

SAMB for “graphene”

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- Group: No. 191 D_{6h}^1 $P6/mmm$ [hexagonal]
 - Associated point group: No. 27 D_{6h} $6/mmm$ [hexagonal]
 - Generation condition
 - model type: **tight_binding**
 - time-reversal type: **electric**
 - irrep: **[A1g]**
 - **spinless**
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- Unit cell:
 - $a = 1.0$, $b = 1.0$, $c = 4.0$, $\alpha = 90.0$, $\beta = 90.0$, $\gamma = 120.0$
- Lattice vectors:
 - $\mathbf{a}_1 = (1.0 \ 0 \ 0)$
 - $\mathbf{a}_2 = (-0.5 \ 0.86602540378444 \ 0)$
 - $\mathbf{a}_3 = (0 \ 0 \ 4.0)$

Table 1: High-symmetry line: Γ -K-M- Γ .

	symbol	position	symbol	position	symbol	position
	Γ	$\begin{pmatrix} 0 & 0 & 0 \end{pmatrix}$	M	$\begin{pmatrix} \frac{1}{2} & 0 & 0 \end{pmatrix}$	K	$\begin{pmatrix} \frac{1}{3} & \frac{1}{3} & 0 \end{pmatrix}$

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- Kets: dimension = 2

Table 2: Hilbert space for full matrix.

No.	ket	No.	ket
1	$p_z @ C_1$	2	$p_z @ C_2$

- Sites in (primitive) unit cell:

Table 3: Site-clusters.

site	position	mapping
S ₁ [2c: -6m2]	C ₁ $\begin{pmatrix} \frac{1}{3} & \frac{2}{3} & 0 \end{pmatrix}$	[1,6,7,8,9,10,14,15,16,17,23,24]
	C ₂ $\begin{pmatrix} \frac{2}{3} & \frac{1}{3} & 0 \end{pmatrix}$	[2,3,4,5,11,12,13,18,19,20,21,22]

- Bonds in (primitive) unit cell:

Table 4: Bond-clusters.

	bond	tail	head	n	#	$\mathbf{b@c}$	mapping
B ₁ [3f: mmm]	b ₁	C ₁	C ₂	1	1	$\begin{pmatrix} \frac{1}{3} & \frac{2}{3} & 0 \end{pmatrix} @ \begin{pmatrix} \frac{1}{2} & 0 & 0 \end{pmatrix}$	[1,-2,-3,6,-13,14,17,-18]
	b ₂	C ₁	C ₂	1	1	$\begin{pmatrix} \frac{1}{3} & -\frac{1}{3} & 0 \end{pmatrix} @ \begin{pmatrix} \frac{1}{2} & \frac{1}{2} & 0 \end{pmatrix}$	[-4,7,10,-11,15,-19,-22,23]
	b ₃	C ₁	C ₂	1	1	$\begin{pmatrix} -\frac{2}{3} & -\frac{1}{3} & 0 \end{pmatrix} @ \begin{pmatrix} 0 & \frac{1}{2} & 0 \end{pmatrix}$	[-5,8,9,-12,16,-20,-21,24]
B ₂ [6l: mm2]	b ₄	C ₁	C ₁	2	1	$\begin{pmatrix} 0 & 1 & 0 \end{pmatrix} @ \begin{pmatrix} \frac{1}{3} & \frac{1}{6} & 0 \end{pmatrix}$	[1,-7,-15,17]
	b ₅	C ₂	C ₂	2	1	$\begin{pmatrix} 0 & 1 & 0 \end{pmatrix} @ \begin{pmatrix} \frac{2}{3} & \frac{5}{6} & 0 \end{pmatrix}$	[-2,4,-13,19]
	b ₆	C ₂	C ₂	2	1	$\begin{pmatrix} 1 & 1 & 0 \end{pmatrix} @ \begin{pmatrix} \frac{1}{6} & \frac{5}{6} & 0 \end{pmatrix}$	[-3,12,-18,21]
	b ₇	C ₂	C ₂	2	1	$\begin{pmatrix} 1 & 0 & 0 \end{pmatrix} @ \begin{pmatrix} \frac{1}{6} & \frac{1}{3} & 0 \end{pmatrix}$	[5,-11,20,-22]
	b ₈	C ₁	C ₁	2	1	$\begin{pmatrix} 1 & 1 & 0 \end{pmatrix} @ \begin{pmatrix} \frac{5}{6} & \frac{1}{6} & 0 \end{pmatrix}$	[6,-9,14,-24]
	b ₉	C ₁	C ₁	2	1	$\begin{pmatrix} 1 & 0 & 0 \end{pmatrix} @ \begin{pmatrix} \frac{5}{6} & \frac{2}{3} & 0 \end{pmatrix}$	[-8,10,-16,23]
B ₃ [1a: 6/mmm]	b ₁₀	C ₁	C ₂	3	1	$\begin{pmatrix} \frac{4}{3} & \frac{2}{3} & 0 \end{pmatrix} @ \begin{pmatrix} 0 & 0 & 0 \end{pmatrix}$	[1,-2,-4,7,-13,15,17,-19]

continued ...

