Model for "graphene"

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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	$\{\mathrm{m}_{001}\|0\}$	17	$\{-6^{-}_{001}\|0\}$	18	$\{-6^{+}_{001}\|0\}$	19	$\{\mathrm{m}_{110}\|0\}$	20	$\{\mathrm{m}_{100}\|0\}$
21	$\{\mathrm{m}_{010}\|0\}$	22	$\{\mathrm{m}_{1-10}\|0\}$	23	$\{\mathrm{m}_{120}\|0\}$	24	$\{\mathrm{m}_{210}\|0\}$		

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	-	-	$\frac{\sqrt{10}x\left(x^2-3y^2\right)}{4}$
6	$\mathbb{Q}_{1,1}(E_{1u})$	E_{1u}	1	Q, T	-	1	x

continued ...

Table 2

#	symbol	irrep.	rank	X	multiplicity	component	symmetry
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	$\frac{\sqrt{35}(x^2-2xy-y^2)(x^2+2xy-y^2)}{8}$
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	$\|p_z\rangle$ @C(1)	1	$\|p_z\rangle$ @C(2)

Table 4: Atomic basis (orbital part only)

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

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

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

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

- `C;C_001_1` : 'C'-'C' bond-cluster
  * bra: $\langle p_z|$
  * ket: $|p_z\rangle$
  * wyckoff: `3a@3f`

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

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

  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_002_1` : 'C'-'C' bond-cluster
  * bra: $\langle p_z|$
  * ket: $|p_z\rangle$
  * wyckoff: `6b@6l`

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

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

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

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

z27 $\mathbb{Q}^{(c)}_{2,1}(E_{2g}) = \dfrac{\sqrt{2}\mathbb{Q}^{(a)}_{0}(A_{1g})\mathbb{Q}^{(b)}_{2,1}(E_{2g})}{2}$

z28 $\mathbb{Q}^{(c)}_{2,2}(E_{2g}) = \dfrac{\sqrt{2}\mathbb{Q}^{(a)}_{0}(A_{1g})\mathbb{Q}^{(b)}_{2,2}(E_{2g})}{2}$

- `C;C_003_1` : 'C'-'C' bond-cluster
  * bra: $\langle p_z|$
  * ket: $|p_z\rangle$
  * wyckoff: `3b@1a`

  z4 $\mathbb{Q}^{(c)}_{0}(A_{1g}) = \mathbb{Q}^{(a)}_{0}(A_{1g})\mathbb{Q}^{(b)}_{0}(A_{1g})$

  z13 $\mathbb{Q}^{(c)}_{2,1}(E_{2g}) = \dfrac{\sqrt{2}\mathbb{Q}^{(a)}_{0}(A_{1g})\mathbb{Q}^{(b)}_{2,1}(E_{2g})}{2}$

  z14 $\mathbb{Q}^{(c)}_{2,2}(E_{2g}) = \dfrac{\sqrt{2}\mathbb{Q}^{(a)}_{0}(A_{1g})\mathbb{Q}^{(b)}_{2,2}(E_{2g})}{2}$

- `C;C_004_1` : 'C'-'C' bond-cluster
  * bra: $\langle p_z|$
  * ket: $|p_z\rangle$
  * wyckoff: `6d@3f`

  z5 $\mathbb{Q}^{(c)}_{0}(A_{1g}) = \mathbb{Q}^{(a)}_{0}(A_{1g})\mathbb{Q}^{(b)}_{0}(A_{1g})$

  z8 $\mathbb{Q}^{(c)}_{6}(A_{2g}) = \mathbb{Q}^{(a)}_{0}(A_{1g})\mathbb{Q}^{(b)}_{6}(A_{2g})$

  z15 $\mathbb{Q}^{(c)}_{2,1}(E_{2g}) = \dfrac{\sqrt{2}\mathbb{Q}^{(a)}_{0}(A_{1g})\mathbb{Q}^{(b)}_{2,1}(E_{2g})}{2}$

  z16 $\mathbb{Q}^{(c)}_{2,2}(E_{2g}) = \dfrac{\sqrt{2}\mathbb{Q}^{(a)}_{0}(A_{1g})\mathbb{Q}^{(b)}_{2,2}(E_{2g})}{2}$

  z17 $\mathbb{Q}^{(c)}_{4,1}(E_{2g},1) = \dfrac{\sqrt{2}\mathbb{Q}^{(a)}_{0}(A_{1g})\mathbb{Q}^{(b)}_{4,1}(E_{2g},1)}{2}$

  z18 $\mathbb{Q}^{(c)}_{4,2}(E_{2g},1) = \dfrac{\sqrt{2}\mathbb{Q}^{(a)}_{0}(A_{1g})\mathbb{Q}^{(b)}_{4,2}(E_{2g},1)}{2}$

- `C;C_005_1` : 'C'-'C' bond-cluster
  * bra: $\langle p_z|$
  * ket: $|p_z\rangle$
  * wyckoff: `6a@61`

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

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

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

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

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

  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_006_1` : '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 $\mathbb{Q}^{(c)}_{2,2}(E_{2g}) = \dfrac{\sqrt{2}\mathbb{Q}^{(a)}_{0}(A_{1g})\mathbb{Q}^{(b)}_{2,2}(E_{2g})}{2}$

