

# 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**

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## 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:
  - $a = 2.43500$ ,  $b = 2.43500$ ,  $c = 10.00000$ ,  $\alpha = 90.0$ ,  $\beta = 90.0$ ,  $\gamma = 120.0$
- Lattice vectors (conventional cell):
  - $\mathbf{a}_1 = [ 2.43500, 0.00000, 0.00000 ]$
  - $\mathbf{a}_2 = [ -1.21750, 2.10877, 0.00000 ]$
  - $\mathbf{a}_3 = [ 0.00000, 0.00000, 10.00000 ]$

## 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	$\mathbb{Q}_{5,1}(E_{1u}, 1)$	$E_{1u}$	5	$Q, T$	1	1	$\frac{3\sqrt{14}x(x^4-10x^2y^2+5y^4)}{16}$
9	$\mathbb{Q}_{5,2}(E_{1u}, 1)$					2	$-\frac{3\sqrt{14}y(5x^4-10x^2y^2+y^4)}{16}$
10	$\mathbb{Q}_{2,1}(E_{2g})$	$E_{2g}$	2	$Q, T$	-	1	$\frac{\sqrt{3}(x-y)(x+y)}{2}$
11	$\mathbb{Q}_{2,2}(E_{2g})$					2	$-\sqrt{3}xy$
12	$\mathbb{Q}_{4,1}(E_{2g}, 1)$	$E_{2g}$	4	$Q, T$	1	1	$\frac{\sqrt{35}(x^2-2xy-y^2)(x^2+2xy-y^2)}{8}$
13	$\mathbb{Q}_{4,2}(E_{2g}, 1)$					2	$\frac{\sqrt{35}xy(x-y)(x+y)}{2}$

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Basis in full matrix

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Table 3: dimension = 2

#	orbital@atom(SL)	#	orbital@atom(SL)
0	$ p_z\rangle @A(1)$	1	$ p_z\rangle @A(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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30 (all 59) SAMBs

- 'A' site-cluster

- \* bra:  $\langle p_z|$

- \* ket:  $|p_z\rangle$

- \* wyckoff: **2c**

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

$$\boxed{\text{z44}} \quad \mathbb{Q}_3^{(c)}(B_{1u}) = \mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_3^{(s)}(B_{1u})$$

- 'A'-'A' bond-cluster

- \* bra:  $\langle p_z|$

- \* ket:  $|p_z\rangle$

- \* wyckoff: **3a@3f**

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

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

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

- 'A'-'A' bond-cluster

\* bra:  $\langle p_z |$

\* ket:  $|p_z\rangle$

\* wyckoff: 6b061

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

$$\boxed{\text{z18}} \quad \mathbb{Q}_3^{(c)}(B_{1u}) = \mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_3^{(b)}(B_{1u})$$

$$\boxed{\text{z19}} \quad \mathbb{Q}_{1,1}^{(c)}(E_{1u}) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{2}$$

$$\boxed{\text{z45}} \quad \mathbb{Q}_{1,2}^{(c)}(E_{1u}) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{2}$$

$$\boxed{\text{z50}} \quad \mathbb{Q}_{2,1}^{(c)}(E_{2g}) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2}$$

$$\boxed{\text{z51}} \quad \mathbb{Q}_{2,2}^{(c)}(E_{2g}) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2}$$

- 'A'-'A' bond-cluster

\* bra:  $\langle p_z |$

\* ket:  $|p_z\rangle$

\* wyckoff: 3b01a

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

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

$$\boxed{\text{z21}} \quad \mathbb{Q}_{2,2}^{(c)}(E_{2g}) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2}$$

\* common SAMBs

(z4, z9), (z20, z34), (z21, z35)

- 'A'-'A' bond-cluster

\* bra:  $\langle p_z |$

\* ket:  $|p_z\rangle$

\* wyckoff: **6d03f**

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

$$\boxed{\text{z12}} \quad \mathbb{Q}_6^{(c)}(A_{2g}) = \mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_6^{(b)}(A_{2g})$$

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

$$\boxed{\text{z23}} \quad \mathbb{Q}_{2,2}^{(c)}(E_{2g}) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2}$$

$$\boxed{\text{z24}} \quad \mathbb{Q}_{4,1}^{(c)}(E_{2g}, 1) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{4,1}^{(b)}(E_{2g}, 1)}{2}$$

$$\boxed{\text{z25}} \quad \mathbb{Q}_{4,2}^{(c)}(E_{2g}, 1) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{4,2}^{(b)}(E_{2g}, 1)}{2}$$