Table 4

	bond	tail	head	n	#	$\mathbf{b@c}$	mapping
	b ₁₁	C ₁	C ₂	3	1	$\begin{pmatrix} -\frac{2}{3} & \frac{2}{3} & 0 \end{pmatrix} @ \begin{pmatrix} 0 & 0 & 0 \end{pmatrix}$	[-3,6,9,-12,14,-18,-21,24]
	b ₁₂	C ₁	C ₂	3	1	$\begin{pmatrix} -\frac{2}{3} & -\frac{4}{3} & 0 \end{pmatrix} @ \begin{pmatrix} 0 & 0 & 0 \end{pmatrix}$	[-5,8,10,-11,16,-20,-22,23]
B ₄ [3f: mmm]	b ₁₃	C ₁	C ₂	4	1	$\begin{pmatrix} \frac{4}{3} & \frac{5}{3} & 0 \end{pmatrix} @ \begin{pmatrix} 0 & \frac{1}{2} & 0 \end{pmatrix}$	[1,-2,-13,17]
	b ₁₄	C ₁	C ₂	4	1	$\begin{pmatrix} \frac{1}{3} & \frac{5}{3} & 0 \end{pmatrix} @ \begin{pmatrix} \frac{1}{2} & \frac{1}{2} & 0 \end{pmatrix}$	[-3,6,14,-18]
	b ₁₅	C ₁	C ₂	4	1	$\begin{pmatrix} \frac{4}{3} & -\frac{1}{3} & 0 \end{pmatrix} @ \begin{pmatrix} 0 & \frac{1}{2} & 0 \end{pmatrix}$	[-4,7,15,-19]
	b ₁₆	C ₁	C ₂	4	1	$\begin{pmatrix} -\frac{5}{3} & -\frac{4}{3} & 0 \end{pmatrix} @ \begin{pmatrix} \frac{1}{2} & 0 & 0 \end{pmatrix}$	[-5,8,16,-20]
	b ₁₇	C ₁	C ₂	4	1	$\begin{pmatrix} -\frac{5}{3} & -\frac{1}{3} & 0 \end{pmatrix} @ \begin{pmatrix} \frac{1}{2} & \frac{1}{2} & 0 \end{pmatrix}$	[9,-12,-21,24]
	b ₁₈	C ₁	C ₂	4	1	$\begin{pmatrix} \frac{1}{3} & -\frac{4}{3} & 0 \end{pmatrix} @ \begin{pmatrix} \frac{1}{2} & 0 & 0 \end{pmatrix}$	[10,-11,-22,23]
B ₅ [6l: mm2]	b ₁₉	C ₁	C ₁	5	1	$\begin{pmatrix} 1 & 2 & 0 \end{pmatrix} @ \begin{pmatrix} \frac{5}{6} & \frac{2}{3} & 0 \end{pmatrix}$	[1,6,14,17]
	b ₂₀	C ₂	C ₂	5	1	$\begin{pmatrix} -1 & -2 & 0 \end{pmatrix} @ \begin{pmatrix} \frac{1}{6} & \frac{1}{3} & 0 \end{pmatrix}$	[2,3,13,18]
	b ₂₁	C ₂	C ₂	5	1	$\begin{pmatrix} -1 & 1 & 0 \end{pmatrix} @ \begin{pmatrix} \frac{1}{6} & \frac{5}{6} & 0 \end{pmatrix}$	[4,11,19,22]
	b ₂₂	C ₂	C ₂	5	1	$\begin{pmatrix} 2 & 1 & 0 \end{pmatrix} @ \begin{pmatrix} \frac{2}{3} & \frac{5}{6} & 0 \end{pmatrix}$	[5,12,20,21]
	b ₂₃	C ₁	C ₁	5	1	$\begin{pmatrix} 1 & -1 & 0 \end{pmatrix} @ \begin{pmatrix} \frac{5}{6} & \frac{1}{6} & 0 \end{pmatrix}$	[7,10,15,23]
	b ₂₄	C ₁	C ₁	5	1	$\begin{pmatrix} -2 & -1 & 0 \end{pmatrix} @ \begin{pmatrix} \frac{1}{3} & \frac{1}{6} & 0 \end{pmatrix}$	[8,9,16,24]
B ₆ [2c: -6m2]	b ₂₅	C ₁	C ₁	6	1	$\begin{pmatrix} 2 & 2 & 0 \end{pmatrix} @ \begin{pmatrix} \frac{1}{3} & \frac{2}{3} & 0 \end{pmatrix}$	[1,-8,-16,17]
	b ₂₆	C ₂	C ₂	6	1	$\begin{pmatrix} 2 & 2 & 0 \end{pmatrix} @ \begin{pmatrix} \frac{2}{3} & \frac{1}{3} & 0 \end{pmatrix}$	[-2,5,-13,20]
	b ₂₇	C ₂	C ₂	6	1	$\begin{pmatrix} 0 & 2 & 0 \end{pmatrix} @ \begin{pmatrix} \frac{2}{3} & \frac{1}{3} & 0 \end{pmatrix}$	[-3,11,-18,22]
	b ₂₈	C ₂	C ₂	6	1	$\begin{pmatrix} 2 & 0 & 0 \end{pmatrix} @ \begin{pmatrix} \frac{2}{3} & \frac{1}{3} & 0 \end{pmatrix}$	[-4,12,-19,21]
	b ₂₉	C ₁	C ₁	6	1	$\begin{pmatrix} 0 & 2 & 0 \end{pmatrix} @ \begin{pmatrix} \frac{1}{3} & \frac{2}{3} & 0 \end{pmatrix}$	[6,-10,14,-23]
	b ₃₀	C ₁	C ₁	6	1	$\begin{pmatrix} 2 & 0 & 0 \end{pmatrix} @ \begin{pmatrix} \frac{1}{3} & \frac{2}{3} & 0 \end{pmatrix}$	[7,-9,15,-24]

