SAMB for "graphene"

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- Generation condition

 - time-reversal type: electric
 - irrep: [A1g]
 - spinless
- Unit cell:

$$a=2.435,\ b=2.435,\ c=10.0,\ \alpha=90.0,\ \beta=90.0,\ \gamma=120.0$$

• Lattice vectors:

$$a_1 = (2.435 \quad 0 \quad 0)$$

$$a_2 = \begin{pmatrix} -1.2175 & 2.10877185821511 & 0 \end{pmatrix}$$

$$\boldsymbol{a}_3 = \begin{pmatrix} 0 & 0 & 10.0 \end{pmatrix}$$

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

symbol	position	symbol	position	symbol	position
Г К'	$ \begin{pmatrix} 0 & 0 & 0 \\ -\frac{1}{3} & -\frac{1}{3} & 0 \end{pmatrix} $	М	$\begin{pmatrix} \frac{1}{2} & 0 & 0 \end{pmatrix}$	K	$\begin{pmatrix} \frac{1}{3} & \frac{1}{3} & 0 \end{pmatrix}$

• Kets: dimension = 2

Table 2: Hilbert space for full matrix.

No.	ket	No.	ket
1	$p_z@A_1$	2	$p_z@A_2$

• Sites in (primitive) unit cell:

Table 3: Site-clusters.

	site	position	mapping
S_1 [2c: -6m2]	A_1	$\begin{pmatrix} \frac{1}{3} & \frac{2}{3} & 0 \end{pmatrix}$	[1,6,7,8,9,10,14,15,16,17,23,24]
	A_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	#	b@c	mapping
B ₁ [3f: mmm]	b ₁	A_2	A_1	1	1	$\left(\begin{array}{cccc} \frac{1}{3} & \frac{2}{3} & 0 \end{array}\right) @ \left(\begin{array}{cccc} \frac{1}{2} & 0 & 0 \end{array}\right)$	[1,-2,-3,6,-13,14,17,-18]
	b_2	A_2	A_1	1	1	$\left[\begin{array}{cccc} \left(\frac{1}{3} & -\frac{1}{3} & 0\right) @ \left(\frac{1}{2} & \frac{1}{2} & 0\right) \end{array}\right]$	[-4,7,10,-11,15,-19,-22,23]
	b_3	A_2	A_1	1	1	$\left[\begin{array}{cccc} \left(-\frac{2}{3} & -\frac{1}{3} & 0 \right) @ \left(0 & \frac{1}{2} & 0 \right) \end{array} \right]$	[-5,8,9,-12,16,-20,-21,24]
B ₂ [6l: mm2]	b_4	A_1	A_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	A_2	A_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	A_2	A_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	A_2	A_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	A_1	A_1	2	1		[6,-9,14,-24]
	b_9	A_1	A_1	2	1		[-8,10,-16,23]

• SAMB:

$$\begin{split} & \boxed{ \text{No. 1} } & \hat{\mathbb{Q}}_0^{(A_{1g})} \text{ } [M_1, S_1] \\ & \hat{\mathbb{Z}}_1 = \mathbb{X}_1[\mathbb{Q}_0^{(a, A_{1g})}] \otimes \mathbb{Y}_1[\mathbb{Q}_0^{(s, A_{1g})}] \end{split}$$

No. 2
$$\hat{\mathbb{Q}}_0^{(A_{1g})}$$
 [M₁, B₁]

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

No. 3
$$\hat{\mathbb{Q}}_0^{(A_{1g})}$$
 [M₁, B₂]

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

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	(1)

Table 7: Cluster SAMB.

symbol	type	cluster	form
\mathbb{Y}_1	$\mathbb{Q}_0^{(s,A_{1g})}$	S_1	$\begin{pmatrix} \sqrt{2} & \sqrt{2} \\ 2 & 2 \end{pmatrix}$
\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{array}{c ccccccccccccccccccccccccccccccccccc$

Table 8: Polar harmonics.

