Model for “graphene”

Generated on 2026-01-20 13:25:06 by MultiPie 2.0.1

General Condition

- Basis type: `lg`
- SAMB selection:
  - Type: `[Q, G]`
  - Rank: `[0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11]`
  - Irrep.: [A_{1g}, A_{2g}, B_{1g}, B_{2g}, E_{1g}, E_{2g}, A_{1u}, A_{2u}, B_{1u}, B_{2u}, E_{1u}, E_{2u}]
  - Spin (s): `[0, 1]`
- Atomic selection:
  - Type: `[Q, G, M, T]`
  - Rank: `[0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11]`
  - Irrep.: [A_{1g}, A_{2g}, B_{1g}, B_{2g}, E_{1g}, E_{2g}, A_{1u}, A_{2u}, B_{1u}, B_{2u}, E_{1u}, E_{2u}]
  - Spin (s): `[0, 1]`
- Site-cluster selection:
  - Rank: `[0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11]`
  - Irrep.: [A_{1g}, A_{2g}, B_{1g}, B_{2g}, E_{1g}, E_{2g}, A_{1u}, A_{2u}, B_{1u}, B_{2u}, E_{1u}, E_{2u}]
- Bond-cluster selection:
  - Type: `[Q, G, M, T]`
  - Rank: `[0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11]`
  - Irrep.: [A_{1g}, A_{2g}, B_{1g}, B_{2g}, E_{1g}, E_{2g}, A_{1u}, A_{2u}, B_{1u}, B_{2u}, E_{1u}, E_{2u}]
- Max. neighbor: `10`
- Search cell range: `(-2, 3), (-2, 3), (-2, 3)`
- Toroidal priority: `false`

Group and Unit Cell

- Group: SG No. 191 D_{6h}^{1} $P6/mmm$ [hexagonal]
- Associated point group: PG No. 191 D_{6h} $6/mmm$ [hexagonal]
- Unit cell:
  $a =$ 1.00000, $b =$ 1.00000, $c =$ 4.00000, $\alpha = 90.0$, $\beta = 90.0$, $\gamma = 120.0$
- Lattice vectors (conventional cell):
  $\boldsymbol{a}_1 =$ [1.00000, 0.00000, 0.00000]
  $\boldsymbol{a}_2 =$ [-0.50000, 0.86603, 0.00000]
  $\boldsymbol{a}_3 =$ [0.00000, 0.00000, 4.00000]

Symmetry Operation

Table 1: Symmetry operation

#	SO	#	SO	#	SO	#	SO	#	SO
1	$\{1\|0\}$	2	$\{3^{+}_{001}\|0\}$	3	$\{3^{-}_{001}\|0\}$	4	$\{2_{001}\|0\}$	5	$\{6^{-}_{001}\|0\}$
6	$\{6^{+}_{001}\|0\}$	7	$\{2_{110}\|0\}$	8	$\{2_{100}\|0\}$	9	$\{2_{010}\|0\}$	10	$\{2_{1-10}\|0\}$
11	$\{2_{120}\|0\}$	12	$\{2_{210}\|0\}$	13	$\{-1\|0\}$	14	$\{-3^{+}_{001}\|0\}$	15	$\{-3^{-}_{001}\|0\}$
16	$\{m_{001}\|0\}$	17	$\{-6^{-}_{001}\|0\}$	18	$\{-6^{+}_{001}\|0\}$	19	$\{m_{110}\|0\}$	20	$\{m_{100}\|0\}$
21	$\{m_{010}\|0\}$	22	$\{m_{1-10}\|0\}$	23	$\{m_{120}\|0\}$	24	$\{m_{210}\|0\}$		

Harmonics

Table 2: Harmonics

#	symbol	irrep.	rank	X	multiplicity	component	symmetry
1	$\mathbb{Q}_0(A_{1g})$	A_{1g}	0	Q, T	-	-	1
2	$\mathbb{G}_1(A_{2g})$	A_{2g}	1	G, M	-	-	z
3	$\mathbb{Q}_6(A_{2g})$	A_{2g}	6	Q, T	-	-	$\frac{\sqrt{462}xy\left(x^2-3y^2\right)\left(3x^2-y^2\right)}{16}$
4	$\mathbb{Q}_3(B_{1u})$	B_{1u}	3	Q, T	-	-	$\frac{\sqrt{10}y\left(3x^2-y^2\right)}{4}$
5	$\mathbb{Q}_3(B_{2u})$	B_{2u}	3	Q, T	-	-	$\frac{\sqrt{10}x\left(x^2-3y^2\right)}{4}$

continued ...