- SAMB:

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

$$\hat{\mathbb{Z}}_1 = \mathbb{X}_{001}[\mathbb{Q}_0^{(a,A_{1g})}] \otimes \mathbb{Y}_{001}[\mathbb{Q}_0^{(s,A_{1g})}]$$

$$\boxed{\text{No. 2}} \quad \hat{Q}_0^{(A_{1g})} [M_1, B_1]$$

$$\hat{Z}_2 = X_{001}[Q_0^{(a, A_{1g})}] \otimes Y_{002}[Q_0^{(b, A_{1g})}]$$

$$\boxed{\text{No. 3}} \quad \hat{Q}_0^{(A_{1g})} [M_1, B_2]$$

$$\hat{Z}_3 = X_{001}[Q_0^{(a, A_{1g})}] \otimes Y_{003}[Q_0^{(b, A_{1g})}]$$

$$\boxed{\text{No. 4}} \quad \hat{Q}_0^{(A_{1g})} [M_1, B_3]$$

$$\hat{Z}_4 = X_{001}[Q_0^{(a, A_{1g})}] \otimes Y_{004}[Q_0^{(b, A_{1g})}]$$

$$\boxed{\text{No. 5}} \quad \hat{Q}_0^{(A_{1g})} [M_1, B_4]$$

$$\hat{Z}_5 = X_{001}[Q_0^{(a, A_{1g})}] \otimes Y_{005}[Q_0^{(b, A_{1g})}]$$

$$\boxed{\text{No. 6}} \quad \hat{Q}_0^{(A_{1g})} [M_1, B_5]$$

$$\hat{Z}_6 = X_{001}[Q_0^{(a, A_{1g})}] \otimes Y_{006}[Q_0^{(b, A_{1g})}]$$

$$\boxed{\text{No. 7}} \quad \hat{Q}_0^{(A_{1g})} [M_1, B_6]$$

$$\hat{Z}_7 = X_{001}[Q_0^{(a, A_{1g})}] \otimes Y_{007}[Q_0^{(b, A_{1g})}]$$

Table 5: Atomic SAMB group.

group	bra	ket
M ₁	p_z	p_z

Table 6: Atomic SAMB.

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

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	$\mathbb{Q}_0^{(b, A_{1g})}$	B_1	$\begin{pmatrix} \frac{\sqrt{3}}{3} & \frac{\sqrt{3}}{3} & \frac{\sqrt{3}}{3} \end{pmatrix}$
\mathbb{Y}_3	$\mathbb{Q}_0^{(b, A_{1g})}$	B_2	$\begin{pmatrix} \frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} \end{pmatrix}$
\mathbb{Y}_4	$\mathbb{Q}_0^{(b, A_{1g})}$	B_3	$\begin{pmatrix} \frac{\sqrt{3}}{3} & \frac{\sqrt{3}}{3} & \frac{\sqrt{3}}{3} \end{pmatrix}$
\mathbb{Y}_5	$\mathbb{Q}_0^{(b, A_{1g})}$	B_4	$\begin{pmatrix} \frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} \end{pmatrix}$
\mathbb{Y}_6	$\mathbb{Q}_0^{(b, A_{1g})}$	B_5	$\begin{pmatrix} \frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} \end{pmatrix}$
\mathbb{Y}_7	$\mathbb{Q}_0^{(b, A_{1g})}$	B_6	$\begin{pmatrix} \frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} \end{pmatrix}$

Table 8: Polar harmonics.

No.	symbol	rank	irrep.	mul.	comp.	form
1	$\mathbb{Q}_0^{(A_{1g})}$	0	A_{1g}	—	—	1

- Group info.: Generator = $\{3_{001}^+|0\}$, $\{2_{001}|0\}$, $\{2_{110}|0\}$, $\{-1|0\}$

Table 9: Conjugacy class (point-group part).

rep. SO	symmetry operations
$\{1 0\}$	$\{1 0\}$
$\{2_{001} 0\}$	$\{2_{001} 0\}$
$\{2_{100} 0\}$	$\{2_{100} 0\}, \{2_{010} 0\}, \{2_{110} 0\}$
$\{2_{120} 0\}$	$\{2_{120} 0\}, \{2_{210} 0\}, \{2_{1-10} 0\}$
$\{3_{001}^+ 0\}$	$\{3_{001}^+ 0\}, \{3_{001}^- 0\}$
$\{6_{001}^+ 0\}$	$\{6_{001}^+ 0\}, \{6_{001}^- 0\}$
$\{-1 0\}$	$\{-1 0\}$
$\{m_{100} 0\}$	$\{m_{100} 0\}, \{m_{010} 0\}, \{m_{110} 0\}$
$\{m_{001} 0\}$	$\{m_{001} 0\}$
$\{m_{120} 0\}$	$\{m_{120} 0\}, \{m_{210} 0\}, \{m_{1-10} 0\}$
$\{-3_{001}^+ 0\}$	$\{-3_{001}^+ 0\}, \{-3_{001}^- 0\}$
$\{-6_{001}^+ 0\}$	$\{-6_{001}^+ 0\}, \{-6_{001}^- 0\}$

