Model for "graphene"

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 $\quad D_{6h}^1 \quad P6/mmm$ [hexagonal]
- Associated point group: PG No. 191 $\quad D_{6h} \quad 6/mmm$ [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):
  $\boldsymbol{a}_1 = [\ 2.43500,\ 0.00000,\ 0.00000]$
  $\boldsymbol{a}_2 = [-1.21750,\ 2.10877,\ 0.00000]$
  $\boldsymbol{a}_3 = [\ 0.00000,\ 0.00000, 10.00000]$

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	$\{m_{210}\|0\}$		

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	-	-	$\frac{\sqrt{10}x(x^2-3y^2)}{4}$
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	$\mathbb{Q}_{5,1}(E_{1u},1)$	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	$\frac{\sqrt{35}xy(x-y)(x+y)}{2}$

━━ **Basis in full matrix** ━━━

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

continued …

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Table 4

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

--- **SAMB: 44 (all 59)** ---

- `A` : 'A' site-cluster
  * bra: $\langle p_z \rvert$
  * ket: $\lvert p_z \rangle$
  * 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_001_1` : 'A'-'A' bond-cluster
  * bra: $\langle p_z \rvert$
  * ket: $\lvert p_z \rangle$
  * wyckoff: `3a@3f`

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

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

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

- `A;A_002_1` : 'A'-'A' bond-cluster
  * bra: $\langle p_z \rvert$
  * ket: $\lvert p_z \rangle$

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* wyckoff: `6b@6l`

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

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

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

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

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

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

- `A;A_003_1` : 'A'-'A' bond-cluster
  * bra: $\langle p_z |$
  * ket: $| p_z \rangle$
  * wyckoff: `3b@1a`

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

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

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

  * common SAMBs
  (`A;A_003_1`, `A;A_008_1`), (z4, z9), (z20, z34), (z21, z35)

- `A;A_004_1` : 'A'-'A' bond-cluster
  * bra: $\langle p_z |$
  * ket: $| p_z \rangle$
  * wyckoff: `6d@3f`

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

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

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

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

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

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

* common SAMBs
(A;A_004_1, A;A_007_1, A;A_009_1), (z5, z8, z10), (z12, z13, z14), (z22, z30, z36), (z23, z31, z37), (z24, z32, z38), (z25, z33, z39)

- A;A_005_1 : 'A'-'A' bond-cluster
  * bra: $\langle p_z|$
  * ket: $|p_z\rangle$
  * wyckoff: 6a@6l

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

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

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

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

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

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

- A;A_006_1 : 'A'-'A' bond-cluster

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

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

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

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

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

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

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

- `A;A_010_1` : 'A'-'A' bond-cluster
  * bra: $\langle p_z |$
  * ket: $| p_z \rangle$
  * wyckoff: `12d@6l`

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

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

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

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

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

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

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

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

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

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

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

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

—— **Atomic SAMB** ————————————————————————————————————

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

x1 $\mathbb{Q}_0^{(a)}(A_{1g}) = \begin{bmatrix} 1 \end{bmatrix}$

—— **Cluster SAMB** ————————————————————————————————————

- Site cluster

** Wyckoff: **2c**

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

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

- Bond cluster

** Wyckoff: `3b@1a`

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

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

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

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

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

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

** Wyckoff: `3a@3f`

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

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

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

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

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

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

** Wyckoff: `6b@6l`

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

$\boxed{\text{y16}}$ $\quad \mathbb{M}_{1}^{(s)}(A_{2g}) = \left[\dfrac{\sqrt{6}i}{6}, \dfrac{\sqrt{6}i}{6}, \dfrac{\sqrt{6}i}{6}, \dfrac{\sqrt{6}i}{6}, \dfrac{\sqrt{6}i}{6}, \dfrac{\sqrt{6}i}{6} \right]$

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

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

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

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

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

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

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

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

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

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

** Wyckoff: `6a@6l`

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

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

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

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

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

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

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

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

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

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

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

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

** Wyckoff: `6c@2c`

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

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

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

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

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

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

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

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

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

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

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

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

** Wyckoff: `6d@3f`

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

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

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

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

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

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

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

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

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

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

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

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

** Wyckoff: `12d@6l`

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

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

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

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

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

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

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

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

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

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

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

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

y75 $\quad \mathbb{T}_{1,1}^{(s)}(E_{1u}, b) = \left[\dfrac{\sqrt{14}i}{28}, \dfrac{\sqrt{14}i}{14}, -\dfrac{3\sqrt{14}i}{28}, -\dfrac{\sqrt{14}i}{28}, -\dfrac{\sqrt{14}i}{14}, \dfrac{3\sqrt{14}i}{28}, -\dfrac{3\sqrt{14}i}{28}, \dfrac{\sqrt{14}i}{28}, \dfrac{\sqrt{14}i}{14}, \dfrac{3\sqrt{14}i}{28}, -\dfrac{\sqrt{14}i}{28}, -\dfrac{\sqrt{14}i}{14} \right]$