Table 2

#	symbol	irrep.	rank	X	multiplicity	component	symmetry
6	$\mathbb{Q}_{1,1}(E_{1u})$	E_{1u}	1	Q, T	-	1	x
7	$\mathbb{Q}_{1,2}(E_{1u})$					2	y
8	$\mathbb{Q}_{2,1}(E_{2g})$	E_{2g}	2	Q, T	-	1	$\frac{\sqrt{3}(x-y)(x+y)}{2}$
9	$\mathbb{Q}_{2,2}(E_{2g})$					2	$-\sqrt{3}xy$
10	$\mathbb{Q}_{4,1}(E_{2g},1)$	E_{2g}	4	Q, T	1	1	$\frac{\sqrt{35}\left(x^2-2xy-y^2\right)\left(x^2+2xy-y^2\right)}{8}$
11	$\mathbb{Q}_{4,2}(E_{2g},1)$					2	$\frac{\sqrt{35}xy(x-y)(x+y)}{2}$

Basis in full matrix

Table 3: dimension = 2

#	orbital@atom(SL)	#	orbital@atom(SL)
0	$\lvert p_z\rangle$ @C(1)	1	$\lvert p_z\rangle$ @C(2)

Table 4: Atomic basis (orbital part only)

orbital	definition
$\lvert p_x \rangle$	x
$\lvert p_y \rangle$	y
$\lvert p_z \rangle$	z

SAMB

22 (all 32) SAMBs

- 'C' site-cluster
  * bra: $\langle p_z \rvert$
  * ket: $\lvert p_z \rangle$
  * wyckoff: `2c`

$\boxed{\text{z1}}$ $\mathbb{Q}_0^{(c)}(A_{1g}) = \mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_0^{(s)}(A_{1g})$

$\boxed{\text{z23}}$ $\mathbb{Q}_3^{(c)}(B_{1u}) = \mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_3^{(s)}(B_{1u})$

- 'C'-'C' bond-cluster
  * bra: $\langle p_z \rvert$
  * ket: $\lvert p_z \rangle$
  * wyckoff: `3a@3f`

$\boxed{\text{z2}}$ $\mathbb{Q}_0^{(c)}(A_{1g}) = \mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_0^{(b)}(A_{1g})$

$\boxed{\text{z9}}$ $\mathbb{Q}_{2,1}^{(c)}(E_{2g}) = \dfrac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2}$

$\boxed{\text{z10}}$ $\mathbb{Q}_{2,2}^{(c)}(E_{2g}) = \dfrac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2}$

- 'C'-'C' bond-cluster
  * bra: $\langle p_z|$
  * ket: $|p_z\rangle$
  * wyckoff: `6b@6l`

$\boxed{\text{z3}}$ $\mathbb{Q}_0^{(c)}(A_{1g}) = \mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_0^{(b)}(A_{1g})$

$\boxed{\text{z11}}$ $\mathbb{Q}_3^{(c)}(B_{1u}) = \mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_3^{(b)}(B_{1u})$

$\boxed{\text{z12}}$ $\mathbb{Q}_{1,1}^{(c)}(E_{1u}) = \dfrac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{2}$

$\boxed{\text{z24}}$ $\mathbb{Q}_{1,2}^{(c)}(E_{1u}) = \dfrac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{2}$

$\boxed{\text{z27}}$ $\mathbb{Q}_{2,1}^{(c)}(E_{2g}) = \dfrac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2}$

$\boxed{\text{z28}}$ $\mathbb{Q}_{2,2}^{(c)}(E_{2g}) = \dfrac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2}$

- 'C'-'C' bond-cluster
  * bra: $\langle p_z|$
  * ket: $|p_z\rangle$
  * wyckoff: `3b@1a`

$\boxed{\text{z4}}$ $\mathbb{Q}_0^{(c)}(A_{1g}) = \mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_0^{(b)}(A_{1g})$

$\boxed{\text{z13}}$ $\mathbb{Q}_{2,1}^{(c)}(E_{2g}) = \dfrac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2}$

$\boxed{\text{z14}}$ $\mathbb{Q}_{2,2}^{(c)}(E_{2g}) = \dfrac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2}$

- 'C'-'C' bond-cluster
  * bra: $\langle p_z|$
  * ket: $|p_z\rangle$
  * wyckoff: `6d@3f`

$\boxed{\text{z5}}$ $\mathbb{Q}_0^{(c)}(A_{1g}) = \mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_0^{(b)}(A_{1g})$

$\boxed{\text{z8}}$ $\mathbb{Q}_6^{(c)}(A_{2g}) = \mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_6^{(b)}(A_{2g})$

$\boxed{\text{z15}}$ $\mathbb{Q}_{2,1}^{(c)}(E_{2g}) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2}$

