

Model for “graphene”

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General Condition

- Basis type: **1g**
- 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):
 - $\mathbf{a}_1 = [1.00000, 0.00000, 0.00000]$
 - $\mathbf{a}_2 = [-0.50000, 0.86603, 0.00000]$
 - $\mathbf{a}_3 = [0.00000, 0.00000, 4.00000]$

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	-	-	$\frac{\sqrt{462}xy(x^2-3y^2)(3x^2-y^2)}{16}$
4	$\mathbb{Q}_3(B_{1u})$	B_{1u}	3	Q, T	-	-	$\frac{\sqrt{10}y(3x^2-y^2)}{4}$
5	$\mathbb{Q}_3(B_{2u})$	B_{2u}	3	Q, T	-	-	$\frac{\sqrt{10}x(x^2-3y^2)}{4}$

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	$\frac{\sqrt{35}(x^2-2xy-y^2)(x^2+2xy-y^2)}{8}$
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

SAMB

32 (all 32) SAMBs

- 'C' site-cluster : C

* bra: $\langle p_z|$

* ket: $|p_z\rangle$

* wyckoff: 2c

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

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

- 'C'-'C' bond-cluster : C;C_001_1

* bra: $\langle p_z|$

* ket: $|p_z\rangle$

* wyckoff: 3a@3f

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

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

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

- 'C'-'C' bond-cluster : C;C_002_1

* bra: $\langle p_z |$

* ket: $|p_z\rangle$

* wyckoff: 6b061

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

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

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

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

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

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

- 'C'-'C' bond-cluster : C;C_003_1

* bra: $\langle p_z |$

* ket: $|p_z\rangle$

* wyckoff: 3b01a

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

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

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

- 'C'-'C' bond-cluster : C;C_004_1

* bra: $\langle p_z |$

* ket: $|p_z\rangle$

* wyckoff: 6d03f

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

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

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

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

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

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

• 'C'-'C' bond-cluster : C;C_005_1

* bra: $\langle p_z |$

* ket: $|p_z\rangle$

* wyckoff: 6a@61

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

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

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

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

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

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

• 'C'-'C' bond-cluster : C;C_006_1

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

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

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

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

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

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

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

Atomic SAMB

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

$$\boxed{\text{x1}} \quad \mathbb{Q}_0^{(a)}(A_{1g}) = [1]$$

Cluster SAMB

- Site cluster

** Wyckoff: 2c

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

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

- Bond cluster

** Wyckoff: **3b@1a**

$$\boxed{\text{y3}} \quad \mathbb{Q}_0^{(s)}(A_{1g}) = \left[\frac{\sqrt{3}}{3}, \frac{\sqrt{3}}{3}, \frac{\sqrt{3}}{3} \right]$$

$$\boxed{\text{y4}} \quad \mathbb{T}_3^{(s)}(B_{1u}) = \left[\frac{\sqrt{3}i}{3}, \frac{\sqrt{3}i}{3}, \frac{\sqrt{3}i}{3} \right]$$

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

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

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

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

** Wyckoff: **3a@3f**

$$\boxed{\text{y9}} \quad \mathbb{Q}_0^{(s)}(A_{1g}) = \left[\frac{\sqrt{3}}{3}, \frac{\sqrt{3}}{3}, \frac{\sqrt{3}}{3} \right]$$

$$\boxed{\text{y10}} \quad \mathbb{T}_3^{(s)}(B_{1u}) = \left[\frac{\sqrt{3}i}{3}, \frac{\sqrt{3}i}{3}, \frac{\sqrt{3}i}{3} \right]$$

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

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

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

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

** Wyckoff: 6b061

$$\boxed{\text{y15}} \quad \mathbb{Q}_0^{(s)}(A_{1g}) = \left[\frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6} \right]$$

$$\boxed{\text{y16}} \quad \mathbb{M}_1^{(s)}(A_{2g}) = \left[\frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6} \right]$$

$$\boxed{\text{y17}} \quad \mathbb{Q}_3^{(s)}(B_{1u}) = \left[\frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, -\frac{\sqrt{6}}{6}, -\frac{\sqrt{6}}{6}, -\frac{\sqrt{6}}{6} \right]$$

$$\boxed{\text{y18}} \quad \mathbb{T}_3^{(s)}(B_{2u}) = \left[\frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, -\frac{\sqrt{6}i}{6}, -\frac{\sqrt{6}i}{6}, -\frac{\sqrt{6}i}{6} \right]$$