y76 $\quad \mathbb{T}_{1,2}^{(s)}(E_{1u}, b) = \left[-\dfrac{5\sqrt{42}i}{84}, \dfrac{\sqrt{42}i}{21}, \dfrac{\sqrt{42}i}{84}, \dfrac{5\sqrt{42}i}{84}, -\dfrac{\sqrt{42}i}{21}, -\dfrac{\sqrt{42}i}{84}, -\dfrac{\sqrt{42}i}{84}, \dfrac{5\sqrt{42}i}{84}, -\dfrac{\sqrt{42}i}{21}, \dfrac{\sqrt{42}i}{84}, -\dfrac{5\sqrt{42}i}{84}, \dfrac{\sqrt{42}i}{21} \right]$

y77 $\quad \mathbb{Q}_{5,1}^{(s)}(E_{1u}, 1) = \left[\dfrac{\sqrt{14}}{28}, \dfrac{\sqrt{14}}{14}, -\dfrac{3\sqrt{14}}{28}, -\dfrac{\sqrt{14}}{28}, -\dfrac{\sqrt{14}}{14}, \dfrac{3\sqrt{14}}{28}, -\dfrac{3\sqrt{14}}{28}, \dfrac{\sqrt{14}}{28}, \dfrac{\sqrt{14}}{14}, \dfrac{3\sqrt{14}}{28}, -\dfrac{\sqrt{14}}{28}, -\dfrac{\sqrt{14}}{14} \right]$

y78 $\quad \mathbb{Q}_{5,2}^{(s)}(E_{1u}, 1) = \left[-\dfrac{5\sqrt{42}}{84}, \dfrac{\sqrt{42}}{21}, \dfrac{\sqrt{42}}{84}, \dfrac{5\sqrt{42}}{84}, -\dfrac{\sqrt{42}}{21}, -\dfrac{\sqrt{42}}{84}, -\dfrac{\sqrt{42}}{84}, \dfrac{5\sqrt{42}}{84}, -\dfrac{\sqrt{42}}{21}, \dfrac{\sqrt{42}}{84}, -\dfrac{5\sqrt{42}}{84}, \dfrac{\sqrt{42}}{21} \right]$

y79 $\quad \mathbb{Q}_{2,1}^{(s)}(E_{2g}) = \left[\dfrac{11\sqrt{6}}{84}, \dfrac{\sqrt{6}}{42}, -\dfrac{13\sqrt{6}}{84}, \dfrac{11\sqrt{6}}{84}, \dfrac{\sqrt{6}}{42}, -\dfrac{13\sqrt{6}}{84}, -\dfrac{13\sqrt{6}}{84}, \dfrac{11\sqrt{6}}{84}, \dfrac{\sqrt{6}}{42}, -\dfrac{13\sqrt{6}}{84}, \dfrac{11\sqrt{6}}{84}, \dfrac{\sqrt{6}}{42} \right]$

y80 $\quad \mathbb{Q}_{2,2}^{(s)}(E_{2g}) = \left[-\dfrac{5\sqrt{2}}{28}, \dfrac{2\sqrt{2}}{7}, -\dfrac{3\sqrt{2}}{28}, -\dfrac{5\sqrt{2}}{28}, \dfrac{2\sqrt{2}}{7}, -\dfrac{3\sqrt{2}}{28}, \dfrac{3\sqrt{2}}{28}, \dfrac{5\sqrt{2}}{28}, -\dfrac{2\sqrt{2}}{7}, \dfrac{3\sqrt{2}}{28}, \dfrac{5\sqrt{2}}{28}, -\dfrac{2\sqrt{2}}{7} \right]$

y81 $\quad \mathbb{T}_{2,1}^{(s)}(E_{2g}, a) = \left[\dfrac{11\sqrt{6}i}{84}, \dfrac{\sqrt{6}i}{42}, -\dfrac{13\sqrt{6}i}{84}, \dfrac{11\sqrt{6}i}{84}, \dfrac{\sqrt{6}i}{42}, -\dfrac{13\sqrt{6}i}{84}, -\dfrac{13\sqrt{6}i}{84}, \dfrac{11\sqrt{6}i}{84}, \dfrac{\sqrt{6}i}{42}, -\dfrac{13\sqrt{6}i}{84}, \dfrac{11\sqrt{6}i}{84}, \dfrac{\sqrt{6}i}{42} \right]$