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

 \bullet 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}	$\{-1 0\}$
$\{m_{100} 0\}$	$\{m_{100} 0\},\ \{m_{010} 0\},\ \{m_{110} 0\}$

 $continued\ \dots$

Table 9

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

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	2001	2100	2120	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
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	$\begin{pmatrix} 1+\sqrt{3} & -1+\sqrt{3} & 1 \end{pmatrix}$	2	$\left(-\sqrt{3}-1 1-\sqrt{3} 1\right)$	3	$\begin{pmatrix} 2 & 1 - \sqrt{3} & -1 \end{pmatrix}$	4	$\left(-\sqrt{3}-1 -2 -1\right)$
5	$\begin{pmatrix} -1 + \sqrt{3} & 1 + \sqrt{3} & -1 \end{pmatrix}$	6	$\begin{pmatrix} -2 & -1 + \sqrt{3} & -1 \end{pmatrix}$	7	$\begin{pmatrix} 1+\sqrt{3} & 2 & -1 \end{pmatrix}$	8	$\begin{pmatrix} 1-\sqrt{3} & -\sqrt{3}-1 & -1 \end{pmatrix}$
9	$\begin{pmatrix} 1 - \sqrt{3} & 2 & 1 \end{pmatrix}$	10	$\begin{pmatrix} -2 & -\sqrt{3} - 1 & 1 \end{pmatrix}$	11	$\begin{pmatrix} 2 & 1 + \sqrt{3} & 1 \end{pmatrix}$	12	$\begin{pmatrix} -1 + \sqrt{3} & -2 & 1 \end{pmatrix}$
13	$\left(-\sqrt{3}-1 1-\sqrt{3} -1\right)$	14	$\begin{pmatrix} -2 & -1 + \sqrt{3} & 1 \end{pmatrix}$	15	$\begin{pmatrix} 1+\sqrt{3} & 2 & 1 \end{pmatrix}$	16	$\begin{pmatrix} 1 - \sqrt{3} & -\sqrt{3} - 1 & 1 \end{pmatrix}$
17	$\begin{pmatrix} 1+\sqrt{3} & -1+\sqrt{3} & -1 \end{pmatrix}$	18	$\begin{pmatrix} 2 & 1 - \sqrt{3} & 1 \end{pmatrix}$	19	$\left(-\sqrt{3}-1 -2 1\right)$	20	$\begin{pmatrix} -1 + \sqrt{3} & 1 + \sqrt{3} & 1 \end{pmatrix}$
21	$\left(-1+\sqrt{3} -2 -1\right)$	22	$\begin{pmatrix} 2 & 1 + \sqrt{3} & -1 \end{pmatrix}$	23	$\begin{pmatrix} -2 & -\sqrt{3} - 1 & -1 \end{pmatrix}$	24	$\begin{pmatrix} 1-\sqrt{3} & 2 & -1 \end{pmatrix}$

Table 16: Virtual-cluster basis.