Table 10: 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	$\{2_{120} 0\}$	7	$\{2_{210} 0\}$	8	$\{2_{1-10} 0\}$	9	$\{3_{001}^+ 0\}$	10	$\{3_{001}^- 0\}$
11	$\{6_{001}^+ 0\}$	12	$\{6_{001}^- 0\}$	13	$\{-1 0\}$	14	$\{m_{100} 0\}$	15	$\{m_{010} 0\}$
16	$\{m_{110} 0\}$	17	$\{m_{001} 0\}$	18	$\{m_{120} 0\}$	19	$\{m_{210} 0\}$	20	$\{m_{1-10} 0\}$
21	$\{-3_{001}^+ 0\}$	22	$\{-3_{001}^- 0\}$	23	$\{-6_{001}^+ 0\}$	24	$\{-6_{001}^- 0\}$		

Table 11: Character table (point-group part).

	1	2_{001}	2_{100}	2_{120}	3_{001}^+	6_{001}^+	-1	m_{100}	m_{001}	m_{120}	-3_{001}^+	-6_{001}^+
A_{1g}	1	1	1	1	1	1	1	1	1	1	1	1

continued ...

Table 11

	1	2 ₀₀₁	2 ₁₀₀	2 ₁₂₀	3 ₀₀₁ ⁺	6 ₀₀₁ ⁺	-1	m ₁₀₀	m ₀₀₁	m ₁₂₀	-3 ₀₀₁ ⁺	-6 ₀₀₁ ⁺
A_{2g}	1	1	-1	-1	1	1	1	-1	1	-1	1	1
B_{1g}	1	-1	-1	1	1	-1	1	-1	-1	1	1	-1
B_{2g}	1	-1	1	-1	1	-1	1	1	-1	-1	1	-1
E_{1g}	2	-2	0	0	-1	1	2	0	-2	0	-1	1
E_{2g}	2	2	0	0	-1	-1	2	0	2	0	-1	-1
A_{1u}	1	1	1	1	1	1	-1	-1	-1	-1	-1	-1
A_{2u}	1	1	-1	-1	1	1	-1	1	-1	1	-1	-1
B_{1u}	1	-1	-1	1	1	-1	-1	1	1	-1	-1	1
B_{2u}	1	-1	1	-1	1	-1	-1	-1	1	1	-1	1
E_{1u}	2	-2	0	0	-1	1	-2	0	2	0	1	-1
E_{2u}	2	2	0	0	-1	-1	-2	0	-2	0	1	1

Table 12: Parity conversion.

\leftrightarrow	\leftrightarrow	\leftrightarrow	\leftrightarrow	\leftrightarrow
A_{1g} (A_{1u})	A_{2g} (A_{2u})	B_{1g} (B_{1u})	B_{2g} (B_{2u})	E_{1g} (E_{1u})
E_{2g} (E_{2u})	A_{1u} (A_{1g})	A_{2u} (A_{2g})	B_{1u} (B_{1g})	B_{2u} (B_{2g})
E_{1u} (E_{1g})	E_{2u} (E_{2g})			

Table 13: Symmetric product, $[\Gamma \otimes \Gamma']_+$.

	A_{1g}	A_{2g}	B_{1g}	B_{2g}	E_{1g}	E_{2g}	A_{1u}	A_{2u}	B_{1u}	B_{2u}	E_{1u}	E_{2u}
A_{1g}	A_{1g}	A_{2g}	B_{1g}	B_{2g}	E_{1g}	E_{2g}	A_{1u}	A_{2u}	B_{1u}	B_{2u}	E_{1u}	E_{2u}
A_{2g}		A_{1g}	B_{2g}	B_{1g}	E_{1g}	E_{2g}	A_{2u}	A_{1u}	B_{2u}	B_{1u}	E_{1u}	E_{2u}
B_{1g}			A_{1g}	A_{2g}	E_{2g}	E_{1g}	B_{1u}	B_{2u}	A_{1u}	A_{2u}	E_{2u}	E_{1u}
B_{2g}				A_{1g}	E_{2g}	E_{1g}	B_{2u}	B_{1u}	A_{2u}	A_{1u}	E_{2u}	E_{1u}
E_{1g}					$A_{1g} + E_{2g}$	$B_{1g} + B_{2g} + E_{1g}$	E_{1u}	E_{1u}	E_{2u}	E_{2u}	$A_{1u} + A_{2u} + E_{2u}$	$B_{1u} + B_{2u} + E_{1u}$
E_{2g}						$A_{1g} + E_{2g}$	E_{2u}	E_{2u}	E_{1u}	E_{1u}	$B_{1u} + B_{2u} + E_{1u}$	$A_{1u} + A_{2u} + E_{2u}$
A_{1u}							A_{1g}	A_{2g}	B_{1g}	B_{2g}	E_{1g}	E_{2g}
A_{2u}								A_{1g}	B_{2g}	B_{1g}	E_{1g}	E_{2g}
B_{1u}									A_{1g}	A_{2g}	E_{2g}	E_{1g}
B_{2u}										A_{1g}	E_{2g}	E_{1g}
E_{1u}											$A_{1g} + E_{2g}$	$B_{1g} + B_{2g} + E_{1g}$
E_{2u}												$A_{1g} + E_{2g}$

Table 14: Anti-symmetric product, $[\Gamma \otimes \Gamma]_-$.

