

# 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**

- Unit cell:
  - $a = 2.435$ ,  $b = 2.435$ ,  $c = 10.0$ ,  $\alpha = 90.0$ ,  $\beta = 90.0$ ,  $\gamma = 120.0$
- Lattice vectors:
  - $\mathbf{a}_1 = (2.435 \ 0 \ 0)$
  - $\mathbf{a}_2 = (-1.2175 \ 2.10877185821511 \ 0)$
  - $\mathbf{a}_3 = (0 \ 0 \ 10.0)$

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

symbol	position	symbol	position	symbol	position
$\Gamma$	$\begin{pmatrix} 0 & 0 & 0 \end{pmatrix}$	M	$\begin{pmatrix} \frac{1}{2} & 0 & 0 \end{pmatrix}$	K	$\begin{pmatrix} \frac{1}{3} & \frac{1}{3} & 0 \end{pmatrix}$
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 <sub>1</sub> A <sub>1</sub>	$\begin{pmatrix} \frac{1}{3} & \frac{2}{3} & 0 \end{pmatrix}$	[1,6,7,8,9,10,14,15,16,17,23,24]
A <sub>2</sub>	$\begin{pmatrix} \frac{2}{3} & \frac{1}{3} & 0 \end{pmatrix}$	[2,3,4,5,11,12,13,18,19,20,21,22]

- Bonds in (primitive) unit cell:

Table 4: Bond-clusters.

bond	tail	head	$n$	#	$\mathbf{b} @ \mathbf{c}$	mapping	
B <sub>1</sub>	b <sub>1</sub>	A <sub>2</sub>	A <sub>1</sub>	1	1	$\left(\frac{1}{3} \quad \frac{2}{3} \quad 0\right) @ \left(\frac{1}{2} \quad 0 \quad 0\right)$	[1,-2,-3,6,-13,14,17,-18]
	b <sub>2</sub>	A <sub>2</sub>	A <sub>1</sub>	1	1	$\left(\frac{1}{3} \quad -\frac{1}{3} \quad 0\right) @ \left(\frac{1}{2} \quad \frac{1}{2} \quad 0\right)$	[-4,7,10,-11,15,-19,-22,23]
	b <sub>3</sub>	A <sub>2</sub>	A <sub>1</sub>	1	1	$\left(-\frac{2}{3} \quad -\frac{1}{3} \quad 0\right) @ \left(0 \quad \frac{1}{2} \quad 0\right)$	[-5,8,9,-12,16,-20,-21,24]
B <sub>2</sub>	b <sub>4</sub>	A <sub>1</sub>	A <sub>1</sub>	2	1	$\left(0 \quad 1 \quad 0\right) @ \left(\frac{1}{3} \quad \frac{1}{6} \quad 0\right)$	[1,-7,-15,17]
	b <sub>5</sub>	A <sub>2</sub>	A <sub>2</sub>	2	1	$\left(0 \quad 1 \quad 0\right) @ \left(\frac{2}{3} \quad \frac{5}{6} \quad 0\right)$	[-2,4,-13,19]
	b <sub>6</sub>	A <sub>2</sub>	A <sub>2</sub>	2	1	$\left(1 \quad 1 \quad 0\right) @ \left(\frac{1}{6} \quad \frac{5}{6} \quad 0\right)$	[-3,12,-18,21]
	b <sub>7</sub>	A <sub>2</sub>	A <sub>2</sub>	2	1	$\left(1 \quad 0 \quad 0\right) @ \left(\frac{1}{6} \quad \frac{1}{3} \quad 0\right)$	[5,-11,20,-22]
	b <sub>8</sub>	A <sub>1</sub>	A <sub>1</sub>	2	1	$\left(1 \quad 1 \quad 0\right) @ \left(\frac{5}{6} \quad \frac{1}{6} \quad 0\right)$	[6,-9,14,-24]
	b <sub>9</sub>	A <sub>1</sub>	A <sub>1</sub>	2	1	$\left(1 \quad 0 \quad 0\right) @ \left(\frac{5}{6} \quad \frac{2}{3} \quad 0\right)$	[-8,10,-16,23]

- SAMB:

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

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

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

$$\boxed{\text{No. 2}} \quad \hat{\mathbb{Q}}_0^{(A_{1g})} [\text{M}_1, \text{B}_1]$$

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

$$\hat{\mathbb{Z}}_2(\mathbf{k}) = \frac{\sqrt{2}\mathbb{X}_1[\mathbb{Q}_0^{(a, A_{1g})}] \otimes \mathbb{U}_2[\mathbb{Q}_0^{(u, A_{1g})}] \otimes \mathbb{F}_1[\mathbb{Q}_0^{(k, A_{1g})}]}{2} - \frac{\sqrt{2}\mathbb{X}_1[\mathbb{Q}_0^{(a, A_{1g})}] \otimes \mathbb{U}_3[\mathbb{T}_3^{(u, B_{1u})}] \otimes \mathbb{F}_2[\mathbb{T}_3^{(k, B_{1u})}]}{2}$$

$$\boxed{\text{No. 3}} \quad \hat{\mathbb{Q}}_0^{(A_{1g})} [\text{M}_1, \text{B}_2]$$

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

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

Table 5: Atomic SAMB group.