$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$											
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$		1	2	3	4	5	6	7	8	9	10
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	$\mathbb{Q}_0^{(A_{1g})}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$							
$ \mathbb{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}$		$\frac{\sqrt{6}}{12}$		$\frac{\sqrt{6}}{12}$			$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$
$ \mathbb{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}$		$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$						
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	$\mathbb{Q}_{1}^{(A_{2u})}$	$\frac{\sqrt{6}}{12}$		$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$			$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	
$ \begin{array}{ c c c c c c }\hline \mathbb{Q}_{1,0}^{(E1u)} & \frac{\sqrt{6}}{24} + \frac{\sqrt{2}}{8} & -\frac{\sqrt{2}}{8} - \frac{\sqrt{6}}{24} & \frac{\sqrt{6}}{24} + \frac{\sqrt{2}}{8} & -\frac{\sqrt{6}}{12} & -\frac{\sqrt{2}}{8} + \frac{\sqrt{6}}{24} & -\frac{\sqrt{2}}{8} - \frac{\sqrt{6}}{24} & \frac{\sqrt{6}}{12} & -\frac{\sqrt{2}}{8} + \frac{\sqrt{2}}{24} \\ & -\frac{\sqrt{6}}{24} + \frac{\sqrt{2}}{8} & \frac{\sqrt{6}}{12} & -\frac{\sqrt{2}}{8} - \frac{\sqrt{6}}{24} & -\frac{\sqrt{2}}{8} - \frac{\sqrt{6}}{24} & \frac{\sqrt{6}}{12} & -\frac{\sqrt{2}}{4} + \frac{\sqrt{2}}{8} & \frac{\sqrt{6}}{24} + \frac{\sqrt{2}}{8} & -\frac{\sqrt{6}}{12} & -\frac{\sqrt{2}}{8} + \frac{\sqrt{2}}{24} \\ & \frac{\sqrt{6}}{12} & -\frac{\sqrt{2}}{24} + \frac{\sqrt{2}}{8} & -\frac{\sqrt{2}}{8} + \frac{\sqrt{6}}{24} & -\frac{\sqrt{6}}{12} \\ & & & & & & & & & & & & & & & & & & $		$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$		$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$						
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	$\mathbb{Q}_{1,0}^{(E_{1u})}$		$-\frac{\sqrt{2}}{8} - \frac{\sqrt{6}}{24}$			$-\frac{\sqrt{2}}{8} + \frac{\sqrt{6}}{24}$	$-\frac{\sqrt{2}}{8} - \frac{\sqrt{6}}{24}$				
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$\frac{\sqrt{6}}{24} + \frac{\sqrt{2}}{8} \qquad -\frac{\sqrt{6}}{12} \qquad -\frac{\sqrt{2}}{8} + \frac{\sqrt{6}}{24} \qquad -\frac{\sqrt{6}}{24} + \frac{\sqrt{2}}{8} \qquad \frac{\sqrt{6}}{12} \qquad -\frac{\sqrt{2}}{8} - \frac{\sqrt{6}}{24} \qquad -\frac{\sqrt{6}}{24} + \frac{\sqrt{2}}{8} \qquad -\frac{\sqrt{2}}{8} + \frac{\sqrt{6}}{24} \qquad -\frac{\sqrt{6}}{12} \qquad \frac{\sqrt{6}}{24} + \frac{\sqrt{2}}{8} \qquad -\frac{\sqrt{6}}{12} \qquad -\sqrt{6$		$\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{24} + \frac{\sqrt{2}}{8}$	$-\frac{\sqrt{2}}{8} + \frac{\sqrt{6}}{24}$	$-\frac{\sqrt{6}}{12}$						
$\frac{\sqrt{6}}{24} + \frac{\sqrt{2}}{8} \qquad -\frac{\sqrt{6}}{12} \qquad -\frac{\sqrt{2}}{8} + \frac{\sqrt{6}}{24} \qquad -\frac{\sqrt{6}}{24} + \frac{\sqrt{2}}{8} \qquad \frac{\sqrt{6}}{12} \qquad -\frac{\sqrt{2}}{8} - \frac{\sqrt{6}}{24} \qquad -\frac{\sqrt{6}}{24} + \frac{\sqrt{2}}{8} \qquad -\frac{\sqrt{2}}{8} + \frac{\sqrt{6}}{24} \qquad -\frac{\sqrt{6}}{12} \qquad \frac{\sqrt{6}}{24} + \frac{\sqrt{2}}{8} \qquad -\frac{\sqrt{6}}{12} \qquad -\sqrt{6$	$\mathbb{Q}_{1,1}^{(E_{1u})}$		$-\frac{\sqrt{2}}{8} + \frac{\sqrt{6}}{24}$		$-\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{24} + \frac{\sqrt{2}}{8}$				$\frac{\sqrt{6}}{12}$	