$$\boxed{\text{y19}} \quad \mathbb{Q}_{1,1}^{(s)}(E_{1u}) = \left[0, -\frac{1}{2}, \frac{1}{2}, 0, \frac{1}{2}, -\frac{1}{2} \right]$$

$$\boxed{\text{y20}} \quad \mathbb{Q}_{1,2}^{(s)}(E_{1u}) = \left[\frac{\sqrt{3}}{3}, -\frac{\sqrt{3}}{6}, -\frac{\sqrt{3}}{6}, -\frac{\sqrt{3}}{3}, \frac{\sqrt{3}}{6}, \frac{\sqrt{3}}{6} \right]$$

$$\boxed{\text{y21}} \quad \mathbb{T}_{1,1}^{(s)}(E_{1u}) = \left[\frac{\sqrt{3}i}{3}, -\frac{\sqrt{3}i}{6}, -\frac{\sqrt{3}i}{6}, -\frac{\sqrt{3}i}{3}, \frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{6} \right]$$

$$\boxed{\text{y22}} \quad \mathbb{T}_{1,2}^{(s)}(E_{1u}) = \left[0, \frac{i}{2}, -\frac{i}{2}, 0, -\frac{i}{2}, \frac{i}{2} \right]$$

$$\boxed{\text{y23}} \quad \mathbb{Q}_{2,1}^{(s)}(E_{2g}) = \left[\frac{\sqrt{3}}{3}, -\frac{\sqrt{3}}{6}, -\frac{\sqrt{3}}{6}, \frac{\sqrt{3}}{3}, -\frac{\sqrt{3}}{6}, -\frac{\sqrt{3}}{6} \right]$$

$$\boxed{\text{y24}} \quad \mathbb{Q}_{2,2}^{(s)}(E_{2g}) = \left[0, \frac{1}{2}, -\frac{1}{2}, 0, \frac{1}{2}, -\frac{1}{2} \right]$$

$$\boxed{\text{y25}} \quad \mathbb{T}_{2,1}^{(s)}(E_{2g}) = \left[0, \frac{i}{2}, -\frac{i}{2}, 0, \frac{i}{2}, -\frac{i}{2} \right]$$

$$\boxed{\text{y26}} \quad \mathbb{T}_{2,2}^{(s)}(E_{2g}) = \left[-\frac{\sqrt{3}i}{3}, \frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{6}, -\frac{\sqrt{3}i}{3}, \frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{6} \right]$$

** Wyckoff: 6a@61

$$\boxed{\text{y27}} \quad \mathbb{Q}_0^{(s)}(A_{1g}) = \left[\frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6} \right]$$

$$\boxed{\text{y28}} \quad \mathbb{T}_0^{(s)}(A_{1g}) = \left[\frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6} \right]$$

$$\boxed{\text{y29}} \quad \mathbb{Q}_3^{(s)}(B_{1u}) = \left[\frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, -\frac{\sqrt{6}}{6}, -\frac{\sqrt{6}}{6}, -\frac{\sqrt{6}}{6} \right]$$

$$\boxed{\text{y30}} \quad \mathbb{T}_3^{(s)}(B_{1u}) = \left[\frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, -\frac{\sqrt{6}i}{6}, -\frac{\sqrt{6}i}{6}, -\frac{\sqrt{6}i}{6} \right]$$

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

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

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

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

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

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

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

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

** Wyckoff: 6c@2c

$$\boxed{\text{y49}} \quad \mathbb{Q}_0^{(s)}(A_{1g}) = \left[\frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6} \right]$$

$$\boxed{\text{y40}} \quad \mathbb{M}_1^{(s)}(A_{2g}) = \left[\frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6} \right]$$

$$\boxed{\text{y41}} \quad \mathbb{Q}_3^{(s)}(B_{1u}) = \left[\frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, -\frac{\sqrt{6}}{6}, -\frac{\sqrt{6}}{6}, -\frac{\sqrt{6}}{6} \right]$$

$$\boxed{\text{y42}} \quad \mathbb{T}_3^{(s)}(B_{2u}) = \left[\frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, -\frac{\sqrt{6}i}{6}, -\frac{\sqrt{6}i}{6}, -\frac{\sqrt{6}i}{6} \right]$$