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

Table 6: Atomic SAMB.

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

Table 7: Cluster SAMB.

symbol	type	cluster	form
$\mathbb{Y}_1$	$\mathbb{Q}_0^{(s, A_{1g})}$	$S_1$	$\begin{pmatrix} \frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2} \end{pmatrix}$
$\mathbb{Y}_2$	$\mathbb{Q}_0^{(b, A_{1g})}$	$B_1$	$\begin{pmatrix} \frac{\sqrt{3}}{3} & \frac{\sqrt{3}}{3} & \frac{\sqrt{3}}{3} \end{pmatrix}$
$\mathbb{Y}_3$	$\mathbb{Q}_0^{(b, A_{1g})}$	$B_2$	$\begin{pmatrix} \frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} \end{pmatrix}$

Table 8: Uniform SAMB.

symbol	type	cluster	form
$\mathbb{U}_1$	$\mathbb{Q}_0^{(s, A_{1g})}$	$S_1$	$\begin{pmatrix} \frac{\sqrt{2}}{2} & 0 \\ 0 & \frac{\sqrt{2}}{2} \end{pmatrix}$
$\mathbb{U}_2$	$\mathbb{Q}_0^{(u, A_{1g})}$	$B_1$	$\begin{pmatrix} 0 & \frac{\sqrt{2}}{2} \\ \frac{\sqrt{2}}{2} & 0 \end{pmatrix}$
$\mathbb{U}_3$	$\mathbb{T}_3^{(u, B_{1u})}$	$B_1$	$\begin{pmatrix} 0 & -\frac{\sqrt{2}i}{2} \\ \frac{\sqrt{2}i}{2} & 0 \end{pmatrix}$

Table 9: Structure SAMB.

symbol	type	cluster	form
$\mathbb{F}_1$	$\mathbb{Q}_0^{(k, A_{1g})}$	$B_1$	$\frac{\sqrt{6}c_{001}}{3} + \frac{\sqrt{6}c_{002}}{3} + \frac{\sqrt{6}c_{003}}{3}$
$\mathbb{F}_2$	$\mathbb{T}_3^{(k, B_{1u})}$	$B_1$	$\frac{\sqrt{6}s_{001}}{3} + \frac{\sqrt{6}s_{002}}{3} + \frac{\sqrt{6}s_{003}}{3}$
$\mathbb{F}_3$	$\mathbb{Q}_0^{(k, A_{1g})}$	$B_2$	$\frac{\sqrt{6}c_{004}}{3} + \frac{\sqrt{6}c_{006}}{3} + \frac{\sqrt{6}c_{007}}{3}$

Table 10: Polar harmonics.

No.	symbol	rank	irrep.	mul.	comp.	form
1	$\mathbb{Q}_0^{(A_{1g})}$	0	$A_{1g}$	—	—	1
2	$\mathbb{Q}_3^{(B_{1u})}$	3	$B_{1u}$	—	—	$\frac{\sqrt{10}y(3x^2 - y^2)}{4}$

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

Table 11: Conjugacy class (point-group part).

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

*continued ...*

Table 11

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

Table 12: Symmetry operations.

No.	SO	No.	SO	No.	SO	No.	SO	No.	SO
1	$\{1 0\}$	2	$\{2_{001} 0\}$	3	$\{2_{100} 0\}$	4	$\{2_{010} 0\}$	5	$\{2_{110} 0\}$
6	$\{2_{120} 0\}$	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	$\{\mathbf{m}_{100} 0\}$	15	$\{\mathbf{m}_{010} 0\}$
16	$\{\mathbf{m}_{110} 0\}$	17	$\{\mathbf{m}_{001} 0\}$	18	$\{\mathbf{m}_{120} 0\}$	19	$\{\mathbf{m}_{210} 0\}$	20	$\{\mathbf{m}_{1-10} 0\}$
21	$\{-3_{001}^+ 0\}$	22	$\{-3_{001}^- 0\}$	23	$\{-6_{001}^+ 0\}$	24	$\{-6_{001}^- 0\}$		

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

	1	$2_{001}$	$2_{100}$	$2_{120}$	$3_{001}^+$	$6_{001}^+$	-1	$\mathbf{m}_{100}$	$\mathbf{m}_{001}$	$\mathbf{m}_{120}$	$-3_{001}^+$	$-6_{001}^+$
$A_{1g}$	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

continued ...

Table 13

	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>
$E_{2u}$	2	2	0	0	-1	-1	-2	0	-2	0	1	1

Table 14: 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 15: 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 16: 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 17: Virtual-cluster sites.