$\boxed{\text{z16}}$ $\mathbb{Q}_{2,2}^{(c)}(E_{2g}) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2}$

$\boxed{\text{z17}}$ $\mathbb{Q}_{4,1}^{(c)}(E_{2g},1) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{4,1}^{(b)}(E_{2g},1)}{2}$

$\boxed{\text{z18}}$ $\mathbb{Q}_{4,2}^{(c)}(E_{2g},1) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{4,2}^{(b)}(E_{2g},1)}{2}$

- 'C'-'C' bond-cluster
  * bra: $\langle p_z|$
  * ket: $|p_z\rangle$
  * wyckoff: `6a@6l`

$\boxed{\text{z6}}$ $\mathbb{Q}_0^{(c)}(A_{1g}) = \mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_0^{(b)}(A_{1g})$

$\boxed{\text{z19}}$ $\mathbb{Q}_3^{(c)}(B_{1u}) = \mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_3^{(b)}(B_{1u})$

$\boxed{\text{z20}}$ $\mathbb{Q}_{1,1}^{(c)}(E_{1u}) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{2}$

$\boxed{\text{z25}}$ $\mathbb{Q}_{1,2}^{(c)}(E_{1u}) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{2}$

$\boxed{\text{z29}}$ $\mathbb{Q}_{2,1}^{(c)}(E_{2g}) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2}$

$\boxed{\text{z30}}$ $\mathbb{Q}_{2,2}^{(c)}(E_{2g}) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2}$

- 'C'-'C' bond-cluster

* bra: $\langle p_z|$
* ket: $|p_z\rangle$
* wyckoff: `6c@2c`

z7 $\mathbb{Q}_0^{(c)}(A_{1g}) = \mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_0^{(b)}(A_{1g})$

z21 $\mathbb{Q}_3^{(c)}(B_{1u}) = \mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_3^{(b)}(B_{1u})$

z22 $\mathbb{Q}_{1,1}^{(c)}(E_{1u}) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{2}$

z26 $\mathbb{Q}_{1,2}^{(c)}(E_{1u}) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{2}$

z31 $\mathbb{Q}_{2,1}^{(c)}(E_{2g}) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2}$

z32 $\mathbb{Q}_{2,2}^{(c)}(E_{2g}) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2}$

Atomic SAMB

- bra: $\langle p_z|$
- ket: $|p_z\rangle$

x1 $\mathbb{Q}_0^{(a)}(A_{1g}) = \left[1\right]$

Cluster SAMB

- Site cluster

** Wyckoff: `2c`

y1 $\mathbb{Q}_0^{(s)}(A_{1g}) = \left[\frac{\sqrt{2}}{2}, \frac{\sqrt{2}}{2}\right]$

y2 $\mathbb{Q}_3^{(s)}(B_{1u}) = \left[\frac{\sqrt{2}}{2}, -\frac{\sqrt{2}}{2}\right]$

- Bond cluster

** Wyckoff: `3a@3f`

$\boxed{\text{y3}}$ $\mathbb{Q}_{0}^{(s)}(A_{1g}) = \left[\frac{\sqrt{3}}{3}, \frac{\sqrt{3}}{3}, \frac{\sqrt{3}}{3}\right]$

$\boxed{\text{y4}}$ $\mathbb{T}_{3}^{(s)}(B_{1u}) = \left[\frac{\sqrt{3}i}{3}, \frac{\sqrt{3}i}{3}, \frac{\sqrt{3}i}{3}\right]$

$\boxed{\text{y5}}$ $\mathbb{T}_{1,1}^{(s)}(E_{1u}) = \left[0, -\frac{\sqrt{2}i}{2}, \frac{\sqrt{2}i}{2}\right]$

$\boxed{\text{y6}}$ $\mathbb{T}_{1,2}^{(s)}(E_{1u}) = \left[\frac{\sqrt{6}i}{3}, -\frac{\sqrt{6}i}{6}, -\frac{\sqrt{6}i}{6}\right]$

$\boxed{\text{y7}}$ $\mathbb{Q}_{2,1}^{(s)}(E_{2g}) = \left[\frac{\sqrt{6}}{3}, -\frac{\sqrt{6}}{6}, -\frac{\sqrt{6}}{6}\right]$

$\boxed{\text{y8}}$ $\mathbb{Q}_{2,2}^{(s)}(E_{2g}) = \left[0, \frac{\sqrt{2}}{2}, -\frac{\sqrt{2}}{2}\right]$

** Wyckoff: `3b@1a`

$\boxed{\text{y9}}$ $\mathbb{Q}_{0}^{(s)}(A_{1g}) = \left[\frac{\sqrt{3}}{3}, \frac{\sqrt{3}}{3}, \frac{\sqrt{3}}{3}\right]$

