B}_3]$

$$\hat{\mathbb{Z}}_{20} = \mathbb{X}_7[\mathbb{T}_1^{(a,A_{2u})}(1,0)] \otimes \mathbb{Y}_{15}[\mathbb{T}_1^{(b,A_{2u})}]$$

$\boxed{\text{No. 21}}$ $\hat{\mathbb{Q}}_0^{(A_{1g})}$ $[\mathrm{M}_3, \mathrm{B}_3]$

$$\hat{\mathbb{Z}}_{21} = \mathbb{X}_8[\mathbb{Q}_0^{(a,A_{1g})}] \otimes \mathbb{Y}_{14}[\mathbb{Q}_0^{(b,A_{1g})}]$$

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

$$\hat{\mathbb{Z}}_{22} = \mathbb{X}_9[\mathbb{Q}_0^{(a,A_{1g})}(1,1)] \otimes \mathbb{Y}_{14}[\mathbb{Q}_0^{(b,A_{1g})}]$$

Table 5: Atomic SAMB group.

group	bra	ket
M_1	$(s,\uparrow),(s,\downarrow)$	$(s,\uparrow),(s,\downarrow)$
M_2	$(s,\uparrow),(s,\downarrow)$	$(p_x,\uparrow),(p_x,\downarrow),(p_y,\uparrow),(p_y,\downarrow)$
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	$\begin{pmatrix} \frac{\sqrt{2}}{2} & 0 \\ 0 & \frac{\sqrt{2}}{2} \end{pmatrix}$
$\mathbb{X}_2$	$\mathbb{M}_2^{(a,B_{1u})}(1,-1)$	M_2	$\begin{pmatrix} 0 & \frac{1}{2} & 0 & \frac{i}{2} \\ \frac{1}{2} & 0 & -\frac{i}{2} & 0 \end{pmatrix}$
$\mathbb{X}_3$	$\mathbb{M}_{2,0}^{(a,E_u)}(1,-1)$	M_2	$\begin{pmatrix} 0 & 0 & \frac{\sqrt{2}}{2} & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{2}}{2} \end{pmatrix}$
$\mathbb{X}_4$	$\mathbb{M}_{2,1}^{(a,E_u)}(1,-1)$	M_2	$\begin{pmatrix} \frac{\sqrt{2}}{2} & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{2}}{2} & 0 & 0 \end{pmatrix}$
$\mathbb{X}_5$	$\mathbb{T}_{1,0}^{(a,E_u)}$	M_2	$\begin{pmatrix} \frac{\sqrt{2}i}{2} & 0 & 0 & 0 \\ 0 & \frac{\sqrt{2}i}{2} & 0 & 0 \end{pmatrix}$
$\mathbb{X}_6$	$\mathbb{T}_{1,1}^{(a,E_u)}$	M_2	$\begin{pmatrix} 0 & 0 & \frac{\sqrt{2}i}{2} & 0 \\ 0 & 0 & 0 & \frac{\sqrt{2}i}{2} \end{pmatrix}$
$\mathbb{X}_7$	$\mathbb{T}_1^{(a,A_{2u})}(1,0)$	M_2	$\begin{pmatrix} 0 & \frac{i}{2} & 0 & \frac{1}{2} \\ -\frac{i}{2} & 0 & \frac{1}{2} & 0 \end{pmatrix}$
$\mathbb{X}_8$	$\mathbb{Q}_0^{(a,A_{1g})}$	M_3	$\begin{pmatrix} \frac{1}{2} & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 \\ 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & \frac{1}{2} \end{pmatrix}$
$\mathbb{X}_9$	$\mathbb{Q}_0^{(a,A_{1g})}(1,1)$	M_3	$\begin{pmatrix} 0 & 0 & -\frac{i}{2} & 0 \\ 0 & 0 & 0 & \frac{i}{2} \\ \frac{i}{2} & 0 & 0 & 0 \\ 0 & -\frac{i}{2} & 0 & 0 \end{pmatrix}$
$\mathbb{X}_{10}$	$\mathbb{Q}_2^{(a,B_{1g})}$	M_3	$\begin{pmatrix} \frac{1}{2} & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 \\ 0 & 0 & -\frac{1}{2} & 0 \\ 0 & 0 & 0 & -\frac{1}{2} \end{pmatrix}$
$\mathbb{X}_{11}$	$\mathbb{Q}_2^{(a,B_{2g})}$	M_3	$\begin{pmatrix} 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & \frac{1}{2} \\ \frac{1}{2} & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 \end{pmatrix}$

continued ...