\* common SAMBs

(z5, z8, z10), (z12, z13, z14), (z22, z30, z36), (z23, z31, z37), (z24, z32, z38), (z25, z33, z39)

• 'A'-'A' bond-cluster

\* bra:  $\langle p_z |$

\* ket:  $|p_z\rangle$

\* wyckoff: **6a061**

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

$$\boxed{\text{z26}} \quad \mathbb{Q}_3^{(c)}(B_{1u}) = \mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_3^{(b)}(B_{1u})$$

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

$$\boxed{\text{z46}} \quad \mathbb{Q}_{1,2}^{(c)}(E_{1u}) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{2}$$

$$\boxed{\text{z52}} \quad \mathbb{Q}_{2,1}^{(c)}(E_{2g}) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2}$$

$$\boxed{\text{z53}} \quad \mathbb{Q}_{2,2}^{(c)}(E_{2g}) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2}$$

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

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

$$\boxed{\text{z28}} \quad \mathbb{Q}_3^{(c)}(B_{1u}) = \mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_3^{(b)}(B_{1u})$$

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

$$\boxed{\text{z47}} \quad \mathbb{Q}_{1,2}^{(c)}(E_{1u}) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{2}$$

$$\boxed{\text{z54}} \quad \mathbb{Q}_{2,1}^{(c)}(E_{2g}) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2}$$

$$\boxed{\text{z55}} \quad \mathbb{Q}_{2,2}^{(c)}(E_{2g}) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2}$$

- 'A'-'A' bond-cluster
  - \* bra:  $\langle p_z |$
  - \* ket:  $|p_z\rangle$
  - \* wyckoff: **12d@61**

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

$$\boxed{\text{z15}} \quad \mathbb{Q}_6^{(c)}(A_{2g}) = \mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_6^{(b)}(A_{2g})$$

$$\boxed{\text{z40}} \quad \mathbb{Q}_3^{(c)}(B_{1u}) = \mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_3^{(b)}(B_{1u})$$

$$\boxed{\text{z41}} \quad \mathbb{Q}_3^{(c)}(B_{2u}) = \mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_3^{(b)}(B_{2u})$$

$$\boxed{\text{z42}} \quad \mathbb{Q}_{1,1}^{(c)}(E_{1u}) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{2}$$

$$\boxed{\text{z43}} \quad \mathbb{Q}_{1,2}^{(c)}(E_{1u}) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{2}$$

$$\boxed{\text{z48}} \quad \mathbb{Q}_{5,1}^{(c)}(E_{1u}, 1) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{5,1}^{(b)}(E_{1u}, 1)}{2}$$

$$\boxed{\text{z49}} \quad \mathbb{Q}_{5,2}^{(c)}(E_{1u}, 1) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{5,2}^{(b)}(E_{1u}, 1)}{2}$$

$$\boxed{\text{z56}} \quad \mathbb{Q}_{2,1}^{(c)}(E_{2g}) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2}$$

$$\boxed{\text{z57}} \quad \mathbb{Q}_{2,2}^{(c)}(E_{2g}) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2}$$

$$\boxed{\text{z58}} \quad \mathbb{Q}_{4,1}^{(c)}(E_{2g}, 1) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{4,1}^{(b)}(E_{2g}, 1)}{2}$$

$$\boxed{\text{z59}} \quad \mathbb{Q}_{4,2}^{(c)}(E_{2g}, 1) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{4,2}^{(b)}(E_{2g}, 1)}{2}$$

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### Atomic SAMB

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

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

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### Cluster SAMB

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- 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: 6a@61

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

$$\boxed{\text{y16}} \quad \mathbb{T}_0^{(s)}(A_{1g}) = \left[ \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6} \right]$$

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

$$\boxed{\text{y18}} \quad \mathbb{T}_3^{(s)}(B_{1u}) = \left[ \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, -\frac{\sqrt{6}i}{6}, -\frac{\sqrt{6}i}{6}, -\frac{\sqrt{6}i}{6} \right]$$

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

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

$$\boxed{\text{y21}} \quad \mathbb{T}_{1,1}^{(s)}(E_{1u}) = \left[ 0, -\frac{i}{2}, \frac{i}{2}, 0, \frac{i}{2}, -\frac{i}{2} \right]$$

$$\boxed{\text{y22}} \quad \mathbb{T}_{1,2}^{(s)}(E_{1u}) = \left[ \frac{\sqrt{3}i}{3}, -\frac{\sqrt{3}i}{6}, -\frac{\sqrt{3}i}{6}, -\frac{\sqrt{3}i}{3}, \frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{6} \right]$$