$\boxed{\text{y10}}$ $\mathbb{T}_{3}^{(s)}(B_{1u}) = \left[\frac{\sqrt{3}i}{3}, \frac{\sqrt{3}i}{3}, \frac{\sqrt{3}i}{3}\right]$

$\boxed{\text{y11}}$ $\mathbb{T}_{1,1}^{(s)}(E_{1u}) = \left[0, -\frac{\sqrt{2}i}{2}, \frac{\sqrt{2}i}{2}\right]$

$\boxed{\text{y12}}$ $\mathbb{T}_{1,2}^{(s)}(E_{1u}) = \left[\frac{\sqrt{6}i}{3}, -\frac{\sqrt{6}i}{6}, -\frac{\sqrt{6}i}{6}\right]$

$\boxed{\text{y13}}$ $\mathbb{Q}_{2,1}^{(s)}(E_{2g}) = \left[\frac{\sqrt{6}}{3}, -\frac{\sqrt{6}}{6}, -\frac{\sqrt{6}}{6}\right]$

$\boxed{\text{y14}}$ $\mathbb{Q}_{2,2}^{(s)}(E_{2g}) = \left[0,\ \frac{\sqrt{2}}{2},\ -\frac{\sqrt{2}}{2}\right]$

** Wyckoff: `6d@3f`

$\boxed{\text{y15}}$ $\mathbb{Q}_{0}^{(s)}(A_{1g}) = \left[\frac{\sqrt{6}}{6},\ \frac{\sqrt{6}}{6},\ \frac{\sqrt{6}}{6},\ \frac{\sqrt{6}}{6},\ \frac{\sqrt{6}}{6},\ \frac{\sqrt{6}}{6}\right]$

$\boxed{\text{y16}}$ $\mathbb{Q}_{6}^{(s)}(A_{2g}) = \left[\frac{\sqrt{6}}{6},\ \frac{\sqrt{6}}{6},\ \frac{\sqrt{6}}{6},\ -\frac{\sqrt{6}}{6},\ -\frac{\sqrt{6}}{6},\ -\frac{\sqrt{6}}{6}\right]$

$\boxed{\text{y17}}$ $\mathbb{T}_{3}^{(s)}(B_{1u}) = \left[\frac{\sqrt{6}i}{6},\ \frac{\sqrt{6}i}{6},\ \frac{\sqrt{6}i}{6},\ -\frac{\sqrt{6}i}{6},\ -\frac{\sqrt{6}i}{6},\ -\frac{\sqrt{6}i}{6}\right]$

$\boxed{\text{y18}}$ $\mathbb{T}_{3}^{(s)}(B_{2u}) = \left[\frac{\sqrt{6}i}{6},\ \frac{\sqrt{6}i}{6},\ \frac{\sqrt{6}i}{6},\ \frac{\sqrt{6}i}{6},\ \frac{\sqrt{6}i}{6},\ \frac{\sqrt{6}i}{6}\right]$

$\boxed{\text{y19}}$ $\mathbb{T}_{1,1}^{(s)}(E_{1u}, a) = \left[\frac{5\sqrt{21}i}{42},\ -\frac{2\sqrt{21}i}{21},\ -\frac{\sqrt{21}i}{42},\ -\frac{\sqrt{21}i}{42},\ \frac{5\sqrt{21}i}{42},\ -\frac{2\sqrt{21}i}{21}\right]$

$\boxed{\text{y20}}$ $\mathbb{T}_{1,2}^{(s)}(E_{1u}, a) = \left[\frac{\sqrt{7}i}{14},\ \frac{\sqrt{7}i}{7},\ -\frac{3\sqrt{7}i}{14},\ \frac{3\sqrt{7}i}{14},\ -\frac{\sqrt{7}i}{14},\ -\frac{\sqrt{7}i}{7}\right]$

$\boxed{\text{y21}}$ $\mathbb{T}_{1,1}^{(s)}(E_{1u}, b) = \left[\frac{\sqrt{7}i}{14},\ \frac{\sqrt{7}i}{7},\ -\frac{3\sqrt{7}i}{14},\ -\frac{3\sqrt{7}i}{14},\ \frac{\sqrt{7}i}{14},\ \frac{\sqrt{7}i}{7}\right]$

$\boxed{\text{y22}}$ $\mathbb{T}_{1,2}^{(s)}(E_{1u}, b) = \left[-\frac{5\sqrt{21}i}{42},\ \frac{2\sqrt{21}i}{21},\ \frac{\sqrt{21}i}{42},\ -\frac{\sqrt{21}i}{42},\ \frac{5\sqrt{21}i}{42},\ -\frac{2\sqrt{21}i}{21}\right]$