A_{1g}	A_{2g}	B_{1g}	B_{2g}	E_{1g}	E_{2g}	A_{1u}	A_{2u}	B_{1u}	B_{2u}	E_{1u}	E_{2u}
—	—	—	—	A_{2g}	A_{2g}	—	—	—	—	A_{2g}	A_{2g}

Table 15: Virtual-cluster sites.

No.	position	No.	position	No.	position	No.	position
1	$\begin{pmatrix} 3 & 1 & 1 \end{pmatrix}$	2	$\begin{pmatrix} -3 & -1 & 1 \end{pmatrix}$	3	$\begin{pmatrix} 2 & -1 & -1 \end{pmatrix}$	4	$\begin{pmatrix} -3 & -2 & -1 \end{pmatrix}$
5	$\begin{pmatrix} 1 & 3 & -1 \end{pmatrix}$	6	$\begin{pmatrix} -2 & 1 & -1 \end{pmatrix}$	7	$\begin{pmatrix} 3 & 2 & -1 \end{pmatrix}$	8	$\begin{pmatrix} -1 & -3 & -1 \end{pmatrix}$
9	$\begin{pmatrix} -1 & 2 & 1 \end{pmatrix}$	10	$\begin{pmatrix} -2 & -3 & 1 \end{pmatrix}$	11	$\begin{pmatrix} 2 & 3 & 1 \end{pmatrix}$	12	$\begin{pmatrix} 1 & -2 & 1 \end{pmatrix}$
13	$\begin{pmatrix} -3 & -1 & -1 \end{pmatrix}$	14	$\begin{pmatrix} -2 & 1 & 1 \end{pmatrix}$	15	$\begin{pmatrix} 3 & 2 & 1 \end{pmatrix}$	16	$\begin{pmatrix} -1 & -3 & 1 \end{pmatrix}$
17	$\begin{pmatrix} 3 & 1 & -1 \end{pmatrix}$	18	$\begin{pmatrix} 2 & -1 & 1 \end{pmatrix}$	19	$\begin{pmatrix} -3 & -2 & 1 \end{pmatrix}$	20	$\begin{pmatrix} 1 & 3 & 1 \end{pmatrix}$
21	$\begin{pmatrix} 1 & -2 & -1 \end{pmatrix}$	22	$\begin{pmatrix} 2 & 3 & -1 \end{pmatrix}$	23	$\begin{pmatrix} -2 & -3 & -1 \end{pmatrix}$	24	$\begin{pmatrix} -1 & 2 & -1 \end{pmatrix}$

Table 16: Virtual-cluster basis.

symbol	1	2	3	4	5	6	7	8	9	10
$Q_0^{(A_{1g})}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$
	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$
	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$						
$Q_1^{(A_{2u})}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$
	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$
	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$						

continued ...

