

# Model for “graphene”

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## General Condition

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- Basis type: 1g
- SAMB selection:
  - Type: [Q, G]
  - Rank: [0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11]
  - Irrep.: [A<sub>1g</sub>, A<sub>2g</sub>, B<sub>1g</sub>, B<sub>2g</sub>, E<sub>1g</sub>, E<sub>2g</sub>, A<sub>1u</sub>, A<sub>2u</sub>, B<sub>1u</sub>, B<sub>2u</sub>, E<sub>1u</sub>, E<sub>2u</sub>]
  - 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<sub>1g</sub>, A<sub>2g</sub>, B<sub>1g</sub>, B<sub>2g</sub>, E<sub>1g</sub>, E<sub>2g</sub>, A<sub>1u</sub>, A<sub>2u</sub>, B<sub>1u</sub>, B<sub>2u</sub>, E<sub>1u</sub>, E<sub>2u</sub>]
  - Spin (s): [0, 1]
- Site-cluster selection:
  - Rank: [0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11]
  - Irrep.: [A<sub>1g</sub>, A<sub>2g</sub>, B<sub>1g</sub>, B<sub>2g</sub>, E<sub>1g</sub>, E<sub>2g</sub>, A<sub>1u</sub>, A<sub>2u</sub>, B<sub>1u</sub>, B<sub>2u</sub>, E<sub>1u</sub>, E<sub>2u</sub>]
- Bond-cluster selection:
  - Type: [Q, G, M, T]
  - Rank: [0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11]
  - Irrep.: [A<sub>1g</sub>, A<sub>2g</sub>, B<sub>1g</sub>, B<sub>2g</sub>, E<sub>1g</sub>, E<sub>2g</sub>, A<sub>1u</sub>, A<sub>2u</sub>, B<sub>1u</sub>, B<sub>2u</sub>, E<sub>1u</sub>, E<sub>2u</sub>]
- Max. neighbor: 10
- Search cell range: (-2, 3), (-2, 3), (-2, 3)
- Toroidal priority: false

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## Group and Unit Cell

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- Group: SG No. 191 D<sub>6h</sub><sup>1</sup> P6/mmm [ hexagonal ]
- Associated point group: PG No. 191 D<sub>6h</sub> 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):

$a_1$  = [ 1.00000, 0.00000, 0.00000]  
 $a_2$  = [-0.50000, 0.86603, 0.00000]  
 $a_3$  = [ 0.00000, 0.00000, 4.00000]

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 — Symmetry Operation —

Table 1: Symmetry operation

#	SO	#	SO	#	SO	#	SO	#	SO
1	{1 0}	2	{3 <sup>+</sup> <sub>001</sub>  0}	3	{3 <sup>-</sup> <sub>001</sub>  0}	4	{2 <sub>001</sub>  0}	5	{6 <sup>-</sup> <sub>001</sub>  0}
6	{6 <sup>+</sup> <sub>001</sub>  0}	7	{2 <sub>110</sub>  0}	8	{2 <sub>100</sub>  0}	9	{2 <sub>010</sub>  0}	10	{2 <sub>1-10</sub>  0}
11	{2 <sub>120</sub>  0}	12	{2 <sub>210</sub>  0}	13	{-1 0}	14	{-3 <sup>+</sup> <sub>001</sub>  0}	15	{-3 <sup>-</sup> <sub>001</sub>  0}
16	{m <sub>001</sub>  0}	17	{-6 <sup>-</sup> <sub>001</sub>  0}	18	{-6 <sup>+</sup> <sub>001</sub>  0}	19	{m <sub>110</sub>  0}	20	{m <sub>100</sub>  0}
21	{m <sub>010</sub>  0}	22	{m <sub>1-10</sub>  0}	23	{m <sub>120</sub>  0}	24	{m <sub>210</sub>  0}		

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 — 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	$\frac{\sqrt{35}xy(x-y)(x+y)}{2}$

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— 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$	$z$

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## SAMB

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32 (all 32) SAMBs

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

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

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

- 'C'-'C' bond-cluster : C;C\_001\_1

- \* bra:  $\langle p_z |$
- \* ket:  $|p_z \rangle$
- \* wyckoff: 3a@3f

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

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

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

- 'C'-'C' bond-cluster : C;C\_002\_1

\* bra:  $\langle p_z |$   
 \* ket:  $| p_z \rangle$   
 \* wyckoff: 6b@6l

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

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

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

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

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

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

- 'C-'C' bond-cluster : C;C\_003\_1

\* bra:  $\langle p_z |$   
 \* ket:  $| p_z \rangle$   
 \* wyckoff: 3b@1a

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

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

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

- 'C-'C' bond-cluster : C;C\_004\_1

\* bra:  $\langle p_z |$   
 \* ket:  $| p_z \rangle$   
 \* wyckoff: 6d@3f

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

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

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

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

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

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

• '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**

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

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

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

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

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

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

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### — Atomic SAMB —

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

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

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### — Cluster SAMB —

- Site cluster

\*\* Wyckoff: 2c

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

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

- Bond cluster

\*\* Wyckoff: 3b@1a

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

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

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

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

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

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

\*\* Wyckoff: 3a@3f

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

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

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

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

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

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

\*\* Wyckoff: 6b@61

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

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

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

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

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

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

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

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

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

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

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

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

\*\* Wyckoff: **6c@2c**

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

$$\boxed{\text{y28}} \quad \mathbb{M}_1^{(s)}(A_{2g}) = \left[ \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6} \right]$$