$\boxed{\text{y23}}$ $\mathbb{Q}_{2,1}^{(s)}(E_{2g}) = \left[\frac{11\sqrt{3}}{42},\ \frac{\sqrt{3}}{21},\ -\frac{13\sqrt{3}}{42},\ -\frac{13\sqrt{3}}{42},\ \frac{11\sqrt{3}}{42},\ \frac{\sqrt{3}}{21}\right]$

$\boxed{\text{y24}}$ $\mathbb{Q}_{2,2}^{(s)}(E_{2g}) = \left[-\frac{5}{14},\ \frac{4}{7},\ -\frac{3}{14},\ \frac{3}{14},\ \frac{5}{14},\ -\frac{4}{7}\right]$

$\boxed{\text{y25}}$ $\mathbb{Q}_{4,1}^{(s)}(E_{2g}, 1) = \left[\frac{5}{14},\ -\frac{4}{7},\ \frac{3}{14},\ \frac{3}{14},\ \frac{5}{14},\ -\frac{4}{7}\right]$

$\boxed{\text{y26}}$ $\mathbb{Q}_{4,2}^{(s)}(E_{2g},1) = \left[\frac{11\sqrt{3}}{42}, \frac{\sqrt{3}}{21}, -\frac{13\sqrt{3}}{42}, \frac{13\sqrt{3}}{42}, -\frac{11\sqrt{3}}{42}, -\frac{\sqrt{3}}{21}\right]$

** Wyckoff: `6a@6l`

$\boxed{\text{y27}}$ $\mathbb{Q}_{0}^{(s)}(A_{1g}) = \left[\frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}\right]$

$\boxed{\text{y28}}$ $\mathbb{T}_{0}^{(s)}(A_{1g}) = \left[\frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}\right]$

$\boxed{\text{y29}}$ $\mathbb{Q}_{3}^{(s)}(B_{1u}) = \left[\frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, -\frac{\sqrt{6}}{6}, -\frac{\sqrt{6}}{6}, -\frac{\sqrt{6}}{6}\right]$

$\boxed{\text{y30}}$ $\mathbb{T}_{3}^{(s)}(B_{1u}) = \left[\frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, -\frac{\sqrt{6}i}{6}, -\frac{\sqrt{6}i}{6}, -\frac{\sqrt{6}i}{6}\right]$

$\boxed{\text{y31}}$ $\mathbb{Q}_{1,1}^{(s)}(E_{1u}) = \left[0, -\frac{1}{2}, \frac{1}{2}, 0, \frac{1}{2}, -\frac{1}{2}\right]$

$\boxed{\text{y32}}$ $\mathbb{Q}_{1,2}^{(s)}(E_{1u}) = \left[\frac{\sqrt{3}}{3}, -\frac{\sqrt{3}}{6}, -\frac{\sqrt{3}}{6}, -\frac{\sqrt{3}}{3}, \frac{\sqrt{3}}{6}, \frac{\sqrt{3}}{6}\right]$

$\boxed{\text{y33}}$ $\mathbb{T}_{1,1}^{(s)}(E_{1u}) = \left[0, -\frac{i}{2}, \frac{i}{2}, 0, \frac{i}{2}, -\frac{i}{2}\right]$

$\boxed{\text{y34}}$ $\mathbb{T}_{1,2}^{(s)}(E_{1u}) = \left[\frac{\sqrt{3}i}{3}, -\frac{\sqrt{3}i}{6}, -\frac{\sqrt{3}i}{6}, -\frac{\sqrt{3}i}{3}, \frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{6}\right]$

$\boxed{\text{y35}}$ $\mathbb{Q}_{2,1}^{(s)}(E_{2g}) = \left[\frac{\sqrt{3}}{3}, -\frac{\sqrt{3}}{6}, -\frac{\sqrt{3}}{6}, \frac{\sqrt{3}}{3}, -\frac{\sqrt{3}}{6}, -\frac{\sqrt{3}}{6}\right]$

$\boxed{\text{y36}}$ $\mathbb{Q}_{2,2}^{(s)}(E_{2g}) = \left[0, \frac{1}{2}, -\frac{1}{2}, 0, \frac{1}{2}, -\frac{1}{2}\right]$

$\boxed{\text{y37}}$ $\mathbb{T}_{2,1}^{(s)}(E_{2g}) = \left[\frac{\sqrt{3}i}{3}, -\frac{\sqrt{3}i}{6}, -\frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{3}, -\frac{\sqrt{3}i}{6}, -\frac{\sqrt{3}i}{6}\right]$