$\sqrt{6}$ $\sqrt{6}$ $\sqrt{2}$ $\sqrt{2}$ $\sqrt{6}$ $\sqrt{6}$		$\frac{\sqrt{6}}{24} + \frac{\sqrt{2}}{8}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{2}}{8} + \frac{\sqrt{6}}{24}$	$-\frac{\sqrt{6}}{24} + \frac{\sqrt{2}}{8}$	$\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{2}}{8} - \frac{\sqrt{6}}{24}$	$-\frac{\sqrt{6}}{24} + \frac{\sqrt{2}}{8}$	$-\frac{\sqrt{2}}{8} + \frac{\sqrt{6}}{24}$	$-\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{24} + \frac{\sqrt{2}}{8}$
		$-\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{24} + \frac{\sqrt{2}}{8}$	$-\frac{\sqrt{2}}{8} - \frac{\sqrt{6}}{24}$	$\frac{\sqrt{6}}{12}$						
	$\mathbb{Q}_{2,0}^{(E_{1g})}$	$\frac{\sqrt{6}}{24} + \frac{\sqrt{2}}{8}$	$-\frac{\sqrt{2}}{8} - \frac{\sqrt{6}}{24}$			$-\frac{\sqrt{6}}{24} + \frac{\sqrt{2}}{8}$	$\frac{\sqrt{6}}{24} + \frac{\sqrt{2}}{8}$				$-\frac{\sqrt{2}}{8} + \frac{\sqrt{6}}{24}$
$-\frac{\sqrt{6}}{24} + \frac{\sqrt{2}}{8} \qquad \frac{\sqrt{6}}{12} \qquad \frac{\sqrt{6}}{24} + \frac{\sqrt{2}}{8} \qquad -\frac{\sqrt{2}}{8} - \frac{\sqrt{6}}{24} \qquad \frac{\sqrt{6}}{12} \qquad -\frac{\sqrt{6}}{24} + \frac{\sqrt{2}}{8} \qquad -\frac{\sqrt{2}}{8} - \frac{\sqrt{6}}{24} \qquad \frac{\sqrt{6}}{24} + \frac{\sqrt{2}}{8} \qquad -\frac{\sqrt{6}}{12} \qquad -\frac{\sqrt{6}}{8} + \frac{\sqrt{2}}{24} \qquad \frac{\sqrt{6}}{12} \qquad -\frac{\sqrt{6}}{12} \qquad -\frac{\sqrt{6}}$		$-\frac{\sqrt{6}}{24} + \frac{\sqrt{2}}{8}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{24} + \frac{\sqrt{2}}{8}$	$-\frac{\sqrt{2}}{8} - \frac{\sqrt{6}}{24}$	$\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{24} + \frac{\sqrt{2}}{8}$	$-\frac{\sqrt{2}}{8} - \frac{\sqrt{6}}{24}$	$\frac{\sqrt{6}}{24} + \frac{\sqrt{2}}{8}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{2}}{8} + \frac{\sqrt{6}}{24}$
$-\frac{\sqrt{6}}{12}$ $-\frac{\sqrt{2}}{8} + \frac{\sqrt{6}}{24}$ $-\frac{\sqrt{6}}{24} + \frac{\sqrt{2}}{8}$ $\frac{\sqrt{6}}{12}$		$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{2}}{8} + \frac{\sqrt{6}}{24}$	$-\frac{\sqrt{6}}{24} + \frac{\sqrt{2}}{8}$							
$\mathbb{Q}_{2,1}^{(E_{1g})} -\frac{\sqrt{6}}{24} + \frac{\sqrt{2}}{8} -\frac{\sqrt{2}}{8} + \frac{\sqrt{6}}{24} -\frac{\sqrt{6}}{24} + \frac{\sqrt{2}}{8} \frac{\sqrt{6}}{12} -\frac{\sqrt{2}}{8} - \frac{\sqrt{6}}{24} -\frac{\sqrt{2}}{8} + \frac{\sqrt{6}}{24} -\frac{\sqrt{6}}{12} \frac{\sqrt{6}}{24} + \frac{\sqrt{2}}{8} \frac{\sqrt{6}}{12} -\frac{\sqrt{2}}{8} - \frac{\sqrt{2}}{24} + \frac{\sqrt{2}}{24} -\frac{\sqrt{2}}{8} - \frac{\sqrt{2}}{24} + \frac{\sqrt{2}}{8} \frac{\sqrt{6}}{12} -\frac{\sqrt{2}}{8} - \frac{\sqrt{2}}{24} + \frac{\sqrt{2}}{24} -\frac{\sqrt{2}}{8} - \frac{\sqrt{2}}{24} + \frac{\sqrt{2}}{8} \frac{\sqrt{6}}{12} -\frac{\sqrt{2}}{8} - \frac{\sqrt{2}}{24} + \frac{\sqrt{2}}{8} -\frac{\sqrt{2}}{8} - \frac{\sqrt{2}}{8} - \frac$	$\mathbb{Q}_{2,1}^{(E_{1g})}$	$-\frac{\sqrt{6}}{24} + \frac{\sqrt{2}}{8}$	$-\frac{\sqrt{2}}{8} + \frac{\sqrt{6}}{24}$	$-\frac{\sqrt{6}}{24} + \frac{\sqrt{2}}{8}$	$\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{2}}{8} - \frac{\sqrt{6}}{24}$	$-\frac{\sqrt{2}}{8} + \frac{\sqrt{6}}{24}$	$-\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{24} + \frac{\sqrt{2}}{8}$	$\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{2}}{8} - \frac{\sqrt{6}}{24}$

