Model for "CH4"

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General Condition

- Basis type: `lgs`
- SAMB selection:
  - Type: `[Q, G]`
  - Rank: `[0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11]`
  - Irrep.: $[A_1, A_2]$
  - 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.: $[A_1, A_2, E, T_1, T_2]$
  - Spin (s): `[0, 1]`
- Site-cluster selection:
  - Rank: `[0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11]`
  - Irrep.: $[A_1, A_2, E, T_1, T_2]$
- Bond-cluster selection:
  - Type: `[Q, G, M, T]`
  - Rank: `[0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11]`
  - Irrep.: $[A_1, A_2, E, T_1, T_2]$
- Max. neighbor: `10`
- Search cell range: `(-2, 3), (-2, 3), (-2, 3)`
- Toroidal priority: `false`

Group and Unit Cell

- Group: PG No. 31 $T_{\rm d}$ $\bar{4}3m$ [cubic]
- Unit cell:
  $a =$ 1.00000, $b =$ 1.00000, $c =$ 1.00000, $\alpha = 90.0$, $\beta = 90.0$, $\gamma = 90.0$
- Lattice vectors (conventional cell):
  $\boldsymbol{a}_1 =$ [1.00000, 0.00000, 0.00000]
  $\boldsymbol{a}_2 =$ [0.00000, 1.00000, 0.00000]
  $\boldsymbol{a}_3 =$ [0.00000, 0.00000, 1.00000]

Symmetry Operation

Table 1: Symmetry operation

#	SO	#	SO	#	SO	#	SO	#	SO
1	1	2	2_{001}	3	2_{010}	4	2_{100}	5	3^{+}_{111}
6	3^{+}_{-11-1}	7	3^{+}_{1-1-1}	8	3^{+}_{-1-11}	9	3^{-}_{111}	10	3^{-}_{1-1-1}
11	3^{-}_{-1-11}	12	3^{-}_{-11-1}	13	m_{1-10}	14	m_{110}	15	-4^{+}_{001}
16	-4^{-}_{001}	17	m_{01-1}	18	-4^{+}_{100}	19	-4^{-}_{100}	20	m_{011}
21	m_{-101}	22	-4^{-}_{010}	23	m_{101}	24	-4^{+}_{010}		

Harmonics

Table 2: Harmonics

#	symbol	irrep.	rank	X	multiplicity	component	symmetry
1	$\mathbb{Q}_0(A_1)$	A_1	0	Q, T	-	-	1
2	$\mathbb{G}_0(A_2)$	A_2	0	G, M	-	-	1
3	$\mathbb{G}_3(A_2)$	A_2	3	G, M	-	-	$\sqrt{15}xyz$
4	$\mathbb{G}_{2,1}(E)$	E	2	G, M	-	1	$-\frac{\sqrt{3}(x-y)(x+y)}{2}$
5	$\mathbb{G}_{2,2}(E)$					2	$-\frac{x^2}{2}-\frac{y^2}{2}+z^2$

continued ...

Table 2

#	symbol	irrep.	rank	X	multiplicity	component	symmetry
6	$\mathbb{Q}_{2,1}(E)$	E	2	Q, T	-	1	$-\frac{x^2}{2}-\frac{y^2}{2}+z^2$
7	$\mathbb{Q}_{2,2}(E)$					2	$\frac{\sqrt{3}(x-y)(x+y)}{2}$
8	$\mathbb{G}_{1,1}(T_1)$	T_1	1	G, M	-	1	x
9	$\mathbb{G}_{1,2}(T_1)$					2	y
10	$\mathbb{G}_{1,3}(T_1)$					3	z
11	$\mathbb{G}_{2,1}(T_1)$	T_1	2	G, M	-	1	$\sqrt{3}yz$
12	$\mathbb{G}_{2,2}(T_1)$					2	$\sqrt{3}xz$
13	$\mathbb{G}_{2,3}(T_1)$					3	$\sqrt{3}xy$
14	$\mathbb{G}_{3,1}(T_1)$	T_1	3	G, M	-	1	$\frac{x\left(2x^2-3y^2-3z^2\right)}{2}$
15	$\mathbb{G}_{3,2}(T_1)$					2	$-\frac{y\left(3x^2-2y^2+3z^2\right)}{2}$
16	$\mathbb{G}_{3,3}(T_1)$					3	$-\frac{z\left(3x^2+3y^2-2z^2\right)}{2}$
17	$\mathbb{Q}_{1,1}(T_2)$	T_2	1	Q, T	-	1	x
18	$\mathbb{Q}_{1,2}(T_2)$					2	y
19	$\mathbb{Q}_{1,3}(T_2)$					3	z
20	$\mathbb{Q}_{2,1}(T_2)$	T_2	2	Q, T	-	1	$\sqrt{3}yz$
21	$\mathbb{Q}_{2,2}(T_2)$					2	$\sqrt{3}xz$
22	$\mathbb{Q}_{2,3}(T_2)$					3	$\sqrt{3}xy$
23	$\mathbb{G}_{3,1}(T_2)$	T_2	3	G, M	-	1	$\frac{\sqrt{15}x(y-z)(y+z)}{2}$
24	$\mathbb{G}_{3,2}(T_2)$					2	$-\frac{\sqrt{15}y(x-z)(x+z)}{2}$
25	$\mathbb{G}_{3,3}(T_2)$					3	$\frac{\sqrt{15}z(x-y)(x+y)}{2}$

Basis in full matrix

Table 3: dimension = 16

	#	orbital@atom(SL)	#	orbital@atom(SL)	#	orbital@atom(SL)	#	orbital@atom(SL)	#	orbital@atom(SL)
	0	$\lvert s,\uparrow\rangle$ @C(1)	1	$\lvert s,\downarrow\rangle$ @C(1)	2	$\lvert p_x,\uparrow\rangle$ @C(1)	3	$\lvert p_x,\downarrow\rangle$ @C(1)	4	$\lvert p_y,\uparrow\rangle$ @C(1)
	5	$\lvert p_y,\downarrow\rangle$ @C(1)	6	$\lvert p_z,\uparrow\rangle$ @C(1)	7	$\lvert p_z,\downarrow\rangle$ @C(1)	8	$\lvert s,\uparrow\rangle$ @H(1)	9	$\lvert s,\downarrow\rangle$ @H(1)
	10	$\lvert s,\uparrow\rangle$ @H(2)	11	$\lvert s,\downarrow\rangle$ @H(2)	12	$\lvert s,\uparrow\rangle$ @H(3)	13	$\lvert s,\downarrow\rangle$ @H(3)	14	$\lvert s,\uparrow\rangle$ @H(4)
	15	$\lvert s,\downarrow\rangle$ @H(4)								

Table 4: Atomic basis (orbital part only)

orbital	definition
$\lvert s\rangle$	1
$\lvert p_x\rangle$	x
$\lvert p_y\rangle$	y
$\lvert p_z\rangle$	z

SAMB

11 (all 11) SAMBs

- 'C' site-cluster : `C`
  * bra: $\langle s,\uparrow|$, $\langle s,\downarrow|$
  * ket: $|s,\uparrow\rangle$, $|s,\downarrow\rangle$
  * wyckoff: `1o`

$$\boxed{\text{z1}}\quad \mathbb{Q}_0^{(c)}(A_1) = \mathbb{Q}_0^{(a)}(A_1)\mathbb{Q}_0^{(s)}(A_1)$$

- 'C' site-cluster : `C`
  * bra: $\langle s,\uparrow|$, $\langle s,\downarrow|$
  * ket: $|p_x,\uparrow\rangle$, $|p_x,\downarrow\rangle$, $|p_y,\uparrow\rangle$, $|p_y,\downarrow\rangle$, $|p_z,\uparrow\rangle$, $|p_z,\downarrow\rangle$
  * wyckoff: `1o`

$$\boxed{\text{z8}}\quad \mathbb{G}_0^{(1,1;c)}(A_2) = \mathbb{G}_0^{(1,1;a)}(A_2)\mathbb{Q}_0^{(s)}(A_1)$$