$\boxed{\text{y38}}$ $\mathbb{T}_{2,2}^{(s)}(E_{2g}) = \left[0, \frac{i}{2}, -\frac{i}{2}, 0, \frac{i}{2}, -\frac{i}{2}\right]$

** Wyckoff: `6c@2c`

$\boxed{\text{y39}}$ $\mathbb{Q}_{0}^{(s)}(A_{1g}) = \left[\frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}\right]$

$\boxed{\text{y40}}$ $\mathbb{M}_{1}^{(s)}(A_{2g}) = \left[\frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}\right]$

$\boxed{\text{y41}}$ $\mathbb{Q}_{3}^{(s)}(B_{1u}) = \left[\frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, -\frac{\sqrt{6}}{6}, -\frac{\sqrt{6}}{6}, -\frac{\sqrt{6}}{6}\right]$

$\boxed{\text{y42}}$ $\mathbb{T}_{3}^{(s)}(B_{2u}) = \left[\frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, -\frac{\sqrt{6}i}{6}, -\frac{\sqrt{6}i}{6}, -\frac{\sqrt{6}i}{6}\right]$

$\boxed{\text{y43}}$ $\mathbb{Q}_{1,1}^{(s)}(E_{1u}) = \left[0, -\frac{1}{2}, \frac{1}{2}, 0, \frac{1}{2}, -\frac{1}{2}\right]$

$\boxed{\text{y44}}$ $\mathbb{Q}_{1,2}^{(s)}(E_{1u}) = \left[\frac{\sqrt{3}}{3}, -\frac{\sqrt{3}}{6}, -\frac{\sqrt{3}}{6}, -\frac{\sqrt{3}}{3}, \frac{\sqrt{3}}{6}, \frac{\sqrt{3}}{6}\right]$

$\boxed{\text{y45}}$ $\mathbb{T}_{1,1}^{(s)}(E_{1u}) = \left[\frac{\sqrt{3}i}{3}, -\frac{\sqrt{3}i}{6}, -\frac{\sqrt{3}i}{6}, -\frac{\sqrt{3}i}{3}, \frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{6}\right]$

$\boxed{\text{y46}}$ $\mathbb{T}_{1,2}^{(s)}(E_{1u}) = \left[0, \frac{i}{2}, -\frac{i}{2}, 0, -\frac{i}{2}, \frac{i}{2}\right]$

$\boxed{\text{y47}}$ $\mathbb{Q}_{2,1}^{(s)}(E_{2g}) = \left[\frac{\sqrt{3}}{3}, -\frac{\sqrt{3}}{6}, -\frac{\sqrt{3}}{6}, \frac{\sqrt{3}}{3}, -\frac{\sqrt{3}}{6}, -\frac{\sqrt{3}}{6}\right]$

$\boxed{\text{y48}}$ $\mathbb{Q}_{2,2}^{(s)}(E_{2g}) = \left[0, \frac{1}{2}, -\frac{1}{2}, 0, \frac{1}{2}, -\frac{1}{2}\right]$

$\boxed{\text{y49}}$ $\mathbb{T}_{2,1}^{(s)}(E_{2g}) = \left[0, \frac{i}{2}, -\frac{i}{2}, 0, \frac{i}{2}, -\frac{i}{2}\right]$

$\boxed{\text{y50}}$ $\mathbb{T}_{2,2}^{(s)}(E_{2g}) = \left[-\frac{\sqrt{3}i}{3}, \frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{6}, -\frac{\sqrt{3}i}{3}, \frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{6}\right]$

** Wyckoff: `6b@6l`

$\boxed{\text{y51}}$ $\mathbb{Q}_0^{(s)}(A_{1g}) = \left[\frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}\right]$

$\boxed{\text{y52}}$ $\mathbb{M}_1^{(s)}(A_{2g}) = \left[\frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}\right]$

$\boxed{\text{y53}}$ $\mathbb{Q}_3^{(s)}(B_{1u}) = \left[\frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, -\frac{\sqrt{6}}{6}, -\frac{\sqrt{6}}{6}, -\frac{\sqrt{6}}{6}\right]$

$\boxed{\text{y54}}$ $\mathbb{T}_3^{(s)}(B_{2u}) = \left[\frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, -\frac{\sqrt{6}i}{6}, -\frac{\sqrt{6}i}{6}, -\frac{\sqrt{6}i}{6}\right]$

$\boxed{\text{y55}}$ $\mathbb{Q}_{1,1}^{(s)}(E_{1u}) = \left[0, -\frac{1}{2}, \frac{1}{2}, 0, \frac{1}{2}, -\frac{1}{2}\right]$