 $continued\ \dots$

Table 16

symbol	1	2	3	4	5	6	7	8	9	10
	$\frac{\sqrt{6}}{24} + \frac{\sqrt{2}}{8}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{24} + \frac{\sqrt{2}}{8}$	$-\frac{\sqrt{6}}{24} + \frac{\sqrt{2}}{8}$	$\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{2}}{8} - \frac{\sqrt{6}}{24}$	$-\frac{\sqrt{2}}{8} + \frac{\sqrt{6}}{24}$	$-\frac{\sqrt{2}}{8} + \frac{\sqrt{6}}{24}$	$-\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{24} + \frac{\sqrt{2}}{8}$
	$\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{2}}{8} - \frac{\sqrt{6}}{24}$	$\frac{\sqrt{6}}{24} + \frac{\sqrt{2}}{8}$	$-\frac{\sqrt{6}}{12}$	12	0 24	0 24	0 24	12	24 0
$\mathbb{Q}_{2,0}^{(E_{2g})}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	0	$-\frac{1}{4}$	$\frac{1}{4}$	0	$-\frac{1}{4}$	0	$-\frac{1}{4}$
	$-\frac{1}{4}$	0	$\frac{1}{4}$	$\frac{1}{4}$	0	$-\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	0	$-\frac{1}{4}$
	0	$-\frac{1}{4}$	$-\frac{1}{4}$	0						
$\mathbb{Q}_{2,1}^{(E_{2g})}$	$-\frac{\sqrt{3}}{12}$	$-\frac{\sqrt{3}}{12}$	$\frac{\sqrt{3}}{12}$	$-\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{12}$	$\frac{\sqrt{3}}{12}$	$-\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{12}$	$\frac{\sqrt{3}}{6}$	$-\frac{\sqrt{3}}{12}$
	$-\frac{\sqrt{3}}{12}$	$\frac{\sqrt{3}}{6}$	$-\frac{\sqrt{3}}{12}$	$\frac{\sqrt{3}}{12}$	$-\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{12}$	$-\frac{\sqrt{3}}{12}$	$\frac{\sqrt{3}}{12}$	$-\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{12}$
	$\frac{\sqrt{3}}{6}$	$-\frac{\sqrt{3}}{12}$	$-\frac{\sqrt{3}}{12}$	$\frac{\sqrt{3}}{6}$						
$\mathbb{Q}_3^{(B_{1u})}$	$\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$
	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$
	$-\frac{\sqrt{6}}{12}$ $\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$						
$\mathbb{Q}_3^{(B_{2u})}$	$\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$-rac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$
	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$-rac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$
	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$						
$\mathbb{Q}_{3,0}^{(E_{2u})}$	$\frac{1}{4}$	$\frac{1}{4}$	$-\frac{1}{4}$	0	$\frac{1}{4}$	$-\frac{1}{4}$	0	$\frac{1}{4}$	0	$-\frac{1}{4}$
	$-\frac{1}{4}$	0	$-\frac{1}{4}$	$\frac{1}{4}$	0	$-\frac{1}{4}$	$-\frac{1}{4}$	$\frac{1}{4}$	0	$-\frac{1}{4}$
	0	1/4 -	1/4 	0						
$\mathbb{Q}_{3,1}^{(E_{2u})}$	$-\frac{\sqrt{3}}{12}$	$-\frac{\sqrt{3}}{12}$	$-\frac{\sqrt{3}}{12}$	$\frac{\sqrt{3}}{6}$	$-\frac{\sqrt{3}}{12}$	$-\frac{\sqrt{3}}{12}$	$\frac{\sqrt{3}}{6}$	$-\frac{\sqrt{3}}{12}$	$\frac{\sqrt{3}}{6}$	$-\frac{\sqrt{3}}{12}$
	$-\frac{\sqrt{3}}{12}$	$\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{12}$	$\frac{\sqrt{3}}{12}$	$-\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{12}$	$\frac{\sqrt{3}}{12}$	$\frac{\sqrt{3}}{12}$	$-\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{12}$
(P.)	$-\frac{\sqrt{3}}{6}$ $\frac{\sqrt{6}}{12}$	$\frac{\sqrt{3}}{12}$	$\frac{\sqrt{3}}{12}$	$-\frac{\sqrt{3}}{6}$						
$\mathbb{Q}_4^{(B_{1g})}$	$\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$
	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$
(P-)	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$						
$\mathbb{Q}_4^{(B_{2g})}$	$\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$
	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$
(Eq. 1)	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	<u></u>	<i>(</i> 5	<u></u>	<u> </u>		
$\mathbb{Q}_{4,0}^{(E_{2g},1)}$	$\frac{\sqrt{3}}{12}$	$\frac{\sqrt{3}}{12}$	$\frac{\sqrt{3}}{12}$	$-\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{12}$	$\frac{\sqrt{3}}{12}$	$-\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{12}$	$-\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{12}$
	$\frac{\sqrt{3}}{12}$	$-\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{12}$	$\frac{\sqrt{3}}{12}$	$-\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{12}$	$\frac{\sqrt{3}}{12}$	$\frac{\sqrt{3}}{12}$	$-\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{12}$
	$-\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{12}$	$\frac{\sqrt{3}}{12}$	$-\frac{\sqrt{3}}{6}$						