symbol	1	2	3	4	5	6	7	8	9	10
$\mathbb{Q}_{1,0}^{(E_{1u})}$	$\frac{5\sqrt{21}}{84}$ $\frac{\sqrt{21}}{84}$ $\frac{\sqrt{21}}{21}$	$-\frac{5\sqrt{21}}{84}$ $\frac{\sqrt{21}}{21}$ $\frac{\sqrt{21}}{84}$	$\frac{5\sqrt{21}}{84}$ $-\frac{5\sqrt{21}}{84}$ $-\frac{\sqrt{21}}{84}$	$-\frac{\sqrt{21}}{21}$ $-\frac{5\sqrt{21}}{84}$ $-\frac{\sqrt{21}}{21}$	$-\frac{\sqrt{21}}{84}$ $\frac{\sqrt{21}}{21}$ $\frac{\sqrt{21}}{21}$	$-\frac{5\sqrt{21}}{84}$ $\frac{\sqrt{21}}{84}$ $\frac{5\sqrt{21}}{84}$	$\frac{\sqrt{21}}{21}$ $\frac{5\sqrt{21}}{84}$ $\frac{5\sqrt{21}}{84}$	$\frac{\sqrt{21}}{84}$ $\frac{5\sqrt{21}}{84}$ $-\frac{\sqrt{21}}{21}$	$-\frac{\sqrt{21}}{21}$ $-\frac{\sqrt{21}}{21}$ $-\frac{\sqrt{21}}{84}$	$-\frac{\sqrt{21}}{84}$ $-\frac{\sqrt{21}}{84}$ $-\frac{\sqrt{21}}{84}$
$\mathbb{Q}_{1,1}^{(E_{1u})}$	$\frac{\sqrt{7}}{28}$ $\frac{3\sqrt{7}}{28}$ $-\frac{\sqrt{7}}{14}$	$-\frac{\sqrt{7}}{28}$ $-\frac{\sqrt{7}}{14}$ $\frac{3\sqrt{7}}{28}$	$-\frac{\sqrt{7}}{28}$ $-\frac{\sqrt{7}}{28}$ $-\frac{3\sqrt{7}}{28}$	$-\frac{\sqrt{7}}{14}$ $\frac{\sqrt{7}}{28}$ $\frac{\sqrt{7}}{14}$	$\frac{3\sqrt{7}}{28}$ $\frac{\sqrt{7}}{14}$ $\frac{\sqrt{7}}{14}$	$\frac{\sqrt{7}}{28}$ $-\frac{3\sqrt{7}}{28}$ $-\frac{3\sqrt{7}}{28}$	$\frac{\sqrt{7}}{14}$ $\frac{\sqrt{7}}{28}$ $\frac{\sqrt{7}}{28}$	$-\frac{3\sqrt{7}}{28}$ $-\frac{\sqrt{7}}{28}$ $-\frac{\sqrt{7}}{28}$	$\frac{\sqrt{7}}{14}$ $-\frac{\sqrt{7}}{14}$ $-\frac{\sqrt{7}}{14}$	$-\frac{3\sqrt{7}}{28}$ $\frac{3\sqrt{7}}{28}$ $\frac{3\sqrt{7}}{28}$
$\mathbb{Q}_{2,0}^{(E_{1g})}$	$\frac{5\sqrt{21}}{84}$ $\frac{\sqrt{21}}{84}$ $-\frac{\sqrt{21}}{21}$	$-\frac{5\sqrt{21}}{84}$ $\frac{\sqrt{21}}{21}$ $-\frac{\sqrt{21}}{84}$	$-\frac{5\sqrt{21}}{84}$ $\frac{5\sqrt{21}}{84}$ $\frac{\sqrt{21}}{84}$	$\frac{\sqrt{21}}{21}$ $-\frac{5\sqrt{21}}{84}$ $\frac{\sqrt{21}}{21}$	$\frac{\sqrt{21}}{84}$ $\frac{\sqrt{21}}{21}$ $\frac{\sqrt{21}}{21}$	$\frac{5\sqrt{21}}{84}$ $\frac{\sqrt{21}}{84}$ $-\frac{5\sqrt{21}}{84}$	$-\frac{\sqrt{21}}{21}$ $-\frac{5\sqrt{21}}{84}$ $-\frac{5\sqrt{21}}{84}$	$-\frac{\sqrt{21}}{84}$ $\frac{5\sqrt{21}}{84}$ $\frac{5\sqrt{21}}{84}$	$-\frac{\sqrt{21}}{21}$ $-\frac{\sqrt{21}}{21}$ $-\frac{\sqrt{21}}{21}$	$-\frac{\sqrt{21}}{84}$ $-\frac{\sqrt{21}}{84}$ $-\frac{\sqrt{21}}{84}$