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

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

$$\boxed{\text{y25}} \quad \mathbb{T}_{2,1}^{(s)}(E_{2g}) = \left[ \frac{\sqrt{3}i}{3}, -\frac{\sqrt{3}i}{6}, -\frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{3}, -\frac{\sqrt{3}i}{6}, -\frac{\sqrt{3}i}{6} \right]$$

$$\boxed{\text{y26}} \quad \mathbb{T}_{2,2}^{(s)}(E_{2g}) = \left[ 0, \frac{i}{2}, -\frac{i}{2}, 0, \frac{i}{2}, -\frac{i}{2} \right]$$

\*\* Wyckoff: 6c@2c

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

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

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

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

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

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

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

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

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

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

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

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

\*\* 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: **6b061**

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

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

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

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

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

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

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

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

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

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

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

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

\*\* Wyckoff: 12d061

$$\boxed{\text{y63}} \quad \mathbb{Q}_0^{(s)}(A_{1g}) = \left[ \frac{\sqrt{3}}{6}, \frac{\sqrt{3}}{6}, \frac{\sqrt{3}}{6}, \frac{\sqrt{3}}{6}, \frac{\sqrt{3}}{6}, \frac{\sqrt{3}}{6}, \frac{\sqrt{3}}{6}, \frac{\sqrt{3}}{6}, \frac{\sqrt{3}}{6}, \frac{\sqrt{3}}{6}, \frac{\sqrt{3}}{6}, \frac{\sqrt{3}}{6}, \frac{\sqrt{3}}{6} \right]$$

$$\boxed{\text{y64}} \quad \mathbb{T}_0^{(s)}(A_{1g}) = \left[ \frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{6} \right]$$

$$\boxed{\text{y65}} \quad \mathbb{M}_1^{(s)}(A_{2g}) = \left[ \frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{6}, -\frac{\sqrt{3}i}{6}, -\frac{\sqrt{3}i}{6}, -\frac{\sqrt{3}i}{6}, -\frac{\sqrt{3}i}{6}, -\frac{\sqrt{3}i}{6}, -\frac{\sqrt{3}i}{6}, -\frac{\sqrt{3}i}{6} \right]$$

$$\boxed{\text{y66}} \quad \mathbb{Q}_6^{(s)}(A_{2g}) = \left[ \frac{\sqrt{3}}{6}, \frac{\sqrt{3}}{6}, \frac{\sqrt{3}}{6}, \frac{\sqrt{3}}{6}, \frac{\sqrt{3}}{6}, \frac{\sqrt{3}}{6}, -\frac{\sqrt{3}}{6}, -\frac{\sqrt{3}}{6}, -\frac{\sqrt{3}}{6}, -\frac{\sqrt{3}}{6}, -\frac{\sqrt{3}}{6}, -\frac{\sqrt{3}}{6}, -\frac{\sqrt{3}}{6} \right]$$

$$\boxed{\text{y67}} \quad \mathbb{Q}_3^{(s)}(B_{1u}) = \left[ \frac{\sqrt{3}}{6}, \frac{\sqrt{3}}{6}, \frac{\sqrt{3}}{6}, -\frac{\sqrt{3}}{6}, -\frac{\sqrt{3}}{6}, -\frac{\sqrt{3}}{6}, -\frac{\sqrt{3}}{6}, -\frac{\sqrt{3}}{6}, -\frac{\sqrt{3}}{6}, -\frac{\sqrt{3}}{6}, \frac{\sqrt{3}}{6}, \frac{\sqrt{3}}{6}, \frac{\sqrt{3}}{6} \right]$$

$$\boxed{\text{y68}} \quad \mathbb{T}_3^{(s)}(B_{1u}) = \left[ \frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{6}, -\frac{\sqrt{3}i}{6}, -\frac{\sqrt{3}i}{6}, -\frac{\sqrt{3}i}{6}, -\frac{\sqrt{3}i}{6}, -\frac{\sqrt{3}i}{6}, -\frac{\sqrt{3}i}{6}, -\frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{6} \right]$$