y82 $\quad \mathbb{T}_{2,2}^{(s)}(E_{2g}, a) = \left[-\dfrac{5\sqrt{2}i}{28}, \dfrac{2\sqrt{2}i}{7}, -\dfrac{3\sqrt{2}i}{28}, -\dfrac{5\sqrt{2}i}{28}, \dfrac{2\sqrt{2}i}{7}, -\dfrac{3\sqrt{2}i}{28}, \dfrac{3\sqrt{2}i}{28}, \dfrac{5\sqrt{2}i}{28}, -\dfrac{2\sqrt{2}i}{7}, \dfrac{3\sqrt{2}i}{28}, \dfrac{5\sqrt{2}i}{28}, -\dfrac{2\sqrt{2}i}{7} \right]$

y83 $\quad \mathbb{T}_{2,1}^{(s)}(E_{2g}, b) = \left[\dfrac{5\sqrt{2}i}{28}, -\dfrac{2\sqrt{2}i}{7}, \dfrac{3\sqrt{2}i}{28}, \dfrac{5\sqrt{2}i}{28}, -\dfrac{2\sqrt{2}i}{7}, \dfrac{3\sqrt{2}i}{28}, \dfrac{3\sqrt{2}i}{28}, \dfrac{5\sqrt{2}i}{28}, -\dfrac{2\sqrt{2}i}{7}, \dfrac{3\sqrt{2}i}{28}, \dfrac{5\sqrt{2}i}{28}, -\dfrac{2\sqrt{2}i}{7} \right]$

y84 $\quad \mathbb{T}_{2,2}^{(s)}(E_{2g}, b) = \left[\dfrac{11\sqrt{6}i}{84}, \dfrac{\sqrt{6}i}{42}, -\dfrac{13\sqrt{6}i}{84}, \dfrac{11\sqrt{6}i}{84}, \dfrac{\sqrt{6}i}{42}, -\dfrac{13\sqrt{6}i}{84}, \dfrac{13\sqrt{6}i}{84}, -\dfrac{11\sqrt{6}i}{84}, -\dfrac{\sqrt{6}i}{42}, \dfrac{13\sqrt{6}i}{84}, -\dfrac{11\sqrt{6}i}{84}, -\dfrac{\sqrt{6}i}{42} \right]$

y85 $\quad \mathbb{Q}_{4,1}^{(s)}(E_{2g}, 1) = \left[\dfrac{5\sqrt{2}}{28}, -\dfrac{2\sqrt{2}}{7}, \dfrac{3\sqrt{2}}{28}, \dfrac{5\sqrt{2}}{28}, -\dfrac{2\sqrt{2}}{7}, \dfrac{3\sqrt{2}}{28}, \dfrac{3\sqrt{2}}{28}, \dfrac{5\sqrt{2}}{28}, -\dfrac{2\sqrt{2}}{7}, \dfrac{3\sqrt{2}}{28}, \dfrac{5\sqrt{2}}{28}, -\dfrac{2\sqrt{2}}{7} \right]$

y86 $\quad \mathbb{Q}_{4,2}^{(s)}(E_{2g}, 1) = \left[\dfrac{11\sqrt{6}}{84}, \dfrac{\sqrt{6}}{42}, -\dfrac{13\sqrt{6}}{84}, \dfrac{11\sqrt{6}}{84}, \dfrac{\sqrt{6}}{42}, -\dfrac{13\sqrt{6}}{84}, \dfrac{13\sqrt{6}}{84}, -\dfrac{11\sqrt{6}}{84}, -\dfrac{\sqrt{6}}{42}, \dfrac{13\sqrt{6}}{84}, -\dfrac{11\sqrt{6}}{84}, -\dfrac{\sqrt{6}}{42} \right]$

— **Site and Bond** —

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,$\cdots$,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 (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 (3a@3f), ND, $|\boldsymbol{v}|$= 1.40585 (cartesian)

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

Table 9: 2-th 'A'-'A' [1] (#2) bond cluster (6b@6l), ND, $|\boldsymbol{v}|$= 2.435 (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 'A'-'A' [1] (#3) bond cluster (3b@1a), ND, $|\boldsymbol{v}|$= 2.8117 (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]

Table 10

SL	vector ($\boldsymbol{v}$)	center ($\boldsymbol{c}$)	mapping	head	tail	$\boldsymbol{R}$ (primitive)
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, $|\boldsymbol{v}|=$ 3.71952 (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 'A'-'A' [1] (#5) bond cluster (`6a@6l`), D, $|\boldsymbol{v}|=$ 4.21754 (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]

continued ...

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Table 12

SL	vector (v)	center (c)	mapping	head	tail	R (primitive)
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]