- 'C' site-cluster : `C`
  * bra: $\langle p_x,\uparrow|$, $\langle p_x,\downarrow|$, $\langle p_y,\uparrow|$, $\langle p_y,\downarrow|$, $\langle p_z,\uparrow|$, $\langle p_z,\downarrow|$
  * ket: $|p_x,\uparrow\rangle$, $|p_x,\downarrow\rangle$, $|p_y,\uparrow\rangle$, $|p_y,\downarrow\rangle$, $|p_z,\uparrow\rangle$, $|p_z,\downarrow\rangle$
  * wyckoff: `1o`

$$\boxed{\text{z2}}\quad \mathbb{Q}_0^{(c)}(A_1) = \mathbb{Q}_0^{(a)}(A_1)\mathbb{Q}_0^{(s)}(A_1)$$

$$\boxed{\text{z3}}\quad \mathbb{Q}_0^{(1,1;c)}(A_1) = \mathbb{Q}_0^{(1,1;a)}(A_1)\mathbb{Q}_0^{(s)}(A_1)$$

- 'H' site-cluster : `H`
  * bra: $\langle s,\uparrow|$, $\langle s,\downarrow|$
  * ket: $|s,\uparrow\rangle$, $|s,\downarrow\rangle$
  * wyckoff: `4a`

$$\boxed{\text{z4}}\quad \mathbb{Q}_0^{(c)}(A_1) = \mathbb{Q}_0^{(a)}(A_1)\mathbb{Q}_0^{(s)}(A_1)$$

- 'C'-'H' bond-cluster : `H;C_001_1`
  * bra: $\langle s,\uparrow|$, $\langle s,\downarrow|$
  * ket: $|s,\uparrow\rangle$, $|s,\downarrow\rangle$
  * wyckoff: `4a@4a`

$$\boxed{\text{z5}}\quad \mathbb{Q}_0^{(c)}(A_1) = \mathbb{Q}_0^{(a)}(A_1)\mathbb{Q}_0^{(b)}(A_1)$$

$$\boxed{\text{z9}}\quad \mathbb{G}_0^{(1,-1;c)}(A_2) = \frac{\sqrt{3}\mathbb{M}_{1,1}^{(1,-1;a)}(T_1)\mathbb{T}_{1,1}^{(b)}(T_2)}{3} + \frac{\sqrt{3}\mathbb{M}_{1,2}^{(1,-1;a)}(T_1)\mathbb{T}_{1,2}^{(b)}(T_2)}{3} + \frac{\sqrt{3}\mathbb{M}_{1,3}^{(1,-1;a)}(T_1)\mathbb{T}_{1,3}^{(b)}(T_2)}{3}$$

- 'C'-'H' bond-cluster : `H;C_001_1`
  * bra: $\langle p_x, \uparrow|$, $\langle p_x, \downarrow|$, $\langle p_y, \uparrow|$, $\langle p_y, \downarrow|$, $\langle p_z, \uparrow|$, $\langle p_z, \downarrow|$
  * ket: $|s, \uparrow\rangle$, $|s, \downarrow\rangle$
  * wyckoff: `4a@4a`

$\boxed{\text{z6}}$ $$\mathbb{Q}_0^{(c)}(A_1) = \frac{\sqrt{3}\mathbb{Q}_{1,1}^{(a)}(T_2)\mathbb{Q}_{1,1}^{(b)}(T_2)}{3} + \frac{\sqrt{3}\mathbb{Q}_{1,2}^{(a)}(T_2)\mathbb{Q}_{1,2}^{(b)}(T_2)}{3} + \frac{\sqrt{3}\mathbb{Q}_{1,3}^{(a)}(T_2)\mathbb{Q}_{1,3}^{(b)}(T_2)}{3}$$

$\boxed{\text{z7}}$ $$\mathbb{Q}_0^{(1,0;c)}(A_1) = \frac{\sqrt{3}\mathbb{Q}_{1,1}^{(1,0;a)}(T_2)\mathbb{Q}_{1,1}^{(b)}(T_2)}{3} + \frac{\sqrt{3}\mathbb{Q}_{1,2}^{(1,0;a)}(T_2)\mathbb{Q}_{1,2}^{(b)}(T_2)}{3} + \frac{\sqrt{3}\mathbb{Q}_{1,3}^{(1,0;a)}(T_2)\mathbb{Q}_{1,3}^{(b)}(T_2)}{3}$$

$\boxed{\text{z10}}$ $$\mathbb{G}_3^{(1,-1;c)}(A_2) = \frac{\sqrt{3}\mathbb{G}_{2,1}^{(1,-1;a)}(T_1)\mathbb{Q}_{1,1}^{(b)}(T_2)}{3} + \frac{\sqrt{3}\mathbb{G}_{2,2}^{(1,-1;a)}(T_1)\mathbb{Q}_{1,2}^{(b)}(T_2)}{3} + \frac{\sqrt{3}\mathbb{G}_{2,3}^{(1,-1;a)}(T_1)\mathbb{Q}_{1,3}^{(b)}(T_2)}{3}$$

$\boxed{\text{z11}}$ $$\mathbb{G}_0^{(1,1;c)}(A_2) = \mathbb{G}_0^{(1,1;a)}(A_2)\mathbb{Q}_0^{(b)}(A_1)$$

Atomic SAMB

- bra: $\langle s, \uparrow|$, $\langle s, \downarrow|$
- ket: $|s, \uparrow\rangle$, $|s, \downarrow\rangle$

$\boxed{\text{x1}}$ $$\mathbb{Q}_0^{(a)}(A_1) = \begin{bmatrix} \frac{\sqrt{2}}{2} & 0 \\ 0 & \frac{\sqrt{2}}{2} \end{bmatrix}$$

$\boxed{\text{x2}}$ $$\mathbb{M}_{1,1}^{(1,-1;a)}(T_1) = \begin{bmatrix} 0 & \frac{\sqrt{2}}{2} \\ \frac{\sqrt{2}}{2} & 0 \end{bmatrix}$$

$\boxed{\text{x3}}$ $$\mathbb{M}_{1,2}^{(1,-1;a)}(T_1) = \begin{bmatrix} 0 & -\frac{\sqrt{2}i}{2} \\ \frac{\sqrt{2}i}{2} & 0 \end{bmatrix}$$

$\boxed{\text{x4}}$ $$\mathbb{M}_{1,3}^{(1,-1;a)}(T_1) = \begin{bmatrix} \frac{\sqrt{2}}{2} & 0 \\ 0 & -\frac{\sqrt{2}}{2} \end{bmatrix}$$

- bra: $\langle s, \uparrow|$, $\langle s, \downarrow|$
- ket: $|p_x, \uparrow\rangle$, $|p_x, \downarrow\rangle$, $|p_y, \uparrow\rangle$, $|p_y, \downarrow\rangle$, $|p_z, \uparrow\rangle$, $|p_z, \downarrow\rangle$

$\boxed{\text{x5}}$ $\mathbb{Q}_{1,1}^{(a)}(T_2) = \begin{bmatrix} \frac{1}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 & 0 & 0 \end{bmatrix}$

$\boxed{\text{x6}}$ $\mathbb{Q}_{1,2}^{(a)}(T_2) = \begin{bmatrix} 0 & 0 & \frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2} & 0 & 0 \end{bmatrix}$

$\boxed{\text{x7}}$ $\mathbb{Q}_{1,3}^{(a)}(T_2) = \begin{bmatrix} 0 & 0 & 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{2} \end{bmatrix}$

$\boxed{\text{x8}}$ $\mathbb{Q}_{1,1}^{(1,0;a)}(T_2) = \begin{bmatrix} 0 & 0 & -\frac{\sqrt{2}i}{4} & 0 & 0 & \frac{\sqrt{2}}{4} \\ 0 & 0 & 0 & \frac{\sqrt{2}i}{4} & -\frac{\sqrt{2}}{4} & 0 \end{bmatrix}$