$\boxed{\text{y56}}$ $\mathbb{Q}_{1,2}^{(s)}(E_{1u}) = \left[\frac{\sqrt{3}}{3}, -\frac{\sqrt{3}}{6}, -\frac{\sqrt{3}}{6}, -\frac{\sqrt{3}}{3}, \frac{\sqrt{3}}{6}, \frac{\sqrt{3}}{6}\right]$

$\boxed{\text{y57}}$ $\mathbb{T}_{1,1}^{(s)}(E_{1u}) = \left[\frac{\sqrt{3}i}{3}, -\frac{\sqrt{3}i}{6}, -\frac{\sqrt{3}i}{6}, -\frac{\sqrt{3}i}{3}, \frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{6}\right]$

$\boxed{\text{y58}}$ $\mathbb{T}_{1,2}^{(s)}(E_{1u}) = \left[0, \frac{i}{2}, -\frac{i}{2}, 0, -\frac{i}{2}, \frac{i}{2}\right]$

$\boxed{\text{y59}}$ $\mathbb{Q}_{2,1}^{(s)}(E_{2g}) = \left[\frac{\sqrt{3}}{3}, -\frac{\sqrt{3}}{6}, -\frac{\sqrt{3}}{6}, \frac{\sqrt{3}}{3}, -\frac{\sqrt{3}}{6}, -\frac{\sqrt{3}}{6}\right]$

$\boxed{\text{y60}}$ $\mathbb{Q}_{2,2}^{(s)}(E_{2g}) = \left[0, \frac{1}{2}, -\frac{1}{2}, 0, \frac{1}{2}, -\frac{1}{2}\right]$

$\boxed{\text{y61}}$ $\mathbb{T}_{2,1}^{(s)}(E_{2g}) = \left[0, \frac{i}{2}, -\frac{i}{2}, 0, \frac{i}{2}, -\frac{i}{2}\right]$

$\boxed{\text{y62}}$ $\mathbb{T}_{2,2}^{(s)}(E_{2g}) = \left[-\frac{\sqrt{3}i}{3}, \frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{6}, -\frac{\sqrt{3}i}{3}, \frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{6}\right]$

Site and Bond

Table 5: Orbital of each site

#	site	orbital
1	`C`	$\lvert p_z \rangle$

Table 6: Neighbor and bra-ket of each bond

#	head	tail	neighbor	head (bra)	tail (ket)
1	`C`	`C`	`[1,2,3,4,5,6]`	`[p]`	`[p]`

Site in Unit Cell

Sites in (conventional) cell (no plus set), SL = sublattice

Table 7: '`C`' (#1) site cluster (`2c`), `-6m2`

SL	position ($\boldsymbol{s}$)	mapping
1	`[ 0.33333, 0.66667, 0.00000]`	`[1,2,3,10,11,12,16,17,18,19,20,21]`
2	`[ 0.66667, 0.33333, 0.00000]`	`[4,5,6,7,8,9,13,14,15,22,23,24]`

Bonds in (conventional) cell (no plus set): tail, head = (SL, plus set), (N)D = (non)directional (listed up to 5th neighbor at most)

Table 8: 1-th 'C'-'C' [1] (#1) bond cluster (3a@3f), ND, $|\boldsymbol{v}|$= 0.57735 (cartesian)

SL	vector ($\boldsymbol{v}$)	center ($\boldsymbol{c}$)	mapping	head	tail	$\boldsymbol{R}$ (primitive)
1	[0.33333, 0.66667, 0.00000]	[0.50000, 0.00000, 0.00000]	[1,-4,-8,11,-13,16,20,-23]	(2,1)	(1,1)	[0,-1,0]
2	[-0.66667,-0.33333, 0.00000]	[0.00000, 0.50000, 0.00000]	[2,-5,-7,10,-14,17,19,-22]	(2,1)	(1,1)	[1,0,0]
3	[0.33333,-0.33333, 0.00000]	[0.50000, 0.50000, 0.00000]	[3,-6,-9,12,-15,18,21,-24]	(2,1)	(1,1)	[0,0,0]

Table 9: 2-th 'C'-'C' [1] (#2) bond cluster (6b@6l), ND, $|\boldsymbol{v}|$= 1.0 (cartesian)