$\mathbb{Q}_{2,1}^{(E_{1g})}$	$\frac{\sqrt{7}}{28}$ $\frac{3\sqrt{7}}{28}$ $\frac{\sqrt{7}}{14}$	$-\frac{\sqrt{7}}{28}$ $-\frac{\sqrt{7}}{14}$ $-\frac{3\sqrt{7}}{28}$	$\frac{\sqrt{7}}{28}$ $\frac{\sqrt{7}}{28}$ $\frac{3\sqrt{7}}{28}$	$\frac{\sqrt{7}}{14}$ $\frac{\sqrt{7}}{28}$ $-\frac{\sqrt{7}}{14}$	$-\frac{3\sqrt{7}}{28}$ $\frac{\sqrt{7}}{14}$ $\frac{\sqrt{7}}{14}$	$-\frac{\sqrt{7}}{28}$ $-\frac{3\sqrt{7}}{28}$ $-\frac{3\sqrt{7}}{28}$	$-\frac{\sqrt{7}}{14}$ $-\frac{\sqrt{7}}{28}$ $-\frac{\sqrt{7}}{28}$	$\frac{3\sqrt{7}}{28}$ $-\frac{\sqrt{7}}{28}$ $-\frac{\sqrt{7}}{28}$	$\frac{\sqrt{7}}{14}$ $-\frac{\sqrt{7}}{14}$ $-\frac{\sqrt{7}}{14}$	$-\frac{3\sqrt{7}}{28}$ $\frac{3\sqrt{7}}{28}$ $\frac{3\sqrt{7}}{28}$
$\mathbb{Q}_{2,0}^{(E_{2g})}$	$\frac{11\sqrt{3}}{84}$ $-\frac{13\sqrt{3}}{84}$ $\frac{\sqrt{3}}{42}$	$\frac{11\sqrt{3}}{84}$ $\frac{\sqrt{3}}{42}$ $-\frac{13\sqrt{3}}{84}$	$\frac{11\sqrt{3}}{84}$ $\frac{11\sqrt{3}}{84}$ $-\frac{13\sqrt{3}}{84}$	$\frac{\sqrt{3}}{42}$ $\frac{11\sqrt{3}}{84}$ $\frac{\sqrt{3}}{42}$	$-\frac{13\sqrt{3}}{84}$ $\frac{\sqrt{3}}{42}$ $\frac{\sqrt{3}}{42}$	$\frac{11\sqrt{3}}{84}$ $-\frac{13\sqrt{3}}{84}$ $-\frac{13\sqrt{3}}{84}$	$\frac{\sqrt{3}}{42}$ $\frac{11\sqrt{3}}{84}$ $\frac{11\sqrt{3}}{84}$	$-\frac{13\sqrt{3}}{84}$ $\frac{11\sqrt{3}}{84}$ $\frac{11\sqrt{3}}{84}$	$\frac{\sqrt{3}}{42}$ $\frac{\sqrt{3}}{42}$ $\frac{\sqrt{3}}{42}$	$-\frac{13\sqrt{3}}{84}$ $-\frac{13\sqrt{3}}{84}$ $-\frac{13\sqrt{3}}{84}$
$\mathbb{Q}_{2,1}^{(E_{2g})}$	$-\frac{5}{28}$ $-\frac{3}{28}$ $\frac{2}{7}$	$-\frac{5}{28}$ $\frac{2}{7}$ $-\frac{3}{28}$	$\frac{5}{28}$ $-\frac{5}{28}$ $-\frac{3}{28}$	$-\frac{2}{7}$ $\frac{5}{28}$ $\frac{2}{7}$	$\frac{3}{28}$ $-\frac{2}{7}$ $-\frac{2}{7}$	$\frac{5}{28}$ $\frac{3}{28}$ $\frac{3}{28}$	$-\frac{2}{7}$ $-\frac{5}{28}$ $-\frac{5}{28}$	$\frac{3}{28}$ $\frac{5}{28}$ $\frac{5}{28}$	$\frac{2}{7}$ $-\frac{2}{7}$ $-\frac{2}{7}$	$-\frac{3}{28}$ $\frac{3}{28}$ $\frac{3}{28}$
$\mathbb{Q}_3^{(B_{1u})}$	$\frac{\sqrt{6}}{12}$ $-\frac{\sqrt{6}}{12}$ $-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$ $-\frac{\sqrt{6}}{12}$ $-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$ $-\frac{\sqrt{6}}{12}$ $\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$ $\frac{\sqrt{6}}{12}$ $\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$ $\frac{\sqrt{6}}{12}$ $\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$ $\frac{\sqrt{6}}{12}$ $-\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$ $\frac{\sqrt{6}}{12}$ $-\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$ $-\frac{\sqrt{6}}{12}$ $-\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$ $-\frac{\sqrt{6}}{12}$ $-\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$ $-\frac{\sqrt{6}}{12}$ $-\frac{\sqrt{6}}{12}$
$\mathbb{Q}_3^{(B_{2u})}$	$\frac{\sqrt{6}}{12}$ $-\frac{\sqrt{6}}{12}$ $-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$ $-\frac$								