$\boxed{\text{x9}}$ $\mathbb{Q}_{1,2}^{(1,0;a)}(T_2) = \begin{bmatrix} \frac{\sqrt{2}i}{4} & 0 & 0 & 0 & 0 & -\frac{\sqrt{2}i}{4} \\ 0 & -\frac{\sqrt{2}i}{4} & 0 & 0 & -\frac{\sqrt{2}i}{4} & 0 \end{bmatrix}$

$\boxed{\text{x10}}$ $\mathbb{Q}_{1,3}^{(1,0;a)}(T_2) = \begin{bmatrix} 0 & -\frac{\sqrt{2}}{4} & 0 & \frac{\sqrt{2}i}{4} & 0 & 0 \\ \frac{\sqrt{2}}{4} & 0 & \frac{\sqrt{2}i}{4} & 0 & 0 & 0 \end{bmatrix}$

$\boxed{\text{x11}}$ $\mathbb{G}_{2,1}^{(1,-1;a)}(E) = \begin{bmatrix} 0 & -\frac{\sqrt{2}i}{4} & 0 & \frac{\sqrt{2}}{4} & 0 & 0 \\ -\frac{\sqrt{2}i}{4} & 0 & -\frac{\sqrt{2}}{4} & 0 & 0 & 0 \end{bmatrix}$

$\boxed{\text{x12}}$ $\mathbb{G}_{2,2}^{(1,-1;a)}(E) = \begin{bmatrix} 0 & -\frac{\sqrt{6}i}{12} & 0 & -\frac{\sqrt{6}}{12} & \frac{\sqrt{6}i}{6} & 0 \\ -\frac{\sqrt{6}i}{12} & 0 & \frac{\sqrt{6}}{12} & 0 & 0 & -\frac{\sqrt{6}i}{6} \end{bmatrix}$

$\boxed{\text{x13}}$ $\mathbb{G}_{2,1}^{(1,-1;a)}(T_1) = \begin{bmatrix} 0 & 0 & \frac{\sqrt{2}i}{4} & 0 & 0 & \frac{\sqrt{2}}{4} \\ 0 & 0 & 0 & -\frac{\sqrt{2}i}{4} & -\frac{\sqrt{2}}{4} & 0 \end{bmatrix}$

$\boxed{\text{x14}}$ $\mathbb{G}_{2,2}^{(1,-1;a)}(T_1) = \begin{bmatrix} \frac{\sqrt{2}i}{4} & 0 & 0 & 0 & 0 & \frac{\sqrt{2}i}{4} \\ 0 & -\frac{\sqrt{2}i}{4} & 0 & 0 & \frac{\sqrt{2}i}{4} & 0 \end{bmatrix}$

$\boxed{\text{x15}}$ $\mathbb{G}_{2,3}^{(1,-1;a)}(T_1) = \begin{bmatrix} 0 & \frac{\sqrt{2}}{4} & 0 & \frac{\sqrt{2}i}{4} & 0 & 0 \\ -\frac{\sqrt{2}}{4} & 0 & \frac{\sqrt{2}i}{4} & 0 & 0 & 0 \end{bmatrix}$

$\boxed{\text{x16}}$ $\mathbb{G}_{0}^{(1,1;a)}(A_2) = \begin{bmatrix} 0 & \frac{\sqrt{3}i}{6} & 0 & \frac{\sqrt{3}}{6} & \frac{\sqrt{3}i}{6} & 0 \\ \frac{\sqrt{3}i}{6} & 0 & -\frac{\sqrt{3}}{6} & 0 & 0 & -\frac{\sqrt{3}i}{6} \end{bmatrix}$

$\boxed{\text{x17}}$ $\mathbb{M}_{2,1}^{(1,-1;a)}(E) = \begin{bmatrix} 0 & -\frac{\sqrt{2}}{4} & 0 & -\frac{\sqrt{2}i}{4} & 0 & 0 \\ -\frac{\sqrt{2}}{4} & 0 & \frac{\sqrt{2}i}{4} & 0 & 0 & 0 \end{bmatrix}$

$\boxed{\text{x18}}$ $\mathbb{M}_{2,2}^{(1,-1;a)}(E) = \begin{bmatrix} 0 & -\frac{\sqrt{6}}{12} & 0 & \frac{\sqrt{6}i}{12} & \frac{\sqrt{6}}{6} & 0 \\ -\frac{\sqrt{6}}{12} & 0 & -\frac{\sqrt{6}i}{12} & 0 & 0 & -\frac{\sqrt{6}}{6} \end{bmatrix}$

$\boxed{\text{x19}}$ $\mathbb{M}_{2,1}^{(1,-1;a)}(T_1) = \begin{bmatrix} 0 & 0 & \frac{\sqrt{2}}{4} & 0 & 0 & -\frac{\sqrt{2}i}{4} \\ 0 & 0 & 0 & -\frac{\sqrt{2}}{4} & \frac{\sqrt{2}i}{4} & 0 \end{bmatrix}$

$\boxed{\text{x20}}$ $\mathbb{M}_{2,2}^{(1,-1;a)}(T_1) = \begin{bmatrix} \frac{\sqrt{2}}{4} & 0 & 0 & 0 & 0 & \frac{\sqrt{2}}{4} \\ 0 & -\frac{\sqrt{2}}{4} & 0 & 0 & \frac{\sqrt{2}}{4} & 0 \end{bmatrix}$

$\boxed{\text{x21}}$ $\mathbb{M}_{2,3}^{(1,-1;a)}(T_1) = \begin{bmatrix} 0 & -\frac{\sqrt{2}i}{4} & 0 & \frac{\sqrt{2}}{4} & 0 & 0 \\ \frac{\sqrt{2}i}{4} & 0 & \frac{\sqrt{2}}{4} & 0 & 0 & 0 \end{bmatrix}$

$\boxed{\text{x22}}$ $\mathbb{M}_{0}^{(1,1;a)}(A_2) = \begin{bmatrix} 0 & \frac{\sqrt{3}}{6} & 0 & -\frac{\sqrt{3}i}{6} & \frac{\sqrt{3}}{6} & 0 \\ \frac{\sqrt{3}}{6} & 0 & \frac{\sqrt{3}i}{6} & 0 & 0 & -\frac{\sqrt{3}}{6} \end{bmatrix}$

$\boxed{\text{x23}}$ $\mathbb{T}_{1,1}^{(a)}(T_2) = \begin{bmatrix} \frac{i}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{i}{2} & 0 & 0 & 0 & 0 \end{bmatrix}$

$\boxed{\text{x24}}$ $\mathbb{T}_{1,2}^{(a)}(T_2) = \begin{bmatrix} 0 & 0 & \frac{i}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{i}{2} & 0 & 0 \end{bmatrix}$

$\boxed{\text{x25}}$ $\mathbb{T}_{1,3}^{(a)}(T_2) = \begin{bmatrix} 0 & 0 & 0 & 0 & \frac{i}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{i}{2} \end{bmatrix}$

$\boxed{\text{x26}}$ $\mathbb{T}_{1,1}^{(1,0;a)}(T_2) = \begin{bmatrix} 0 & 0 & -\frac{\sqrt{2}}{4} & 0 & 0 & -\frac{\sqrt{2}i}{4} \\ 0 & 0 & 0 & \frac{\sqrt{2}}{4} & \frac{\sqrt{2}i}{4} & 0 \end{bmatrix}$

$\boxed{\text{x27}}$ $\mathbb{T}_{1,2}^{(1,0;a)}(T_2) = \begin{bmatrix} \frac{\sqrt{2}}{4} & 0 & 0 & 0 & 0 & -\frac{\sqrt{2}}{4} \\ 0 & -\frac{\sqrt{2}}{4} & 0 & 0 & -\frac{\sqrt{2}}{4} & 0 \end{bmatrix}$