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

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

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

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

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

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

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

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

** Wyckoff: 6d@3f

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

$$\boxed{\text{y52}} \quad \mathbb{Q}_6^{(s)}(A_{2g}) = \left[\frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, -\frac{\sqrt{6}}{6}, -\frac{\sqrt{6}}{6}, -\frac{\sqrt{6}}{6} \right]$$

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

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

$$\boxed{\text{y55}} \quad \mathbb{T}_{1,1}^{(s)}(E_{1u}, a) = \left[\frac{5\sqrt{21}i}{42}, -\frac{2\sqrt{21}i}{21}, -\frac{\sqrt{21}i}{42}, -\frac{\sqrt{21}i}{42}, \frac{5\sqrt{21}i}{42}, -\frac{2\sqrt{21}i}{21} \right]$$

$$\boxed{\text{y56}} \quad \mathbb{T}_{1,2}^{(s)}(E_{1u}, a) = \left[\frac{\sqrt{7}i}{14}, \frac{\sqrt{7}i}{7}, -\frac{3\sqrt{7}i}{14}, \frac{3\sqrt{7}i}{14}, -\frac{\sqrt{7}i}{14}, -\frac{\sqrt{7}i}{7} \right]$$

$$\boxed{\text{y57}} \quad \mathbb{T}_{1,1}^{(s)}(E_{1u}, b) = \left[\frac{\sqrt{7}i}{14}, \frac{\sqrt{7}i}{7}, -\frac{3\sqrt{7}i}{14}, -\frac{3\sqrt{7}i}{14}, \frac{\sqrt{7}i}{14}, \frac{\sqrt{7}i}{7} \right]$$

$$\boxed{\text{y58}} \quad \mathbb{T}_{1,2}^{(s)}(E_{1u}, b) = \left[-\frac{5\sqrt{21}i}{42}, \frac{2\sqrt{21}i}{21}, \frac{\sqrt{21}i}{42}, -\frac{\sqrt{21}i}{42}, \frac{5\sqrt{21}i}{42}, -\frac{2\sqrt{21}i}{21} \right]$$

$$\boxed{\text{y59}} \quad \mathbb{Q}_{2,1}^{(s)}(E_{2g}) = \left[\frac{11\sqrt{3}}{42}, \frac{\sqrt{3}}{21}, -\frac{13\sqrt{3}}{42}, -\frac{13\sqrt{3}}{42}, \frac{11\sqrt{3}}{42}, \frac{\sqrt{3}}{21} \right]$$

$$\boxed{\text{y60}} \quad \mathbb{Q}_{2,2}^{(s)}(E_{2g}) = \left[-\frac{5}{14}, \frac{4}{7}, -\frac{3}{14}, \frac{3}{14}, \frac{5}{14}, -\frac{4}{7} \right]$$

$$\boxed{\text{y61}} \quad \mathbb{Q}_{4,1}^{(s)}(E_{2g}, 1) = \left[\frac{5}{14}, -\frac{4}{7}, \frac{3}{14}, \frac{3}{14}, \frac{5}{14}, -\frac{4}{7} \right]$$

$$\boxed{\text{y62}} \quad \mathbb{Q}_{4,2}^{(s)}(E_{2g}, 1) = \left[\frac{11\sqrt{3}}{42}, \frac{\sqrt{3}}{21}, -\frac{13\sqrt{3}}{42}, \frac{13\sqrt{3}}{42}, -\frac{11\sqrt{3}}{42}, -\frac{\sqrt{3}}{21} \right]$$

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 (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 (3a03f), ND, $|v| = 0.57735$ (cartesian)

SL	vector (v)	center (c)	mapping	head	tail	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 (6b061), ND, $|v| = 1.0$ (cartesian)

SL	vector (v)	center (c)	mapping	head	tail	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, $|\mathbf{v}|=1.1547$ (cartesian)

SL	vector (\mathbf{v})	center (\mathbf{c})	mapping	head	tail	\mathbf{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, $|\mathbf{v}|=1.52753$ (cartesian)

SL	vector (\mathbf{v})	center (\mathbf{c})	mapping	head	tail	\mathbf{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 (6a061), D, $|\mathbf{v}|= 1.73205$ (cartesian)

SL	vector (\mathbf{v})	center (\mathbf{c})	mapping	head	tail	\mathbf{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]