Table 6

symbol	type	group	form
$\mathbb{X}_{12}$	$\mathbb{Q}_{2,0}^{(a,E_g)}(1,-1)$	M_3	$\begin{pmatrix} 0 & 0 & 0 & -\frac{1}{2} \\ 0 & 0 & \frac{1}{2} & 0 \\ 0 & \frac{1}{2} & 0 & 0 \\ -\frac{1}{2} & 0 & 0 & 0 \end{pmatrix}$
$\mathbb{X}_{13}$	$\mathbb{Q}_{2,1}^{(a,E_g)}(1,-1)$	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	$\begin{pmatrix} \frac{\sqrt{2}}{2} & -\frac{\sqrt{2}}{2} \end{pmatrix}$
$\mathbb{Y}_4$	$\mathbb{T}_{1,0}^{(b,E_u)}$	B_1	$\begin{pmatrix} i & 0 \end{pmatrix}$
$\mathbb{Y}_5$	$\mathbb{T}_{1,1}^{(b,E_u)}$	B_1	$\begin{pmatrix} 0 & i \end{pmatrix}$
$\mathbb{Y}_6$	$\mathbb{Q}_0^{(b,A_{1g})}$	B_2	$\begin{pmatrix} \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \end{pmatrix}$
$\mathbb{Y}_7$	$\mathbb{Q}_2^{(b,B_{2g})}$	B_2	$\begin{pmatrix} \frac{1}{2} & \frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} \end{pmatrix}$
$\mathbb{Y}_8$	$\mathbb{Q}_{2,0}^{(b,E_g)}$	B_2	$\begin{pmatrix} \frac{1}{2} & -\frac{1}{2} & \frac{1}{2} & -\frac{1}{2} \end{pmatrix}$
$\mathbb{Y}_9$	$\mathbb{Q}_{2,1}^{(b,E_g)}$	B_2	$\begin{pmatrix} \frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} & \frac{1}{2} \end{pmatrix}$
$\mathbb{Y}_{10}$	$\mathbb{T}_1^{(b,A_{2u})}$	B_2	$\begin{pmatrix} \frac{i}{2} & -\frac{i}{2} & \frac{i}{2} & \frac{i}{2} \end{pmatrix}$
$\mathbb{Y}_{11}$	$\mathbb{T}_{1,0}^{(b,E_u)}$	B_2	$\begin{pmatrix} \frac{i}{2} & \frac{i}{2} & -\frac{i}{2} & \frac{i}{2} \end{pmatrix}$
$\mathbb{Y}_{12}$	$\mathbb{T}_{1,1}^{(b,E_u)}$	B_2	$\begin{pmatrix} \frac{i}{2} & \frac{i}{2} & \frac{i}{2} & -\frac{i}{2} \end{pmatrix}$
$\mathbb{Y}_{13}$	$\mathbb{T}_3^{(b,B_{1u})}$	B_2	$\begin{pmatrix} \frac{i}{2} & -\frac{i}{2} & -\frac{i}{2} & -\frac{i}{2} \end{pmatrix}$
$\mathbb{Y}_{14}$	$\mathbb{Q}_0^{(b,A_{1g})}$	B_3	$\begin{pmatrix} 1 \end{pmatrix}$
$\mathbb{Y}_{15}$	$\mathbb{T}_1^{(b,A_{2u})}$	B_3	$\begin{pmatrix} i \end{pmatrix}$

Table 8: Polar harmonics.

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

Table 9: Axial harmonics.

No.	symbol	rank	irrep.	mul.	comp.	form
1	$\mathbb{G}_{2}^{(B_{1u})}$	2	B_{1u}	–	–	$\frac{\sqrt{3}(X-Y)(X+Y)}{2}$
2	$\mathbb{G}_{2,0}^{(E_{u})}$	2	E_{u}	–	0	$\sqrt{3}YZ$
3	$\mathbb{G}_{2,1}^{(E_{u})}$	2	E_{u}	–	1	$\sqrt{3}XZ$

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

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

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

Table 11: Symmetry operations.

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

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

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

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