$\boxed{\text{x28}}$ $\mathbb{T}_{1,3}^{(1,0;a)}(T_2) = \begin{bmatrix} 0 & \frac{\sqrt{2}i}{4} & 0 & \frac{\sqrt{2}}{4} & 0 & 0 \\ -\frac{\sqrt{2}i}{4} & 0 & \frac{\sqrt{2}}{4} & 0 & 0 & 0 \end{bmatrix}$

- bra: $\langle p_x, \uparrow|\,,\ \langle p_x, \downarrow|\,,\ \langle p_y, \uparrow|\,,\ \langle p_y, \downarrow|\,,\ \langle p_z, \uparrow|\,,\ \langle p_z, \downarrow|$
- ket: $|p_x, \uparrow\rangle\,,\ |p_x, \downarrow\rangle\,,\ |p_y, \uparrow\rangle\,,\ |p_y, \downarrow\rangle\,,\ |p_z, \uparrow\rangle\,,\ |p_z, \downarrow\rangle$

$\boxed{\text{x29}}$ $$\mathbb{Q}_{0}^{(a)}(A_1) = \begin{bmatrix} \frac{\sqrt{6}}{6} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{6}}{6} & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{6}}{6} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{6}}{6} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{6}}{6} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{6}}{6} \end{bmatrix}$$

$\boxed{\text{x30}}$ $$\mathbb{Q}_{2,1}^{(a)}(E) = \begin{bmatrix} -\frac{\sqrt{3}}{6} & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{3}}{6} & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{3}}{6} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{3}}{6} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{3}}{3} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{3}}{3} \end{bmatrix}$$

$\boxed{\text{x31}}$ $$\mathbb{Q}_{2,2}^{(a)}(E) = \begin{bmatrix} \frac{1}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{1}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$\boxed{\text{x32}}$ $$\mathbb{Q}_{2,1}^{(a)}(T_2) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{2} \\ 0 & 0 & \frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2} & 0 & 0 \end{bmatrix}$$

$\boxed{\text{x33}}$ $$\mathbb{Q}_{2,2}^{(a)}(T_2) = \begin{bmatrix} 0 & 0 & 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{2} \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{1}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 & 0 & 0 \end{bmatrix}$$

$\boxed{\text{x34}}$ $$\mathbb{Q}_{2,3}^{(a)}(T_2) = \begin{bmatrix} 0 & 0 & \frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2} & 0 & 0 \\ \frac{1}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x35}} \quad \mathbb{Q}_{2,1}^{(1,-1;a)}(E) = \begin{bmatrix} 0 & 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 & -\frac{\sqrt{6}}{12} \\ 0 & 0 & 0 & \frac{\sqrt{6}i}{6} & \frac{\sqrt{6}}{12} & 0 \\ \frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 & \frac{\sqrt{6}i}{12} \\ 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 & \frac{\sqrt{6}i}{12} & 0 \\ 0 & \frac{\sqrt{6}}{12} & 0 & -\frac{\sqrt{6}i}{12} & 0 & 0 \\ -\frac{\sqrt{6}}{12} & 0 & -\frac{\sqrt{6}i}{12} & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x36}} \quad \mathbb{Q}_{2,2}^{(1,-1;a)}(E) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{2}}{4} \\ 0 & 0 & 0 & 0 & \frac{\sqrt{2}}{4} & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{2}i}{4} \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{2}i}{4} & 0 \\ 0 & \frac{\sqrt{2}}{4} & 0 & \frac{\sqrt{2}i}{4} & 0 & 0 \\ -\frac{\sqrt{2}}{4} & 0 & \frac{\sqrt{2}i}{4} & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x37}} \quad \mathbb{Q}_{2,1}^{(1,-1;a)}(T_2) = \begin{bmatrix} 0 & 0 & 0 & -\frac{\sqrt{2}}{4} & \frac{\sqrt{2}i}{4} & 0 \\ 0 & 0 & \frac{\sqrt{2}}{4} & 0 & 0 & -\frac{\sqrt{2}i}{4} \\ 0 & \frac{\sqrt{2}}{4} & 0 & 0 & 0 & 0 \\ -\frac{\sqrt{2}}{4} & 0 & 0 & 0 & 0 & 0 \\ -\frac{\sqrt{2}i}{4} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{2}i}{4} & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x38}} \quad \mathbb{Q}_{2,2}^{(1,-1;a)}(T_2) = \begin{bmatrix} 0 & 0 & 0 & -\frac{\sqrt{2}i}{4} & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{2}i}{4} & 0 & 0 & 0 \\ 0 & \frac{\sqrt{2}i}{4} & 0 & 0 & -\frac{\sqrt{2}i}{4} & 0 \\ \frac{\sqrt{2}i}{4} & 0 & 0 & 0 & 0 & \frac{\sqrt{2}i}{4} \\ 0 & 0 & \frac{\sqrt{2}i}{4} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{2}i}{4} & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x39}} \quad \mathbb{Q}_{2,3}^{(1,-1;a)}(T_2) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{2}i}{4} \\ 0 & 0 & 0 & 0 & \frac{\sqrt{2}i}{4} & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{2}}{4} \\ 0 & 0 & 0 & 0 & \frac{\sqrt{2}}{4} & 0 \\ 0 & -\frac{\sqrt{2}i}{4} & 0 & \frac{\sqrt{2}}{4} & 0 & 0 \\ -\frac{\sqrt{2}i}{4} & 0 & -\frac{\sqrt{2}}{4} & 0 & 0 & 0 \end{bmatrix}$$

$\boxed{\text{x40}}$ $$\mathbb{Q}_0^{(1,1;a)}(A_1) = \begin{bmatrix} 0 & 0 & -\frac{\sqrt{3}i}{6} & 0 & 0 & \frac{\sqrt{3}}{6} \\ 0 & 0 & 0 & \frac{\sqrt{3}i}{6} & -\frac{\sqrt{3}}{6} & 0 \\ \frac{\sqrt{3}i}{6} & 0 & 0 & 0 & 0 & -\frac{\sqrt{3}i}{6} \\ 0 & -\frac{\sqrt{3}i}{6} & 0 & 0 & -\frac{\sqrt{3}i}{6} & 0 \\ 0 & -\frac{\sqrt{3}}{6} & 0 & \frac{\sqrt{3}i}{6} & 0 & 0 \\ \frac{\sqrt{3}}{6} & 0 & \frac{\sqrt{3}i}{6} & 0 & 0 & 0 \end{bmatrix}$$

$\boxed{\text{x41}}$ $$\mathbb{G}_{1,1}^{(1,0;a)}(T_1) = \begin{bmatrix} 0 & 0 & 0 & -\frac{\sqrt{2}}{4} & -\frac{\sqrt{2}i}{4} & 0 \\ 0 & 0 & \frac{\sqrt{2}}{4} & 0 & 0 & \frac{\sqrt{2}i}{4} \\ 0 & \frac{\sqrt{2}}{4} & 0 & 0 & 0 & 0 \\ -\frac{\sqrt{2}}{4} & 0 & 0 & 0 & 0 & 0 \\ \frac{\sqrt{2}i}{4} & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{2}i}{4} & 0 & 0 & 0 & 0 \end{bmatrix}$$

$\boxed{\text{x42}}$ $$\mathbb{G}_{1,2}^{(1,0;a)}(T_1) = \begin{bmatrix} 0 & 0 & 0 & \frac{\sqrt{2}i}{4} & 0 & 0 \\ 0 & 0 & \frac{\sqrt{2}i}{4} & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{2}i}{4} & 0 & 0 & -\frac{\sqrt{2}i}{4} & 0 \\ -\frac{\sqrt{2}i}{4} & 0 & 0 & 0 & 0 & \frac{\sqrt{2}i}{4} \\ 0 & 0 & \frac{\sqrt{2}i}{4} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{2}i}{4} & 0 & 0 \end{bmatrix}$$

$\boxed{\text{x43}}$ $$\mathbb{G}_{1,3}^{(1,0;a)}(T_1) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{2}i}{4} \\ 0 & 0 & 0 & 0 & \frac{\sqrt{2}i}{4} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{2}}{4} \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{2}}{4} & 0 \\ 0 & -\frac{\sqrt{2}i}{4} & 0 & -\frac{\sqrt{2}}{4} & 0 & 0 \\ -\frac{\sqrt{2}i}{4} & 0 & \frac{\sqrt{2}}{4} & 0 & 0 & 0 \end{bmatrix}$$