 $continued\ \dots$

Table 16

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$ \begin{array}{ c c c c c c }\hline \mathbb{Q}_{5,0}^{(E_{1u},1)} & -\frac{\sqrt{2}}{\sqrt{6}} + \frac{\sqrt{8}}{8} & -\frac{\sqrt{2}}{\sqrt{2}} + \frac{\sqrt{6}}{\sqrt{4}} & -\frac{\sqrt{4}}{\sqrt{4}} + \frac{\sqrt{8}}{8} & \frac{\sqrt{6}}{\sqrt{2}} & -\frac{\sqrt{2}}{8} - \frac{\sqrt{6}}{\sqrt{4}} & -\frac{\sqrt{2}}{8} + \frac{\sqrt{6}}{\sqrt{2}} & -\frac{\sqrt{6}}{\sqrt{2}} & \frac{\sqrt{6}}{\sqrt{2}} + \frac{\sqrt{2}}{\sqrt{2}} & \frac{\sqrt{6}}{\sqrt{2}} & \sqrt{6$
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$\begin{array}{ c c c c c c }\hline \mathbb{Q}_{5,1}^{(E_{2u},1)} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & 0 & -\frac{1}{4} & \frac{1}{4} & 0 & -\frac{1}{4} & 0 & -\frac{1}{4} \\ & -\frac{1}{4} & 0 & -\frac{1}{4} & -\frac{1}{4} & 0 & \frac{1}{4} & -\frac{1}{4} & 0 & \frac{1}{4} \\ & 0 & \frac{1}{4} & \frac{1}{4} & 0 & & & & & & & & \\ \hline \mathbb{Q}_{6}^{(A_{2g})} & \frac{\sqrt{6}}{12} & \frac{\sqrt{6}}{12} & -\frac{\sqrt{6}}{12} & \frac{\sqrt{6}}{12} & \frac{\sqrt{6}}{12} \\ & \frac{\sqrt{6}}{12} & \frac{\sqrt{6}}{12} & \frac{\sqrt{6}}{12} & -\frac{\sqrt{6}}{12} & -\frac$
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$\begin{array}{ c c c c c c c c c }\hline & 0 & \frac{1}{4} & \frac{1}{4} & 0 \\ \hline \mathbb{Q}_{6}^{(A_{2g})} & \frac{\sqrt{6}}{12} & \frac{\sqrt{6}}{12} & -\frac{\sqrt{6}}{12} & -\frac{\sqrt{6}}{12} & -\frac{\sqrt{6}}{12} & -\frac{\sqrt{6}}{12} & -\frac{\sqrt{6}}{12} & -\frac{\sqrt{6}}{12} & \frac{\sqrt{6}}{12} & \frac{\sqrt{6}}{12} & \frac{\sqrt{6}}{12} & \frac{\sqrt{6}}{12} & \frac{\sqrt{6}}{12} & -\frac{\sqrt{6}}{12} & -\frac{\sqrt{6}}$
$ \begin{array}{ c c c c c c c c }\hline \mathbb{Q}_{6}^{(A_{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}}{1$