$$\boxed{\text{y69}} \quad \mathbb{Q}_3^{(s)}(B_{2u}) = \left[ \frac{\sqrt{3}}{6}, \frac{\sqrt{3}}{6}, \frac{\sqrt{3}}{6}, -\frac{\sqrt{3}}{6}, -\frac{\sqrt{3}}{6}, -\frac{\sqrt{3}}{6}, \frac{\sqrt{3}}{6}, \frac{\sqrt{3}}{6}, \frac{\sqrt{3}}{6}, \frac{\sqrt{3}}{6}, -\frac{\sqrt{3}}{6}, -\frac{\sqrt{3}}{6}, -\frac{\sqrt{3}}{6} \right]$$

$$\boxed{\text{y70}} \quad \mathbb{T}_3^{(s)}(B_{2u}) = \left[ \frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{6}, -\frac{\sqrt{3}i}{6}, -\frac{\sqrt{3}i}{6}, -\frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{6}, -\frac{\sqrt{3}i}{6}, -\frac{\sqrt{3}i}{6}, -\frac{\sqrt{3}i}{6} \right]$$

$$\boxed{\text{y71}} \quad \mathbb{Q}_{1,1}^{(s)}(E_{1u}) = \left[ \frac{5\sqrt{42}}{84}, -\frac{\sqrt{42}}{21}, -\frac{\sqrt{42}}{84}, -\frac{5\sqrt{42}}{84}, \frac{\sqrt{42}}{21}, \frac{\sqrt{42}}{84}, -\frac{\sqrt{42}}{84}, \frac{5\sqrt{42}}{84}, -\frac{\sqrt{42}}{21}, \frac{\sqrt{42}}{84}, -\frac{5\sqrt{42}}{84}, \frac{\sqrt{42}}{21} \right]$$

$$\boxed{\text{y72}} \quad \mathbb{Q}_{1,2}^{(s)}(E_{1u}) = \left[ \frac{\sqrt{14}}{28}, \frac{\sqrt{14}}{14}, -\frac{3\sqrt{14}}{28}, -\frac{\sqrt{14}}{28}, -\frac{\sqrt{14}}{14}, \frac{3\sqrt{14}}{28}, \frac{3\sqrt{14}}{28}, -\frac{\sqrt{14}}{28}, -\frac{\sqrt{14}}{14}, -\frac{3\sqrt{14}}{28}, \frac{\sqrt{14}}{28}, \frac{\sqrt{14}}{14} \right]$$

$$\boxed{\text{y73}} \quad \mathbb{T}_{1,1}^{(s)}(E_{1u}, a) = \left[ \frac{5\sqrt{42}i}{84}, -\frac{\sqrt{42}i}{21}, -\frac{\sqrt{42}i}{84}, -\frac{5\sqrt{42}i}{84}, \frac{\sqrt{42}i}{21}, \frac{\sqrt{42}i}{84}, -\frac{\sqrt{42}i}{84}, \frac{5\sqrt{42}i}{84}, -\frac{\sqrt{42}i}{21}, \frac{\sqrt{42}i}{84}, -\frac{5\sqrt{42}i}{84}, \frac{\sqrt{42}i}{21} \right]$$

$$\boxed{\text{y74}} \quad \mathbb{T}_{1,2}^{(s)}(E_{1u}, a) = \left[ \frac{\sqrt{14}i}{28}, \frac{\sqrt{14}i}{14}, -\frac{3\sqrt{14}i}{28}, -\frac{\sqrt{14}i}{28}, -\frac{\sqrt{14}i}{14}, \frac{3\sqrt{14}i}{28}, \frac{3\sqrt{14}i}{28}, -\frac{\sqrt{14}i}{28}, -\frac{\sqrt{14}i}{14}, -\frac{3\sqrt{14}i}{28}, \frac{\sqrt{14}i}{28}, \frac{\sqrt{14}i}{14} \right]$$