$\boxed{\text{x44}}$ $$\mathbb{M}_{1,1}^{(a)}(T_1) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{i}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{i}{2} \\ 0 & 0 & \frac{i}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{i}{2} & 0 & 0 \end{bmatrix}$$

$\boxed{\text{x45}}$ $$\mathbb{M}_{1,2}^{(a)}(T_1) = \begin{bmatrix} 0 & 0 & 0 & 0 & \frac{i}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{i}{2} \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ -\frac{i}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{i}{2} & 0 & 0 & 0 & 0 \end{bmatrix}$$

$\boxed{\text{x46}}$ $$\mathbb{M}_{1,3}^{(a)}(T_1) = \begin{bmatrix} 0 & 0 & -\frac{i}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{i}{2} & 0 & 0 \\ \frac{i}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{i}{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$\boxed{\text{x47}}$ $$\mathbb{M}_{3}^{(1,-1;a)}(A_2) = \begin{bmatrix} 0 & 0 & \frac{\sqrt{3}}{6} & 0 & 0 & -\frac{\sqrt{3}i}{6} \\ 0 & 0 & 0 & -\frac{\sqrt{3}}{6} & \frac{\sqrt{3}i}{6} & 0 \\ \frac{\sqrt{3}}{6} & 0 & 0 & 0 & 0 & \frac{\sqrt{3}}{6} \\ 0 & -\frac{\sqrt{3}}{6} & 0 & 0 & \frac{\sqrt{3}}{6} & 0 \\ 0 & -\frac{\sqrt{3}i}{6} & 0 & \frac{\sqrt{3}}{6} & 0 & 0 \\ \frac{\sqrt{3}i}{6} & 0 & \frac{\sqrt{3}}{6} & 0 & 0 & 0 \end{bmatrix}$$

$\boxed{\text{x48}}$ $$\mathbb{M}_{1,1}^{(1,-1;a)}(T_1) = \begin{bmatrix} 0 & \frac{\sqrt{6}}{6} & 0 & 0 & 0 & 0 \\ \frac{\sqrt{6}}{6} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{6}}{6} & 0 & 0 \\ 0 & 0 & \frac{\sqrt{6}}{6} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{6}}{6} \\ 0 & 0 & 0 & 0 & \frac{\sqrt{6}}{6} & 0 \end{bmatrix}$$

$\boxed{\text{x49}}$ $$\mathbb{M}_{1,2}^{(1,-1;a)}(T_1) = \begin{bmatrix} 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 \\ \frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 \\ 0 & 0 & \frac{\sqrt{6}i}{6} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{6}i}{6} \\ 0 & 0 & 0 & 0 & \frac{\sqrt{6}i}{6} & 0 \end{bmatrix}$$

$\boxed{\text{x50}}$ $$\mathbb{M}_{1,3}^{(1,-1;a)}(T_1) = \begin{bmatrix} \frac{\sqrt{6}}{6} & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{6}}{6} & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{6}}{6} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{6}}{6} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{6}}{6} & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{6}}{6} \end{bmatrix}$$

$\boxed{\text{x51}}$ $$\mathbb{M}_{3,1}^{(1,-1;a)}(T_1)=\begin{bmatrix} 0 & \frac{\sqrt{5}}{5} & 0 & \frac{\sqrt{5}i}{10} & -\frac{\sqrt{5}}{10} & 0 \\ \frac{\sqrt{5}}{5} & 0 & -\frac{\sqrt{5}i}{10} & 0 & 0 & \frac{\sqrt{5}}{10} \\ 0 & \frac{\sqrt{5}i}{10} & 0 & -\frac{\sqrt{5}}{10} & 0 & 0 \\ -\frac{\sqrt{5}i}{10} & 0 & -\frac{\sqrt{5}}{10} & 0 & 0 & 0 \\ -\frac{\sqrt{5}}{10} & 0 & 0 & 0 & 0 & -\frac{\sqrt{5}}{10} \\ 0 & \frac{\sqrt{5}}{10} & 0 & 0 & -\frac{\sqrt{5}}{10} & 0 \end{bmatrix}$$

$\boxed{\text{x52}}$ $$\mathbb{M}_{3,2}^{(1,-1;a)}(T_1)=\begin{bmatrix} 0 & \frac{\sqrt{5}i}{10} & 0 & -\frac{\sqrt{5}}{10} & 0 & 0 \\ -\frac{\sqrt{5}i}{10} & 0 & -\frac{\sqrt{5}}{10} & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{5}}{10} & 0 & -\frac{\sqrt{5}i}{5} & -\frac{\sqrt{5}}{10} & 0 \\ -\frac{\sqrt{5}}{10} & 0 & \frac{\sqrt{5}i}{5} & 0 & 0 & \frac{\sqrt{5}}{10} \\ 0 & 0 & -\frac{\sqrt{5}}{10} & 0 & 0 & \frac{\sqrt{5}i}{10} \\ 0 & 0 & 0 & \frac{\sqrt{5}}{10} & -\frac{\sqrt{5}i}{10} & 0 \end{bmatrix}$$

$\boxed{\text{x53}}$ $$\mathbb{M}_{3,3}^{(1,-1;a)}(T_1)=\begin{bmatrix} -\frac{\sqrt{5}}{10} & 0 & 0 & 0 & 0 & -\frac{\sqrt{5}}{10} \\ 0 & \frac{\sqrt{5}}{10} & 0 & 0 & -\frac{\sqrt{5}}{10} & 0 \\ 0 & 0 & -\frac{\sqrt{5}}{10} & 0 & 0 & \frac{\sqrt{5}i}{10} \\ 0 & 0 & 0 & \frac{\sqrt{5}}{10} & -\frac{\sqrt{5}i}{10} & 0 \\ 0 & -\frac{\sqrt{5}}{10} & 0 & \frac{\sqrt{5}i}{10} & \frac{\sqrt{5}}{5} & 0 \\ -\frac{\sqrt{5}}{10} & 0 & -\frac{\sqrt{5}i}{10} & 0 & 0 & -\frac{\sqrt{5}}{5} \end{bmatrix}$$

$\boxed{\text{x54}}$ $$\mathbb{M}_{3,1}^{(1,-1;a)}(T_2)=\begin{bmatrix} 0 & 0 & 0 & -\frac{\sqrt{3}i}{6} & -\frac{\sqrt{3}}{6} & 0 \\ 0 & 0 & \frac{\sqrt{3}i}{6} & 0 & 0 & \frac{\sqrt{3}}{6} \\ 0 & -\frac{\sqrt{3}i}{6} & 0 & \frac{\sqrt{3}}{6} & 0 & 0 \\ \frac{\sqrt{3}i}{6} & 0 & \frac{\sqrt{3}}{6} & 0 & 0 & 0 \\ -\frac{\sqrt{3}}{6} & 0 & 0 & 0 & 0 & -\frac{\sqrt{3}}{6} \\ 0 & \frac{\sqrt{3}}{6} & 0 & 0 & -\frac{\sqrt{3}}{6} & 0 \end{bmatrix}$$