No.	position	No.	position	No.	position	No.	position
1	$\begin{pmatrix} 1+\sqrt{3} & -1+\sqrt{3} & 1 \end{pmatrix}$	2	$\begin{pmatrix} -\sqrt{3}-1 & 1-\sqrt{3} & 1 \end{pmatrix}$	3	$\begin{pmatrix} 2 & 1-\sqrt{3} & -1 \end{pmatrix}$	4	$\begin{pmatrix} -\sqrt{3}-1 & -2 & -1 \end{pmatrix}$
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	$\begin{pmatrix} -\sqrt{3}-1 & 1-\sqrt{3} & -1 \end{pmatrix}$	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	$\begin{pmatrix} -\sqrt{3}-1 & -2 & 1 \end{pmatrix}$	20	$\begin{pmatrix} -1+\sqrt{3} & 1+\sqrt{3} & 1 \end{pmatrix}$
21	$\begin{pmatrix} -1+\sqrt{3} & -2 & -1 \end{pmatrix}$	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 18: Virtual-cluster basis.

symbol	1	2	3	4	5	6	7	8	9	10
$\mathbb{Q}_0^{(A_{1g})}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$
	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$
	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$						
$\mathbb{Q}_1^{(A_{2u})}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$
	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$
	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$						
$\mathbb{Q}_{1,0}^{(E_{1u})}$	$\frac{\sqrt{6}}{24} + \frac{\sqrt{2}}{8}$	$-\frac{\sqrt{2}}{8} - \frac{\sqrt{6}}{24}$	$\frac{\sqrt{6}}{24} + \frac{\sqrt{2}}{8}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{2}}{8} + \frac{\sqrt{6}}{24}$	$-\frac{\sqrt{2}}{8} - \frac{\sqrt{6}}{24}$	$\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{24} + \frac{\sqrt{2}}{8}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{2}}{8} + \frac{\sqrt{6}}{24}$
	$-\frac{\sqrt{6}}{24} + \frac{\sqrt{2}}{8}$	$\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{2}}{8} - \frac{\sqrt{6}}{24}$	$-\frac{\sqrt{2}}{8} - \frac{\sqrt{6}}{24}$	$\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{24} + \frac{\sqrt{2}}{8}$	$\frac{\sqrt{6}}{24} + \frac{\sqrt{2}}{8}$	$\frac{\sqrt{6}}{24} + \frac{\sqrt{2}}{8}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{2}}{8} + \frac{\sqrt{6}}{24}$
	$\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{2}}{24} + \frac{\sqrt{6}}{8}$	$-\frac{\sqrt{2}}{8} + \frac{\sqrt{6}}{24}$	$-\frac{\sqrt{6}}{12}$						
$\mathbb{Q}_{1,1}^{(E_{1u})}$	$-\frac{\sqrt{6}}{24} + \frac{\sqrt{2}}{8}$	$-\frac{\sqrt{2}}{8} + \frac{\sqrt{6}}{24}$	$-\frac{\sqrt{2}}{8} + \frac{\sqrt{6}}{24}$	$-\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{24} + \frac{\sqrt{2}}{8}$	$-\frac{\sqrt{6}}{24} + \frac{\sqrt{2}}{8}$	$\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{2}}{8} - \frac{\sqrt{6}}{24}$	$\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{2}}{8} - \frac{\sqrt{6}}{24}$
	$\frac{\sqrt{6}}{24} + \frac{\sqrt{2}}{8}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{2}}{8} + \frac{\sqrt{6}}{24}$	$-\frac{\sqrt{2}}{24} + \frac{\sqrt{6}}{8}$	$\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{2}}{8} - \frac{\sqrt{6}}{24}$	$-\frac{\sqrt{6}}{24} + \frac{\sqrt{2}}{8}$	$-\frac{\sqrt{2}}{8} + \frac{\sqrt{6}}{24}$	$-\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{24} + \frac{\sqrt{2}}{8}$
	$-\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{24} + \frac{\sqrt{2}}{8}$	$-\frac{\sqrt{2}}{8} - \frac{\sqrt{6}}{24}$	$\frac{\sqrt{6}}{12}$						
$\mathbb{Q}_{2,0}^{(E_{1g})}$	$\frac{\sqrt{6}}{24} + \frac{\sqrt{2}}{8}$	$-\frac{\sqrt{2}}{8} - \frac{\sqrt{6}}{24}$	$-\frac{\sqrt{2}}{8} - \frac{\sqrt{6}}{24}$	$\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{24} + \frac{\sqrt{2}}{8}$	$\frac{\sqrt{6}}{24} + \frac{\sqrt{2}}{8}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{2}}{8} + \frac{\sqrt{6}}{24}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{2}}{8} + \frac{\sqrt{6}}{24}$
	$-\frac{\sqrt{6}}{24} + \frac{\sqrt{2}}{8}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{24} + \frac{\sqrt{2}}{8}$	$-\frac{\sqrt{2}}{8} - \frac{\sqrt{6}}{24}$	$\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{24} + \frac{\sqrt{2}}{8}$	$-\frac{\sqrt{2}}{8} - \frac{\sqrt{6}}{24}$	$\frac{\sqrt{6}}{24} + \frac{\sqrt{2}}{8}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{2}}{8} + \frac{\sqrt{6}}{24}$

continued ...



[illegible]

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