$$\begin{aligned}
\boxed{\text{y75}} \quad \mathbb{T}_{1,1}^{(s)}(E_{1u}, b) &= \left[ \frac{\sqrt{14}i}{28}, \frac{\sqrt{14}i}{14}, -\frac{3\sqrt{14}i}{28}, -\frac{\sqrt{14}i}{28}, -\frac{\sqrt{14}i}{14}, \frac{3\sqrt{14}i}{28}, -\frac{3\sqrt{14}i}{28}, \frac{\sqrt{14}i}{28}, \frac{\sqrt{14}i}{14}, \frac{3\sqrt{14}i}{28}, -\frac{\sqrt{14}i}{28}, -\frac{\sqrt{14}i}{14} \right] \\
\boxed{\text{y76}} \quad \mathbb{T}_{1,2}^{(s)}(E_{1u}, b) &= \left[ -\frac{5\sqrt{42}i}{84}, \frac{\sqrt{42}i}{21}, \frac{\sqrt{42}i}{84}, \frac{5\sqrt{42}i}{84}, -\frac{\sqrt{42}i}{21}, -\frac{\sqrt{42}i}{84}, -\frac{\sqrt{42}i}{84}, \frac{5\sqrt{42}i}{84}, -\frac{\sqrt{42}i}{21}, \frac{\sqrt{42}i}{84}, -\frac{5\sqrt{42}i}{84}, \frac{\sqrt{42}i}{21} \right] \\
\boxed{\text{y77}} \quad \mathbb{Q}_{5,1}^{(s)}(E_{1u}, 1) &= \left[ \frac{\sqrt{14}}{28}, \frac{\sqrt{14}}{14}, -\frac{3\sqrt{14}}{28}, -\frac{\sqrt{14}}{28}, -\frac{\sqrt{14}}{14}, \frac{3\sqrt{14}}{28}, -\frac{3\sqrt{14}}{28}, \frac{\sqrt{14}}{28}, \frac{\sqrt{14}}{14}, \frac{3\sqrt{14}}{28}, -\frac{\sqrt{14}}{28}, -\frac{\sqrt{14}}{14} \right] \\
\boxed{\text{y78}} \quad \mathbb{Q}_{5,2}^{(s)}(E_{1u}, 1) &= \left[ -\frac{5\sqrt{42}}{84}, \frac{\sqrt{42}}{21}, \frac{\sqrt{42}}{84}, \frac{5\sqrt{42}}{84}, -\frac{\sqrt{42}}{21}, -\frac{\sqrt{42}}{84}, -\frac{\sqrt{42}}{84}, \frac{5\sqrt{42}}{84}, -\frac{\sqrt{42}}{21}, \frac{\sqrt{42}}{84}, -\frac{5\sqrt{42}}{84}, \frac{\sqrt{42}}{21} \right] \\
\boxed{\text{y79}} \quad \mathbb{Q}_{2,1}^{(s)}(E_{2g}) &= \left[ \frac{11\sqrt{6}}{84}, \frac{\sqrt{6}}{42}, -\frac{13\sqrt{6}}{84}, \frac{11\sqrt{6}}{84}, \frac{\sqrt{6}}{42}, -\frac{13\sqrt{6}}{84}, -\frac{13\sqrt{6}}{84}, \frac{11\sqrt{6}}{84}, \frac{\sqrt{6}}{42}, -\frac{13\sqrt{6}}{84}, \frac{11\sqrt{6}}{84}, \frac{\sqrt{6}}{42} \right] \\
\boxed{\text{y80}} \quad \mathbb{Q}_{2,2}^{(s)}(E_{2g}) &= \left[ -\frac{5\sqrt{2}}{28}, \frac{2\sqrt{2}}{7}, -\frac{3\sqrt{2}}{28}, -\frac{5\sqrt{2}}{28}, \frac{2\sqrt{2}}{7}, -\frac{3\sqrt{2}}{28}, \frac{3\sqrt{2}}{28}, \frac{5\sqrt{2}}{28}, -\frac{2\sqrt{2}}{7}, \frac{3\sqrt{2}}{28}, \frac{5\sqrt{2}}{28}, -\frac{2\sqrt{2}}{7} \right] \\
\boxed{\text{y81}} \quad \mathbb{T}_{2,1}^{(s)}(E_{2g}, a) &= \left[ \frac{11\sqrt{6}i}{84}, \frac{\sqrt{6}i}{42}, -\frac{13\sqrt{6}i}{84}, \frac{11\sqrt{6}i}{84}, \frac{\sqrt{6}i}{42}, -\frac{13\sqrt{6}i}{84}, -\frac{13\sqrt{6}i}{84}, \frac{11\sqrt{6}i}{84}, \frac{\sqrt{6}i}{42}, -\frac{13\sqrt{6}i}{84}, \frac{11\sqrt{6}i}{84}, \frac{\sqrt{6}i}{42} \right] \\