$\boxed{\text{x55}}$ $$\mathbb{M}_{3,2}^{(1,-1;a)}(T_2)=\begin{bmatrix} 0 & \frac{\sqrt{3}i}{6} & 0 & -\frac{\sqrt{3}}{6} & 0 & 0 \\ -\frac{\sqrt{3}i}{6} & 0 & -\frac{\sqrt{3}}{6} & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{3}}{6} & 0 & 0 & \frac{\sqrt{3}}{6} & 0 \\ -\frac{\sqrt{3}}{6} & 0 & 0 & 0 & 0 & -\frac{\sqrt{3}}{6} \\ 0 & 0 & \frac{\sqrt{3}}{6} & 0 & 0 & -\frac{\sqrt{3}i}{6} \\ 0 & 0 & 0 & -\frac{\sqrt{3}}{6} & \frac{\sqrt{3}i}{6} & 0 \end{bmatrix}$$

$$\boxed{\text{x56}} \quad \mathbb{M}_{3,3}^{(1,-1;a)}(T_2) = \begin{bmatrix} \frac{\sqrt{3}}{6} & 0 & 0 & 0 & 0 & \frac{\sqrt{3}}{6} \\ 0 & -\frac{\sqrt{3}}{6} & 0 & 0 & \frac{\sqrt{3}}{6} & 0 \\ 0 & 0 & -\frac{\sqrt{3}}{6} & 0 & 0 & \frac{\sqrt{3}i}{6} \\ 0 & 0 & 0 & \frac{\sqrt{3}}{6} & -\frac{\sqrt{3}i}{6} & 0 \\ 0 & \frac{\sqrt{3}}{6} & 0 & \frac{\sqrt{3}i}{6} & 0 & 0 \\ \frac{\sqrt{3}}{6} & 0 & -\frac{\sqrt{3}i}{6} & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x57}} \quad \mathbb{M}_{1,1}^{(1,1;a)}(T_1) = \begin{bmatrix} 0 & \frac{\sqrt{30}}{15} & 0 & -\frac{\sqrt{30}i}{20} & \frac{\sqrt{30}}{20} & 0 \\ \frac{\sqrt{30}}{15} & 0 & \frac{\sqrt{30}i}{20} & 0 & 0 & -\frac{\sqrt{30}}{20} \\ 0 & -\frac{\sqrt{30}i}{20} & 0 & -\frac{\sqrt{30}}{30} & 0 & 0 \\ \frac{\sqrt{30}i}{20} & 0 & -\frac{\sqrt{30}}{30} & 0 & 0 & 0 \\ \frac{\sqrt{30}}{20} & 0 & 0 & 0 & 0 & -\frac{\sqrt{30}}{30} \\ 0 & -\frac{\sqrt{30}}{20} & 0 & 0 & -\frac{\sqrt{30}}{30} & 0 \end{bmatrix}$$

$$\boxed{\text{x58}} \quad \mathbb{M}_{1,2}^{(1,1;a)}(T_1) = \begin{bmatrix} 0 & \frac{\sqrt{30}i}{30} & 0 & \frac{\sqrt{30}}{20} & 0 & 0 \\ -\frac{\sqrt{30}i}{30} & 0 & \frac{\sqrt{30}}{20} & 0 & 0 & 0 \\ 0 & \frac{\sqrt{30}}{20} & 0 & -\frac{\sqrt{30}i}{15} & \frac{\sqrt{30}}{20} & 0 \\ \frac{\sqrt{30}}{20} & 0 & \frac{\sqrt{30}i}{15} & 0 & 0 & -\frac{\sqrt{30}}{20} \\ 0 & 0 & \frac{\sqrt{30}}{20} & 0 & 0 & \frac{\sqrt{30}i}{30} \\ 0 & 0 & 0 & -\frac{\sqrt{30}}{20} & -\frac{\sqrt{30}i}{30} & 0 \end{bmatrix}$$

$$\boxed{\text{x59}} \quad \mathbb{M}_{1,3}^{(1,1;a)}(T_1) = \begin{bmatrix} -\frac{\sqrt{30}}{30} & 0 & 0 & 0 & 0 & \frac{\sqrt{30}}{20} \\ 0 & \frac{\sqrt{30}}{30} & 0 & 0 & \frac{\sqrt{30}}{20} & 0 \\ 0 & 0 & -\frac{\sqrt{30}}{30} & 0 & 0 & -\frac{\sqrt{30}i}{20} \\ 0 & 0 & 0 & \frac{\sqrt{30}}{30} & \frac{\sqrt{30}i}{20} & 0 \\ 0 & \frac{\sqrt{30}}{20} & 0 & -\frac{\sqrt{30}i}{20} & \frac{\sqrt{30}}{15} & 0 \\ \frac{\sqrt{30}}{20} & 0 & \frac{\sqrt{30}i}{20} & 0 & 0 & -\frac{\sqrt{30}}{15} \end{bmatrix}$$

$$\boxed{\text{x60}} \quad \mathbb{T}_{2,1}^{(1,0;a)}(E) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{2}i}{4} \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{2}i}{4} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{2}}{4} \\ 0 & 0 & 0 & 0 & \frac{\sqrt{2}}{4} & 0 \\ 0 & \frac{\sqrt{2}i}{4} & 0 & \frac{\sqrt{2}}{4} & 0 & 0 \\ -\frac{\sqrt{2}i}{4} & 0 & \frac{\sqrt{2}}{4} & 0 & 0 & 0 \end{bmatrix}$$

$\boxed{\text{x61}}$ $\mathbb{T}_{2,2}^{(1,0;a)}(E) = \begin{bmatrix} 0 & 0 & -\frac{\sqrt{6}}{6} & 0 & 0 & -\frac{\sqrt{6}i}{12} \\ 0 & 0 & 0 & \frac{\sqrt{6}}{6} & \frac{\sqrt{6}i}{12} & 0 \\ -\frac{\sqrt{6}}{6} & 0 & 0 & 0 & 0 & \frac{\sqrt{6}}{12} \\ 0 & \frac{\sqrt{6}}{6} & 0 & 0 & \frac{\sqrt{6}}{12} & 0 \\ 0 & -\frac{\sqrt{6}i}{12} & 0 & \frac{\sqrt{6}}{12} & 0 & 0 \\ \frac{\sqrt{6}i}{12} & 0 & \frac{\sqrt{6}}{12} & 0 & 0 & 0 \end{bmatrix}$

$\boxed{\text{x62}}$ $\mathbb{T}_{2,1}^{(1,0;a)}(T_2) = \begin{bmatrix} 0 & 0 & 0 & \frac{\sqrt{6}i}{12} & \frac{\sqrt{6}}{12} & 0 \\ 0 & 0 & -\frac{\sqrt{6}i}{12} & 0 & 0 & -\frac{\sqrt{6}}{12} \\ 0 & \frac{\sqrt{6}i}{12} & 0 & \frac{\sqrt{6}}{6} & 0 & 0 \\ -\frac{\sqrt{6}i}{12} & 0 & \frac{\sqrt{6}}{6} & 0 & 0 & 0 \\ \frac{\sqrt{6}}{12} & 0 & 0 & 0 & 0 & -\frac{\sqrt{6}}{6} \\ 0 & -\frac{\sqrt{6}}{12} & 0 & 0 & -\frac{\sqrt{6}}{6} & 0 \end{bmatrix}$

$\boxed{\text{x63}}$ $\mathbb{T}_{2,2}^{(1,0;a)}(T_2) = \begin{bmatrix} 0 & \frac{\sqrt{6}i}{6} & 0 & \frac{\sqrt{6}}{12} & 0 & 0 \\ -\frac{\sqrt{6}i}{6} & 0 & \frac{\sqrt{6}}{12} & 0 & 0 & 0 \\ 0 & \frac{\sqrt{6}}{12} & 0 & 0 & -\frac{\sqrt{6}}{12} & 0 \\ \frac{\sqrt{6}}{12} & 0 & 0 & 0 & 0 & \frac{\sqrt{6}}{12} \\ 0 & 0 & -\frac{\sqrt{6}}{12} & 0 & 0 & -\frac{\sqrt{6}i}{6} \\ 0 & 0 & 0 & \frac{\sqrt{6}}{12} & \frac{\sqrt{6}i}{6} & 0 \end{bmatrix}$