SL	vector ($\boldsymbol{v}$)	center ($\boldsymbol{c}$)	mapping	head	tail	$\boldsymbol{R}$ (primitive)
1	[1.00000, 0.00000, 0.00000]	[0.83333, 0.66667, 0.00000]	[1,-11,16,-20]	(1,1)	(1,1)	[-1,0,0]
2	[0.00000, 1.00000, 0.00000]	[0.33333, 0.16667, 0.00000]	[2,-10,17,-19]	(1,1)	(1,1)	[0,-1,0]
3	[-1.00000,-1.00000, 0.00000]	[0.83333, 0.16667, 0.00000]	[3,-12,18,-21]	(1,1)	(1,1)	[1,1,0]
4	[-1.00000, 0.00000, 0.00000]	[0.16667, 0.33333, 0.00000]	[4,-8,13,-23]	(2,1)	(2,1)	[1,0,0]
5	[0.00000,-1.00000, 0.00000]	[0.66667, 0.83333, 0.00000]	[5,-7,14,-22]	(2,1)	(2,1)	[0,1,0]
6	[1.00000, 1.00000, 0.00000]	[0.16667, 0.83333, 0.00000]	[6,-9,15,-24]	(2,1)	(2,1)	[-1,-1,0]

Table 10: 3-th 'C'-'C' [1] (#3) bond cluster (3b@1a), ND, $|\boldsymbol{v}|$= 1.1547 (cartesian)

SL	vector ($\boldsymbol{v}$)	center ($\boldsymbol{c}$)	mapping	head	tail	$\boldsymbol{R}$ (primitive)
1	[-0.66667,-1.33333, 0.00000]	[0.00000, 0.00000, 0.00000]	[1,-4,-8,11,-13,16,20,-23]	(2,1)	(1,1)	[1,1,0]
2	[1.33333, 0.66667, 0.00000]	[0.00000, 0.00000, 0.00000]	[2,-5,-7,10,-14,17,19,-22]	(2,1)	(1,1)	[-1,-1,0]
3	[-0.66667, 0.66667, 0.00000]	[0.00000, 0.00000, 0.00000]	[3,-6,-9,12,-15,18,21,-24]	(2,1)	(1,1)	[1,-1,0]

Table 11: 4-th 'C'-'C' [1] (#4) bond cluster (6d@3f), ND, $|\boldsymbol{v}|$= 1.52753 (cartesian)

SL	vector ($\boldsymbol{v}$)	center ($\boldsymbol{c}$)	mapping	head	tail	$\boldsymbol{R}$ (primitive)
1	[-1.66667,-1.33333, 0.00000]	[0.50000, 0.00000, 0.00000]	[1,-4,-13,16]	(2,1)	(1,1)	[2,1,0]
2	[1.33333,-0.33333, 0.00000]	[0.00000, 0.50000, 0.00000]	[2,-5,-14,17]	(2,1)	(1,1)	[-1,0,0]
3	[0.33333, 1.66667, 0.00000]	[0.50000, 0.50000, 0.00000]	[3,-6,-15,18]	(2,1)	(1,1)	[0,-2,0]
4	[-1.33333,-1.66667, 0.00000]	[0.00000, 0.50000, 0.00000]	[7,-10,-19,22]	(1,1)	(2,1)	[1,2,0]
5	[-0.33333, 1.33333, 0.00000]	[0.50000, 0.00000, 0.00000]	[8,-11,-20,23]	(1,1)	(2,1)	[0,-1,0]
6	[1.66667, 0.33333, 0.00000]	[0.50000, 0.50000, 0.00000]	[9,-12,-21,24]	(1,1)	(2,1)	[-2,0,0]

Table 12: 5-th 'C'-'C' [1] (#5) bond cluster (6a@61), D, $|\boldsymbol{v}|$= 1.73205 (cartesian)

SL	vector ($\boldsymbol{v}$)	center ($\boldsymbol{c}$)	mapping	head	tail	$\boldsymbol{R}$ (primitive)
1	[1.00000, 2.00000, 0.00000]	[0.83333, 0.66667, 0.00000]	[1,11,16,20]	(1,1)	(1,1)	[-1,-2,0]
2	[-2.00000,-1.00000, 0.00000]	[0.33333, 0.16667, 0.00000]	[2,10,17,19]	(1,1)	(1,1)	[2,1,0]
3	[1.00000,-1.00000, 0.00000]	[0.83333, 0.16667, 0.00000]	[3,12,18,21]	(1,1)	(1,1)	[-1,1,0]
4	[-1.00000,-2.00000, 0.00000]	[0.16667, 0.33333, 0.00000]	[4,8,13,23]	(2,1)	(2,1)	[1,2,0]
5	[2.00000, 1.00000, 0.00000]	[0.66667, 0.83333, 0.00000]	[5,7,14,22]	(2,1)	(2,1)	[-2,-1,0]
6	[-1.00000, 1.00000, 0.00000]	[0.16667, 0.83333, 0.00000]	[6,9,15,24]	(2,1)	(2,1)	[1,-1,0]