\boxed{\text{y82}} \quad \mathbb{T}_{2,2}^{(s)}(E_{2g}, a) &= \left[ -\frac{5\sqrt{2}i}{28}, \frac{2\sqrt{2}i}{7}, -\frac{3\sqrt{2}i}{28}, -\frac{5\sqrt{2}i}{28}, \frac{2\sqrt{2}i}{7}, -\frac{3\sqrt{2}i}{28}, \frac{3\sqrt{2}i}{28}, \frac{5\sqrt{2}i}{28}, -\frac{2\sqrt{2}i}{7}, \frac{3\sqrt{2}i}{28}, \frac{5\sqrt{2}i}{28}, -\frac{2\sqrt{2}i}{7} \right] \\
\boxed{\text{y83}} \quad \mathbb{T}_{2,1}^{(s)}(E_{2g}, b) &= \left[ \frac{5\sqrt{2}i}{28}, -\frac{2\sqrt{2}i}{7}, \frac{3\sqrt{2}i}{28}, \frac{5\sqrt{2}i}{28}, -\frac{2\sqrt{2}i}{7}, \frac{3\sqrt{2}i}{28}, \frac{3\sqrt{2}i}{28}, \frac{5\sqrt{2}i}{28}, -\frac{2\sqrt{2}i}{7}, \frac{3\sqrt{2}i}{28}, \frac{5\sqrt{2}i}{28}, -\frac{2\sqrt{2}i}{7} \right] \\
\boxed{\text{y84}} \quad \mathbb{T}_{2,2}^{(s)}(E_{2g}, b) &= \left[ \frac{11\sqrt{6}i}{84}, \frac{\sqrt{6}i}{42}, -\frac{13\sqrt{6}i}{84}, \frac{11\sqrt{6}i}{84}, \frac{\sqrt{6}i}{42}, -\frac{13\sqrt{6}i}{84}, \frac{13\sqrt{6}i}{84}, -\frac{11\sqrt{6}i}{84}, -\frac{\sqrt{6}i}{42}, \frac{13\sqrt{6}i}{84}, -\frac{11\sqrt{6}i}{84}, -\frac{\sqrt{6}i}{42} \right] \\
\boxed{\text{y85}} \quad \mathbb{Q}_{4,1}^{(s)}(E_{2g}, 1) &= \left[ \frac{5\sqrt{2}}{28}, -\frac{2\sqrt{2}}{7}, \frac{3\sqrt{2}}{28}, \frac{5\sqrt{2}}{28}, -\frac{2\sqrt{2}}{7}, \frac{3\sqrt{2}}{28}, \frac{3\sqrt{2}}{28}, \frac{5\sqrt{2}}{28}, -\frac{2\sqrt{2}}{7}, \frac{3\sqrt{2}}{28}, \frac{5\sqrt{2}}{28}, -\frac{2\sqrt{2}}{7} \right] \\
\boxed{\text{y86}} \quad \mathbb{Q}_{4,2}^{(s)}(E_{2g}, 1) &= \left[ \frac{11\sqrt{6}}{84}, \frac{\sqrt{6}}{42}, -\frac{13\sqrt{6}}{84}, \frac{11\sqrt{6}}{84}, \frac{\sqrt{6}}{42}, -\frac{13\sqrt{6}}{84}, \frac{13\sqrt{6}}{84}, -\frac{11\sqrt{6}}{84}, -\frac{\sqrt{6}}{42}, \frac{13\sqrt{6}}{84}, -\frac{11\sqrt{6}}{84}, -\frac{\sqrt{6}}{42} \right]
\end{aligned}$$

Table 5: Orbital of each site

#	site	orbital
1	A	$ p_z\rangle$

Table 6: Neighbor and bra-ket of each bond

#	head	tail	neighbor	head (bra)	tail (ket)
1	A	A	$[1, 2, 3, 4, \dots, 30]$	$[p]$	$[p]$

## Site in Unit Cell

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

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

SL	position ( $\mathbf{s}$ )	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 'A'-'A' [1] (#1) bond cluster (3a03f), ND,  $|v|=1.40585$  (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 'A'-'A' [1] (#2) bond cluster (6b061), ND,  $|v|=2.435$  (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 'A'-'A' [1] (#3) bond cluster (3b@1a), ND,  $|\mathbf{v}|=2.8117$  (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 'A'-'A' [1] (#4) bond cluster (6d@3f), ND,  $|\mathbf{v}|=3.71952$  (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 ' $\mathbf{A}'\text{-}'\mathbf{A}'$  [1] (#5) bond cluster (6a061), D,  $|\mathbf{v}|= 4.21754$  (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]