$\boxed{\text{x64}}$ $\mathbb{T}_{2,3}^{(1,0;a)}(T_2) = \begin{bmatrix} \frac{\sqrt{6}}{6} & 0 & 0 & 0 & 0 & -\frac{\sqrt{6}}{12} \\ 0 & -\frac{\sqrt{6}}{6} & 0 & 0 & -\frac{\sqrt{6}}{12} & 0 \\ 0 & 0 & -\frac{\sqrt{6}}{6} & 0 & 0 & -\frac{\sqrt{6}i}{12} \\ 0 & 0 & 0 & \frac{\sqrt{6}}{6} & \frac{\sqrt{6}i}{12} & 0 \\ 0 & -\frac{\sqrt{6}}{12} & 0 & -\frac{\sqrt{6}i}{12} & 0 & 0 \\ -\frac{\sqrt{6}}{12} & 0 & \frac{\sqrt{6}i}{12} & 0 & 0 & 0 \end{bmatrix}$

- bra: $\langle p_x, \uparrow|$, $\langle p_x, \downarrow|$, $\langle p_y, \uparrow|$, $\langle p_y, \downarrow|$, $\langle p_z, \uparrow|$, $\langle p_z, \downarrow|$
- ket: $|s, \uparrow\rangle$, $|s, \downarrow\rangle$

$\boxed{\text{x65}}$ $\mathbb{Q}_{1,1}^{(a)}(T_2) = \begin{bmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{bmatrix}$

$\boxed{\text{x66}}$ $$\mathbb{Q}_{1,2}^{(a)}(T_2) = \begin{bmatrix} 0 & 0 \\ 0 & 0 \\ \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \\ 0 & 0 \\ 0 & 0 \end{bmatrix}$$

$\boxed{\text{x67}}$ $$\mathbb{Q}_{1,3}^{(a)}(T_2) = \begin{bmatrix} 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{bmatrix}$$

$\boxed{\text{x68}}$ $$\mathbb{Q}_{1,1}^{(1,0;a)}(T_2) = \begin{bmatrix} 0 & 0 \\ 0 & 0 \\ \frac{\sqrt{2}i}{4} & 0 \\ 0 & -\frac{\sqrt{2}i}{4} \\ 0 & -\frac{\sqrt{2}}{4} \\ \frac{\sqrt{2}}{4} & 0 \end{bmatrix}$$

$\boxed{\text{x69}}$ $$\mathbb{Q}_{1,2}^{(1,0;a)}(T_2) = \begin{bmatrix} -\frac{\sqrt{2}i}{4} & 0 \\ 0 & \frac{\sqrt{2}i}{4} \\ 0 & 0 \\ 0 & 0 \\ 0 & \frac{\sqrt{2}i}{4} \\ \frac{\sqrt{2}i}{4} & 0 \end{bmatrix}$$

$\boxed{\text{x70}}$ $$\mathbb{Q}_{1,3}^{(1,0;a)}(T_2) = \begin{bmatrix} 0 & \frac{\sqrt{2}}{4} \\ -\frac{\sqrt{2}}{4} & 0 \\ 0 & -\frac{\sqrt{2}i}{4} \\ -\frac{\sqrt{2}i}{4} & 0 \\ 0 & 0 \\ 0 & 0 \end{bmatrix}$$

$\boxed{\text{x71}}$ $$\mathbb{G}_{2,1}^{(1,-1;a)}(E) = \begin{bmatrix} 0 & \frac{\sqrt{2}i}{4} \\ \frac{\sqrt{2}i}{4} & 0 \\ 0 & -\frac{\sqrt{2}}{4} \\ \frac{\sqrt{2}}{4} & 0 \\ 0 & 0 \\ 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x72}}\quad \mathbb{G}_{2,2}^{(1,-1;a)}(E) = \begin{bmatrix} 0 & \frac{\sqrt{6}i}{12} \\ \frac{\sqrt{6}i}{12} & 0 \\ 0 & \frac{\sqrt{6}}{12} \\ -\frac{\sqrt{6}}{12} & 0 \\ -\frac{\sqrt{6}i}{6} & 0 \\ 0 & \frac{\sqrt{6}i}{6} \end{bmatrix}$$

$$\boxed{\text{x73}}\quad \mathbb{G}_{2,1}^{(1,-1;a)}(T_1) = \begin{bmatrix} 0 & 0 \\ 0 & 0 \\ -\frac{\sqrt{2}i}{4} & 0 \\ 0 & \frac{\sqrt{2}i}{4} \\ 0 & -\frac{\sqrt{2}}{4} \\ \frac{\sqrt{2}}{4} & 0 \end{bmatrix}$$

$$\boxed{\text{x74}}\quad \mathbb{G}_{2,2}^{(1,-1;a)}(T_1) = \begin{bmatrix} -\frac{\sqrt{2}i}{4} & 0 \\ 0 & \frac{\sqrt{2}i}{4} \\ 0 & 0 \\ 0 & 0 \\ 0 & -\frac{\sqrt{2}i}{4} \\ -\frac{\sqrt{2}i}{4} & 0 \end{bmatrix}$$

$$\boxed{\text{x75}}\quad \mathbb{G}_{2,3}^{(1,-1;a)}(T_1) = \begin{bmatrix} 0 & -\frac{\sqrt{2}}{4} \\ \frac{\sqrt{2}}{4} & 0 \\ 0 & -\frac{\sqrt{2}i}{4} \\ -\frac{\sqrt{2}i}{4} & 0 \\ 0 & 0 \\ 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x76}}\quad \mathbb{G}_{0}^{(1,1;a)}(A_2) = \begin{bmatrix} 0 & -\frac{\sqrt{3}i}{6} \\ -\frac{\sqrt{3}i}{6} & 0 \\ 0 & -\frac{\sqrt{3}}{6} \\ \frac{\sqrt{3}}{6} & 0 \\ -\frac{\sqrt{3}i}{6} & 0 \\ 0 & \frac{\sqrt{3}i}{6} \end{bmatrix}$$

$\boxed{\text{x77}}$ $$\mathbb{M}_{2,1}^{(1,-1;a)}(E) = \begin{bmatrix} 0 & -\frac{\sqrt{2}}{4} \\ -\frac{\sqrt{2}}{4} & 0 \\ 0 & -\frac{\sqrt{2}i}{4} \\ \frac{\sqrt{2}i}{4} & 0 \\ 0 & 0 \\ 0 & 0 \end{bmatrix}$$

$\boxed{\text{x78}}$ $$\mathbb{M}_{2,2}^{(1,-1;a)}(E) = \begin{bmatrix} 0 & -\frac{\sqrt{6}}{12} \\ -\frac{\sqrt{6}}{12} & 0 \\ 0 & \frac{\sqrt{6}i}{12} \\ -\frac{\sqrt{6}i}{12} & 0 \\ \frac{\sqrt{6}}{6} & 0 \\ 0 & -\frac{\sqrt{6}}{6} \end{bmatrix}$$

$\boxed{\text{x79}}$ $$\mathbb{M}_{2,1}^{(1,-1;a)}(T_1) = \begin{bmatrix} 0 & 0 \\ 0 & 0 \\ \frac{\sqrt{2}}{4} & 0 \\ 0 & -\frac{\sqrt{2}}{4} \\ 0 & -\frac{\sqrt{2}i}{4} \\ \frac{\sqrt{2}i}{4} & 0 \end{bmatrix}$$

$\boxed{\text{x80}}$ $$\mathbb{M}_{2,2}^{(1,-1;a)}(T_1) = \begin{bmatrix} \frac{\sqrt{2}}{4} & 0 \\ 0 & -\frac{\sqrt{2}}{4} \\ 0 & 0 \\ 0 & 0 \\ 0 & \frac{\sqrt{2}}{4} \\ \frac{\sqrt{2}}{4} & 0 \end{bmatrix}$$

$\boxed{\text{x81}}$ $$\mathbb{M}_{2,3}^{(1,-1;a)}(T_1) = \begin{bmatrix} 0 & -\frac{\sqrt{2}i}{4} \\ \frac{\sqrt{2}i}{4} & 0 \\ 0 & \frac{\sqrt{2}}{4} \\ \frac{\sqrt{2}}{4} & 0 \\ 0 & 0 \\ 0 & 0 \end{bmatrix}$$