Atomic SAMB

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

x1 $\mathbb{Q}^{(a)}_{0}(A_{1g}) = \left[1\right]$

Cluster SAMB

- Site cluster

** Wyckoff: `2c`

y1 $\mathbb{Q}^{(s)}_{0}(A_{1g}) = \left[\dfrac{\sqrt{2}}{2}, \dfrac{\sqrt{2}}{2}\right]$

y2 $\mathbb{Q}^{(s)}_{3}(B_{1u}) = \left[\dfrac{\sqrt{2}}{2}, -\dfrac{\sqrt{2}}{2}\right]$

- Bond cluster

** Wyckoff: `3a@3f`

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

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

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

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

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

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

** Wyckoff: `3b@1a`

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

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

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

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

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

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

** Wyckoff: `6d@3f`

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

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

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

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

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

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

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

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

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

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

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

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: `6c@2c`

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

y28 $\mathbb{M}_{1}^{(s)}(A_{2g}) = \left[\frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}\right]$

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

y30 $\mathbb{T}_{3}^{(s)}(B_{2u}) = \left[\frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, -\frac{\sqrt{6}i}{6}, -\frac{\sqrt{6}i}{6}, -\frac{\sqrt{6}i}{6}\right]$

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

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

y33 $\mathbb{T}_{1,1}^{(s)}(E_{1u}) = \left[\frac{\sqrt{3}i}{3}, -\frac{\sqrt{3}i}{6}, -\frac{\sqrt{3}i}{6}, -\frac{\sqrt{3}i}{3}, \frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{6}\right]$

y34 $\mathbb{T}_{1,2}^{(s)}(E_{1u}) = \left[0, \frac{i}{2}, -\frac{i}{2}, 0, -\frac{i}{2}, \frac{i}{2}\right]$

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

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

y37 $\mathbb{T}_{2,1}^{(s)}(E_{2g}) = \left[0, \frac{i}{2}, -\frac{i}{2}, 0, \frac{i}{2}, -\frac{i}{2}\right]$

y38 $\mathbb{T}_{2,2}^{(s)}(E_{2g}) = \left[-\frac{\sqrt{3}i}{3}, \frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{6}, -\frac{\sqrt{3}i}{3}, \frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{6}\right]$

** Wyckoff: `6b@6l`

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

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

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

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

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

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

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

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

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

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

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

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

** Wyckoff: `6a@6l`

y51 $\mathbb{Q}^{(s)}_{0}(A_{1g}) = \left[\frac{\sqrt{6}}{6},\, \frac{\sqrt{6}}{6},\, \frac{\sqrt{6}}{6},\, \frac{\sqrt{6}}{6},\, \frac{\sqrt{6}}{6},\, \frac{\sqrt{6}}{6}\right]$

y52 $\mathbb{T}^{(s)}_{0}(A_{1g}) = \left[\frac{\sqrt{6}i}{6},\, \frac{\sqrt{6}i}{6},\, \frac{\sqrt{6}i}{6},\, \frac{\sqrt{6}i}{6},\, \frac{\sqrt{6}i}{6},\, \frac{\sqrt{6}i}{6}\right]$

y53 $\mathbb{Q}^{(s)}_{3}(B_{1u}) = \left[\frac{\sqrt{6}}{6},\, \frac{\sqrt{6}}{6},\, \frac{\sqrt{6}}{6},\, -\frac{\sqrt{6}}{6},\, -\frac{\sqrt{6}}{6},\, -\frac{\sqrt{6}}{6}\right]$

y54 $\mathbb{T}^{(s)}_{3}(B_{1u}) = \left[\frac{\sqrt{6}i}{6},\, \frac{\sqrt{6}i}{6},\, \frac{\sqrt{6}i}{6},\, -\frac{\sqrt{6}i}{6},\, -\frac{\sqrt{6}i}{6},\, -\frac{\sqrt{6}i}{6}\right]$

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

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

y57 $\mathbb{T}^{(s)}_{1,1}(E_{1u}) = \left[0, -\frac{i}{2}, \frac{i}{2}, 0, \frac{i}{2}, -\frac{i}{2}\right]$

y58 $\mathbb{T}^{(s)}_{1,2}(E_{1u}) = \left[\frac{\sqrt{3}i}{3}, -\frac{\sqrt{3}i}{6}, -\frac{\sqrt{3}i}{6}, -\frac{\sqrt{3}i}{3}, \frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{6}\right]$

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

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

y61 $\mathbb{T}^{(s)}_{2,1}(E_{2g}) = \left[\frac{\sqrt{3}i}{3}, -\frac{\sqrt{3}i}{6}, -\frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{3}, -\frac{\sqrt{3}i}{6}, -\frac{\sqrt{3}i}{6}\right]$

y62 $\mathbb{T}^{(s)}_{2,2}(E_{2g}) = \left[0, \frac{i}{2}, -\frac{i}{2}, 0, \frac{i}{2}, -\frac{i}{2}\right]$

Site and Bond

Table 5: Orbital of each site

#	site	orbital
1	C	$\|p_z\rangle$

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]

Bond in Unit Cell

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]

continued ...

Table 8

SL	vector ($\boldsymbol{v}$)	center ($\boldsymbol{c}$)	mapping	head	tail	$\boldsymbol{R}$ (primitive)
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@61), 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]