continued ...

symbol	1	2	3	4	5	6	7	8	9	10
$\mathbb{Q}_4^{(B_{1g})}$	$-\frac{2}{7}$	$\frac{3}{28}$	$\frac{3}{28}$	$-\frac{2}{7}$						
	$\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$
	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$
	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$						
$\mathbb{Q}_4^{(B_{2g})}$	$\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$
	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$
	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$						
$\mathbb{Q}_{4,0}^{(E_{2g},1)}$	$\frac{5}{28}$	$\frac{5}{28}$	$\frac{5}{28}$	$-\frac{2}{7}$	$\frac{3}{28}$	$\frac{5}{28}$	$-\frac{2}{7}$	$\frac{3}{28}$	$-\frac{2}{7}$	$\frac{3}{28}$
	$\frac{3}{28}$	$-\frac{2}{7}$	$\frac{5}{28}$	$\frac{5}{28}$	$-\frac{2}{7}$	$\frac{3}{28}$	$\frac{5}{28}$	$\frac{5}{28}$	$-\frac{2}{7}$	$\frac{3}{28}$
	$-\frac{2}{7}$	$\frac{3}{28}$	$\frac{3}{28}$	$-\frac{2}{7}$						
$\mathbb{Q}_{4,1}^{(E_{2g},1)}$	$\frac{11\sqrt{3}}{84}$	$\frac{11\sqrt{3}}{84}$	$-\frac{11\sqrt{3}}{84}$	$-\frac{\sqrt{3}}{42}$	$\frac{13\sqrt{3}}{84}$	$-\frac{11\sqrt{3}}{84}$	$-\frac{\sqrt{3}}{42}$	$\frac{13\sqrt{3}}{84}$	$\frac{\sqrt{3}}{42}$	$-\frac{13\sqrt{3}}{84}$
	$-\frac{13\sqrt{3}}{84}$	$\frac{\sqrt{3}}{42}$	$\frac{11\sqrt{3}}{84}$	$-\frac{11\sqrt{3}}{84}$	$-\frac{\sqrt{3}}{42}$	$\frac{13\sqrt{3}}{84}$	$\frac{11\sqrt{3}}{84}$	$-\frac{11\sqrt{3}}{84}$	$-\frac{\sqrt{3}}{42}$	$\frac{13\sqrt{3}}{84}$
	$\frac{\sqrt{3}}{42}$	$-\frac{13\sqrt{3}}{84}$	$-\frac{13\sqrt{3}}{84}$	$\frac{\sqrt{3}}{42}$						
$\mathbb{Q}_{5,0}^{(E_{1u},1)}$	$\frac{\sqrt{7}}{28}$	$-\frac{\sqrt{7}}{28}$	$\frac{\sqrt{7}}{28}$	$\frac{\sqrt{7}}{14}$	$-\frac{3\sqrt{7}}{28}$	$-\frac{\sqrt{7}}{28}$	$-\frac{\sqrt{7}}{14}$	$\frac{3\sqrt{7}}{28}$	$\frac{\sqrt{7}}{14}$	$-\frac{3\sqrt{7}}{28}$
	$\frac{3\sqrt{7}}{28}$	$-\frac{\sqrt{7}}{14}$	$-\frac{\sqrt{7}}{28}$	$-\frac{\sqrt{7}}{28}$	$-\frac{\sqrt{7}}{14}$	$\frac{3\sqrt{7}}{28}$	$\frac{\sqrt{7}}{28}$	$\frac{\sqrt{7}}{28}$	$\frac{\sqrt{7}}{14}$	$-\frac{3\sqrt{7}}{28}$
	$-\frac{\sqrt{7}}{14}$	$\frac{3\sqrt{7}}{28}$	$-\frac{3\sqrt{7}}{28}$	$\frac{\sqrt{7}}{14}$						
$\mathbb{Q}_{5,1}^{(E_{1u},1)}$	$-\frac{5\sqrt{21}}{84}$	$\frac{5\sqrt{21}}{84}$	$\frac{5\sqrt{21}}{84}$	$-\frac{\sqrt{21}}{21}$	$-\frac{\sqrt{21}}{84}$	$-\frac{5\sqrt{21}}{84}$	$\frac{\sqrt{21}}{21}$	$\frac{\sqrt{21}}{84}$	$\frac{\sqrt{21}}{21}$	$\frac{\sqrt{21}}{84}$
	$-\frac{\sqrt{21}}{84}$	$-\frac{\sqrt{21}}{21}$	$\frac{5\sqrt{21}}{84}$	$-\frac{5\sqrt{21}}{84}$	$\frac{\sqrt{21}}{21}$	$\frac{\sqrt{21}}{84}$	$-\frac{5\sqrt{21}}{84}$	$\frac{5\sqrt{21}}{84}$	$-\frac{\sqrt{21}}{21}$	$-\frac{\sqrt{21}}{84}$
	$-\frac{\sqrt{21}}{21}$	$-\frac{\sqrt{21}}{84}$	$\frac{\sqrt{21}}{84}$	$\frac{\sqrt{21}}{21}$						
$\mathbb{Q}_{5,0}^{(E_{2u},1)}$	$\frac{5}{28}$	$\frac{5}{28}$	$-\frac{5}{28}$	$\frac{2}{7}$	$-\frac{3}{28}$	$-\frac{5}{28}$	$\frac{2}{7}$	$-\frac{3}{28}$	$-\frac{2}{7}$	$\frac{3}{28}$
	$\frac{3}{28}$	$-\frac{2}{7}$	$-\frac{5}{28}$	$\frac{5}{28}$	$-\frac{2}{7}$	$\frac{3}{28}$	$-\frac{5}{28}$	$\frac{5}{28}$	$-\frac{2}{7}$	$\frac{3}{28}$
	$\frac{2}{7}$	$-\frac{3}{28}$ </								

continued ...

Table 16

symbol	1	2	3	4	5	6	7	8	9	10
	$\frac{3\sqrt{7}}{28}$	$-\frac{\sqrt{7}}{14}$	$\frac{\sqrt{7}}{28}$	$-\frac{\sqrt{7}}{28}$	$-\frac{\sqrt{7}}{14}$	$\frac{3\sqrt{7}}{28}$	$-\frac{\sqrt{7}}{28}$	$\frac{\sqrt{7}}{28}$	$\frac{\sqrt{7}}{14}$	$-\frac{3\sqrt{7}}{28}$
	$\frac{\sqrt{7}}{14}$	$-\frac{3\sqrt{7}}{28}$	$\frac{3\sqrt{7}}{28}$	$-\frac{\sqrt{7}}{14}$						
$\mathbb{Q}_{6,1}^{(E_{1g},1)}$	$-\frac{5\sqrt{21}}{84}$	$\frac{5\sqrt{21}}{84}$	$-\frac{5\sqrt{21}}{84}$	$\frac{\sqrt{21}}{21}$	$\frac{\sqrt{21}}{84}$	$\frac{5\sqrt{21}}{84}$	$-\frac{\sqrt{21}}{21}$	$-\frac{\sqrt{21}}{84}$	$\frac{\sqrt{21}}{21}$	$\frac{\sqrt{21}}{84}$
	$-\frac{\sqrt{21}}{84}$	$-\frac{\sqrt{21}}{21}$	$-\frac{5\sqrt{21}}{84}$	$-\frac{5\sqrt{21}}{84}$	$\frac{\sqrt{21}}{21}$	$\frac{\sqrt{21}}{84}$	$\frac{5\sqrt{21}}{84}$	$\frac{5\sqrt{21}}{84}$	$-\frac{\sqrt{21}}{21}$	$-\frac{\sqrt{21}}{84}$
	$\frac{\sqrt{21}}{21}$	$\frac{\sqrt{21}}{84}$	$-\frac{\sqrt{21}}{84}$	$-\frac{\sqrt{21}}{21}$						
$\mathbb{Q}_7^{(A_{1u})}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$
	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$
	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$						