$\boxed{\text{x82}}$ $\mathbb{M}_0^{(1,1;a)}(A_2) = \begin{bmatrix} 0 & \frac{\sqrt{3}}{6} \\ \frac{\sqrt{3}}{6} & 0 \\ 0 & -\frac{\sqrt{3}i}{6} \\ \frac{\sqrt{3}i}{6} & 0 \\ \frac{\sqrt{3}}{6} & 0 \\ 0 & -\frac{\sqrt{3}}{6} \end{bmatrix}$

$\boxed{\text{x83}}$ $\mathbb{T}_{1,1}^{(a)}(T_2) = \begin{bmatrix} -\frac{i}{2} & 0 \\ 0 & -\frac{i}{2} \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{bmatrix}$

$\boxed{\text{x84}}$ $\mathbb{T}_{1,2}^{(a)}(T_2) = \begin{bmatrix} 0 & 0 \\ 0 & 0 \\ -\frac{i}{2} & 0 \\ 0 & -\frac{i}{2} \\ 0 & 0 \\ 0 & 0 \end{bmatrix}$

$\boxed{\text{x85}}$ $\mathbb{T}_{1,3}^{(a)}(T_2) = \begin{bmatrix} 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ -\frac{i}{2} & 0 \\ 0 & -\frac{i}{2} \end{bmatrix}$

$\boxed{\text{x86}}$ $\mathbb{T}_{1,1}^{(1,0;a)}(T_2) = \begin{bmatrix} 0 & 0 \\ 0 & 0 \\ -\frac{\sqrt{2}}{4} & 0 \\ 0 & \frac{\sqrt{2}}{4} \\ 0 & -\frac{\sqrt{2}i}{4} \\ \frac{\sqrt{2}i}{4} & 0 \end{bmatrix}$

$\boxed{\text{x87}}$ $\mathbb{T}_{1,2}^{(1,0;a)}(T_2) = \begin{bmatrix} \frac{\sqrt{2}}{4} & 0 \\ 0 & -\frac{\sqrt{2}}{4} \\ 0 & 0 \\ 0 & 0 \\ 0 & -\frac{\sqrt{2}}{4} \\ -\frac{\sqrt{2}}{4} & 0 \end{bmatrix}$

$\boxed{\text{x88}}$ $\mathbb{T}_{1,3}^{(1,0;a)}(T_2) = \begin{bmatrix} 0 & \frac{\sqrt{2}i}{4} \\ -\frac{\sqrt{2}i}{4} & 0 \\ 0 & \frac{\sqrt{2}}{4} \\ \frac{\sqrt{2}}{4} & 0 \\ 0 & 0 \\ 0 & 0 \end{bmatrix}$

Cluster SAMB

- Site cluster

** Wyckoff: `1o`

$\boxed{\text{y1}}$ $\mathbb{Q}_{0}^{(s)}(A_1) = [1]$

** Wyckoff: `4a`

$\boxed{\text{y2}}$ $\mathbb{Q}_{0}^{(s)}(A_1) = \left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right]$

$\boxed{\text{y3}}$ $\mathbb{Q}_{1,1}^{(s)}(T_2) = \left[\frac{1}{2}, -\frac{1}{2}, -\frac{1}{2}, \frac{1}{2}\right]$

$\boxed{\text{y4}}$ $\mathbb{Q}_{1,2}^{(s)}(T_2) = \left[\frac{1}{2}, -\frac{1}{2}, \frac{1}{2}, -\frac{1}{2}\right]$

$\boxed{\text{y5}}$ $\mathbb{Q}_{1,3}^{(s)}(T_2) = \left[\frac{1}{2}, \frac{1}{2}, -\frac{1}{2}, -\frac{1}{2}\right]$

- Bond cluster

** Wyckoff: `4a@4a`

$\boxed{\text{y6}}$ $\mathbb{Q}_{0}^{(s)}(A_1) = \left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right]$

$\boxed{\text{y7}}$ $\mathbb{T}_{0}^{(s)}(A_1) = \left[\frac{i}{2}, \frac{i}{2}, \frac{i}{2}, \frac{i}{2}\right]$

$\boxed{\text{y8}}$ $\mathbb{Q}_{1,1}^{(s)}(T_2) = \left[\frac{1}{2}, -\frac{1}{2}, -\frac{1}{2}, \frac{1}{2}\right]$

$\boxed{\text{y9}}$ $\mathbb{Q}_{1,2}^{(s)}(T_2) = \left[\frac{1}{2}, -\frac{1}{2}, \frac{1}{2}, -\frac{1}{2}\right]$

$\boxed{\text{y10}}$ $\mathbb{Q}_{1,3}^{(s)}(T_2) = \left[\frac{1}{2}, \frac{1}{2}, -\frac{1}{2}, -\frac{1}{2}\right]$

$\boxed{\text{y11}}$ $\mathbb{T}_{1,1}^{(s)}(T_2) = \left[\frac{i}{2}, -\frac{i}{2}, -\frac{i}{2}, \frac{i}{2}\right]$

$\boxed{\text{y12}}$ $\mathbb{T}_{1,2}^{(s)}(T_2) = \left[\frac{i}{2}, -\frac{i}{2}, \frac{i}{2}, -\frac{i}{2}\right]$

$\boxed{\text{y13}}$ $\mathbb{T}_{1,3}^{(s)}(T_2) = \left[\frac{i}{2}, \frac{i}{2}, -\frac{i}{2}, -\frac{i}{2}\right]$

Site and Bond

Table 5: Orbital of each site

#	site	orbital
1	`C`	$\lvert s,\uparrow\rangle$, $\lvert s,\downarrow\rangle$, $\lvert p_x,\uparrow\rangle$, $\lvert p_x,\downarrow\rangle$, $\lvert p_y,\uparrow\rangle$, $\lvert p_y,\downarrow\rangle$, $\lvert p_z,\uparrow\rangle$, $\lvert p_z,\downarrow\rangle$
2	`H`	$\lvert s,\uparrow\rangle$, $\lvert s,\downarrow\rangle$

Table 6: Neighbor and bra-ket of each bond

#	head	tail	neighbor	head (bra)	tail (ket)
1	`C`	`H`	`[1]`	`[s,p]`	`[s]`

Site in Unit Cell

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

Table 7: 'C' (#1) site cluster (1o), -43m

SL	position ($\boldsymbol{s}$)	mapping
1	[0.00000, 0.00000, 0.00000]	[1,2,3,4,5,6,7,8,9,10,11,12,13,14,15,16,17,18,19,20,21,22,23,24]

Table 8: 'H' (#2) site cluster (4a), .3m

SL	position ($\boldsymbol{s}$)	mapping
1	[0.33333, 0.33333, 0.33333]	[1,5,9,13,17,21]
2	[-0.33333,-0.33333, 0.33333]	[2,7,12,14,19,24]
3	[-0.33333, 0.33333,-0.33333]	[3,8,10,16,18,23]
4	[0.33333,-0.33333,-0.33333]	[4,6,11,15,20,22]

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 9: 1-th 'C'-'H' [1] (#1) bond cluster (4a@4a), D, $|\boldsymbol{v}|$= 0.57735 (cartesian)

SL	vector ($\boldsymbol{v}$)	center ($\boldsymbol{c}$)	mapping	head	tail	$\boldsymbol{R}$ (primitive)
1	[-0.33333,-0.33333,-0.33333]	[0.16667, 0.16667, 0.16667]	[1,5,9,13,17,21]	(1,1)	(1,1)	[0,0,0]
2	[0.33333, 0.33333,-0.33333]	[-0.16667,-0.16667, 0.16667]	[2,7,12,14,19,24]	(1,1)	(2,1)	[0,0,0]
3	[0.33333,-0.33333, 0.33333]	[-0.16667, 0.16667,-0.16667]	[3,8,10,16,18,23]	(1,1)	(3,1)	[0,0,0]
4	[-0.33333, 0.33333, 0.33333]	[0.16667,-0.16667,-0.16667]	[4,6,11,15,20,22]	(1,1)	(4,1)	[0,0,0]