

# 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:
  - $a = 2.435$ ,  $b = 2.435$ ,  $c = 1000.0$ ,  $\alpha = 90.0$ ,  $\beta = 90.0$ ,  $\gamma = 120.0$
- Lattice vectors:
  - $\mathbf{a}_1 = (2.435 \ 0 \ 0)$
  - $\mathbf{a}_2 = (-1.2175 \ 2.10877185821511 \ 0)$
  - $\mathbf{a}_3 = (6.0 \cdot 10^{-14} \ 1.1 \cdot 10^{-13} \ 1000.0)$

Table 1: High-symmetry line:  $\Gamma$ -M-K- $\Gamma$ .

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

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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 <sub>1</sub> [2c: -6m2]	C <sub>1</sub>	$\begin{pmatrix} \frac{2}{3} & \frac{1}{3} & 0 \end{pmatrix}$	[1,6,7,8,9,10,14,15,16,17,23,24]
	C <sub>2</sub>	$\begin{pmatrix} \frac{1}{3} & \frac{2}{3} & 0 \end{pmatrix}$	[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 <sub>1</sub> [3f: mmm]	b <sub>1</sub>	C <sub>1</sub>	C <sub>2</sub>	1	1	$\begin{pmatrix} \frac{2}{3} & \frac{1}{3} & 0 \end{pmatrix} @ \begin{pmatrix} 0 & \frac{1}{2} & 0 \end{pmatrix}$	[1,-2,-4,7,-13,15,17,-19]
	b <sub>2</sub>	C <sub>1</sub>	C <sub>2</sub>	1	1	$\begin{pmatrix} -\frac{1}{3} & \frac{1}{3} & 0 \end{pmatrix} @ \begin{pmatrix} \frac{1}{2} & \frac{1}{2} & 0 \end{pmatrix}$	[-3,6,9,-12,14,-18,-21,24]
	b <sub>3</sub>	C <sub>1</sub>	C <sub>2</sub>	1	1	$\begin{pmatrix} -\frac{1}{3} & -\frac{2}{3} & 0 \end{pmatrix} @ \begin{pmatrix} \frac{1}{2} & 0 & 0 \end{pmatrix}$	[-5,8,10,-11,16,-20,-22,23]
B <sub>2</sub> [6l: mm2]	b <sub>4</sub>	C <sub>1</sub>	C <sub>1</sub>	2	1	$\begin{pmatrix} 1 & 0 & 0 \end{pmatrix} @ \begin{pmatrix} \frac{1}{6} & \frac{1}{3} & 0 \end{pmatrix}$	[1,-6,-14,17]
	b <sub>5</sub>	C <sub>2</sub>	C <sub>2</sub>	2	1	$\begin{pmatrix} 1 & 0 & 0 \end{pmatrix} @ \begin{pmatrix} \frac{5}{6} & \frac{2}{3} & 0 \end{pmatrix}$	[-2,3,-13,18]
	b <sub>6</sub>	C <sub>2</sub>	C <sub>2</sub>	2	1	$\begin{pmatrix} 1 & 1 & 0 \end{pmatrix} @ \begin{pmatrix} \frac{5}{6} & \frac{1}{6} & 0 \end{pmatrix}$	[-4,11,-19,22]
	b <sub>7</sub>	C <sub>2</sub>	C <sub>2</sub>	2	1	$\begin{pmatrix} 0 & 1 & 0 \end{pmatrix} @ \begin{pmatrix} \frac{1}{3} & \frac{1}{6} & 0 \end{pmatrix}$	[5,-12,20,-21]
	b <sub>8</sub>	C <sub>1</sub>	C <sub>1</sub>	2	1	$\begin{pmatrix} 1 & 1 & 0 \end{pmatrix} @ \begin{pmatrix} \frac{1}{6} & \frac{5}{6} & 0 \end{pmatrix}$	[7,-10,15,-23]
	b <sub>9</sub>	C <sub>1</sub>	C <sub>1</sub>	2	1	$\begin{pmatrix} 0 & 1 & 0 \end{pmatrix} @ \begin{pmatrix} \frac{2}{3} & \frac{5}{6} & 0 \end{pmatrix}$	[-8,9,-16,24]
B <sub>3</sub> [1a: 6/mmm]	b <sub>10</sub>	C <sub>1</sub>	C <sub>2</sub>	3	1	$\begin{pmatrix} \frac{2}{3} & \frac{4}{3} & 0 \end{pmatrix} @ \begin{pmatrix} 0 & 0 & 0 \end{pmatrix}$	[1,-2,-3,6,-13,14,17,-18]

continued ...

Table 4

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

- SAMB:

$$\boxed{\text{No. 1}} \quad \hat{Q}_0^{(A_{1g})} [M_1, S_1]$$

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

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

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

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

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

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

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

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

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

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

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

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

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

Table 5: Atomic SAMB group.

group	bra	ket
M <sub>1</sub>	$p_z$	$p_z$

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 <sub>001</sub>	2 <sub>100</sub>	2 <sub>120</sub>	3 <sub>001</sub> <sup>+</sup>	6 <sub>001</sub> <sup>+</sup>	-1	m <sub>100</sub>	m <sub>001</sub>	m <sub>120</sub>	-3 <sub>001</sub> <sup>+</sup>	-6 <sub>001</sub> <sup>+</sup>
$A_{2g}$	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 ...*



[illegible]

*continued ...*

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

*continued ...*

Table 16

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