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$\frac{\sqrt{6}}{24} + \frac{\sqrt{2}}{8} \qquad -\frac{\sqrt{6}}{12} \qquad -\frac{\sqrt{6}}{24} + \frac{\sqrt{2}}{8} \qquad -\frac{\sqrt{2}}{8} + \frac{\sqrt{6}}{24} \qquad -\frac{\sqrt{6}}{12} \qquad \frac{\sqrt{6}}{24} + \frac{\sqrt{2}}{8} \qquad -\frac{\sqrt{2}}{8} + \frac{\sqrt{6}}{24} \qquad -\frac{\sqrt{6}}{24} + \frac{\sqrt{2}}{8} \qquad \frac{\sqrt{6}}{12} \qquad -\frac{\sqrt{2}}{8} - \frac{\sqrt{2}}{24} + \frac{\sqrt{2}}{8} \qquad -\frac{\sqrt{2}}{8} + \frac{\sqrt{2}}{24} \qquad -\frac{\sqrt{2}}{8} + \frac{\sqrt{2}}{8} $
$\frac{\sqrt{6}}{12} \qquad -\frac{\sqrt{2}}{8} - \frac{\sqrt{6}}{24} \qquad \frac{\sqrt{6}}{24} + \frac{\sqrt{2}}{8} \qquad -\frac{\sqrt{6}}{12}$
$\mathbb{Q}_{6.1}^{(£_{1}g_{1})} -\frac{\sqrt{2}}{8} - \frac{\sqrt{6}}{24} \frac{\sqrt{6}}{24} + \frac{\sqrt{2}}{8} -\frac{\sqrt{2}}{8} - \frac{\sqrt{6}}{24} \frac{\sqrt{6}}{12} -\frac{\sqrt{6}}{24} + \frac{\sqrt{2}}{8} \frac{\sqrt{6}}{24} + \frac{\sqrt{2}}{8} -\frac{\sqrt{6}}{12} -\frac{\sqrt{2}}{24} + \frac{\sqrt{6}}{8} \frac{\sqrt{6}}{12} -\frac{\sqrt{2}}{24} + \frac{\sqrt{2}}{8} -\frac{\sqrt{6}}{12} -\frac{\sqrt{2}}{24} + \frac{\sqrt{6}}{8} \frac{\sqrt{6}}{12} -\frac{\sqrt{6}}{24} + \frac{\sqrt{2}}{8} -\frac{\sqrt{6}}{12} -\frac{\sqrt{6}}{24} + \frac{\sqrt{2}}{8} -\frac{\sqrt{6}}{12} -\frac{\sqrt{6}}{24} + \frac{\sqrt{6}}{8} -\frac{\sqrt{6}}{12} -\frac{\sqrt{6}}{12} -\frac{\sqrt{6}}{24} + \frac{\sqrt{6}}{8} -\frac{\sqrt{6}}{12} -\frac{\sqrt{6}}{$
$-\frac{\sqrt{2}}{8} + \frac{\sqrt{6}}{24} \qquad -\frac{\sqrt{6}}{12} \qquad -\frac{\sqrt{2}}{8} - \frac{\sqrt{6}}{24} \qquad -\frac{\sqrt{2}}{8} - \frac{\sqrt{6}}{24} \qquad \frac{\sqrt{6}}{12} \qquad -\frac{\sqrt{6}}{24} + \frac{\sqrt{2}}{8} \qquad \frac{\sqrt{6}}{24} + \frac{\sqrt{2}}{8} \qquad \frac{\sqrt{6}}{24} + \frac{\sqrt{2}}{8} \qquad -\frac{\sqrt{6}}{12} \qquad -\frac{\sqrt{2}}{8} + \frac{\sqrt{2}}{24} \qquad \frac{\sqrt{6}}{12} \qquad -\frac{\sqrt{6}}{12} \qquad -\frac{\sqrt{6}$
$\frac{\sqrt{6}}{12}$ $-\frac{\sqrt{6}}{24} + \frac{\sqrt{2}}{8}$ $-\frac{\sqrt{2}}{8} + \frac{\sqrt{6}}{24}$ $-\frac{\sqrt{6}}{12}$
$\frac{\sqrt{6}}{12} \qquad \frac{\sqrt{6}}{12} \qquad -\frac{\sqrt{6}}{12} \qquad -\frac{\sqrt{6}}{12}$
$-\frac{\sqrt{6}}{12}$ $-\frac{\sqrt{6}}{12}$ $-\frac{\sqrt{6}}{12}$ $-\frac{\sqrt{6}}{12}$