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

$$\boxed{\text{y30}} \quad \mathbb{T}_3^{(s)}(B_{2u}) = \left[ \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, -\frac{\sqrt{6}i}{6}, -\frac{\sqrt{6}i}{6}, -\frac{\sqrt{6}i}{6} \right]$$

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

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

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

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

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

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

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

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

\*\* Wyckoff: **6d@3f**

$$\boxed{\text{y39}} \quad \mathbb{Q}_0^{(s)}(A_{1g}) = \left[ \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6} \right]$$

$$\boxed{\text{y40}} \quad \mathbb{Q}_6^{(s)}(A_{2g}) = \left[ \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, -\frac{\sqrt{6}}{6}, -\frac{\sqrt{6}}{6}, -\frac{\sqrt{6}}{6} \right]$$

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

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

$$\boxed{\text{y43}} \quad \mathbb{T}_{1,1}^{(s)}(E_{1u}, a) = \left[ \frac{5\sqrt{21}i}{42}, -\frac{2\sqrt{21}i}{21}, -\frac{\sqrt{21}i}{42}, -\frac{\sqrt{21}i}{42}, \frac{5\sqrt{21}i}{42}, -\frac{2\sqrt{21}i}{21} \right]$$

$$\boxed{\text{y44}} \quad \mathbb{T}_{1,2}^{(s)}(E_{1u}, a) = \left[ \frac{\sqrt{7}i}{14}, \frac{\sqrt{7}i}{7}, -\frac{3\sqrt{7}i}{14}, \frac{3\sqrt{7}i}{14}, -\frac{\sqrt{7}i}{14}, -\frac{\sqrt{7}i}{7} \right]$$

$$\boxed{\text{y45}} \quad \mathbb{T}_{1,1}^{(s)}(E_{1u}, b) = \left[ \frac{\sqrt{7}i}{14}, \frac{\sqrt{7}i}{7}, -\frac{3\sqrt{7}i}{14}, -\frac{3\sqrt{7}i}{14}, \frac{\sqrt{7}i}{14}, \frac{\sqrt{7}i}{7} \right]$$

$$\boxed{\text{y46}} \quad \mathbb{T}_{1,2}^{(s)}(E_{1u}, b) = \left[ -\frac{5\sqrt{21}i}{42}, \frac{2\sqrt{21}i}{21}, \frac{\sqrt{21}i}{42}, -\frac{\sqrt{21}i}{42}, \frac{5\sqrt{21}i}{42}, -\frac{2\sqrt{21}i}{21} \right]$$

$$\boxed{\text{y47}} \quad \mathbb{Q}_{2,1}^{(s)}(E_{2g}) = \left[ \frac{11\sqrt{3}}{42}, \frac{\sqrt{3}}{21}, -\frac{13\sqrt{3}}{42}, -\frac{13\sqrt{3}}{42}, \frac{11\sqrt{3}}{42}, \frac{\sqrt{3}}{21} \right]$$

$$\boxed{\text{y48}} \quad \mathbb{Q}_{2,2}^{(s)}(E_{2g}) = \left[ -\frac{5}{14}, \frac{4}{7}, -\frac{3}{14}, \frac{3}{14}, \frac{5}{14}, -\frac{4}{7} \right]$$

$$\boxed{\text{y49}} \quad \mathbb{Q}_{4,1}^{(s)}(E_{2g}, 1) = \left[ \frac{5}{14}, -\frac{4}{7}, \frac{3}{14}, \frac{3}{14}, \frac{5}{14}, -\frac{4}{7} \right]$$

$$\boxed{\text{y50}} \quad \mathbb{Q}_{4,2}^{(s)}(E_{2g}, 1) = \left[ \frac{11\sqrt{3}}{42}, \frac{\sqrt{3}}{21}, -\frac{13\sqrt{3}}{42}, \frac{13\sqrt{3}}{42}, -\frac{11\sqrt{3}}{42}, -\frac{\sqrt{3}}{21} \right]$$

\*\* Wyckoff: 6a@61

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

$$\boxed{\text{y52}} \quad \mathbb{T}_0^{(s)}(A_{1g}) = \left[ \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6} \right]$$

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

$$\boxed{\text{y54}} \quad \mathbb{T}_3^{(s)}(B_{1u}) = \left[ \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, -\frac{\sqrt{6}i}{6}, -\frac{\sqrt{6}i}{6}, -\frac{\sqrt{6}i}{6} \right]$$

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

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

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

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

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

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

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

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

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]

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### — 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]

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### Bond in Unit Cell

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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,  $|\mathbf{v}|=0.57735$  (cartesian)

SL	vector ( $\mathbf{v}$ )	center ( $\mathbf{c}$ )	mapping	head	tail	$\mathbf{R}$ (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,  $|\mathbf{v}|=1.0$  (cartesian)

SL	vector ( $\mathbf{v}$ )	center ( $\mathbf{c}$ )	mapping	head	tail	$\mathbf{R}$ (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 (6a@61), 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]