

# Model for “CH4”

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## General Condition

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

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## Group and Unit Cell

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- Group: PG No. 31 T<sub>d</sub>  $\bar{4}3m$  [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):  
 $\mathbf{a}_1 = [1.00000, 0.00000, 0.00000]$   
 $\mathbf{a}_2 = [0.00000, 1.00000, 0.00000]$   
 $\mathbf{a}_3 = [0.00000, 0.00000, 1.00000]$

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**Symmetry Operation**


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Table 1: Symmetry operation

#	SO	#	SO	#	SO	#	SO	#	SO
1	1	2	2 <sub>001</sub>	3	2 <sub>010</sub>	4	2 <sub>100</sub>	5	3 <sub>111</sub> <sup>+</sup>
6	3 <sub>-11-1</sub> <sup>+</sup>	7	3 <sub>1-1-1</sub> <sup>+</sup>	8	3 <sub>-1-11</sub> <sup>+</sup>	9	3 <sub>111</sub> <sup>-</sup>	10	3 <sub>1-1-1</sub> <sup>-</sup>
11	3 <sub>-1-11</sub> <sup>-</sup>	12	3 <sub>-11-1</sub> <sup>-</sup>	13	m <sub>1-10</sub>	14	m <sub>110</sub>	15	-4 <sub>001</sub> <sup>+</sup>
16	-4 <sub>001</sub> <sup>-</sup>	17	m <sub>01-1</sub>	18	-4 <sub>100</sub> <sup>+</sup>	19	-4 <sub>100</sub> <sup>-</sup>	20	m <sub>011</sub>
21	m <sub>-101</sub>	22	-4 <sub>010</sub> <sup>-</sup>	23	m <sub>101</sub>	24	-4 <sub>010</sub> <sup>+</sup>		

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**Harmonics**


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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	$-\frac{x^2}{2} - \frac{y^2}{2} + z^2$
6	$\mathbb{Q}_{2,1}(E)$	$E$	2	$Q, T$	-	1	$-\frac{x^2}{2} - \frac{y^2}{2} + z^2$

*continued ...*

Table 2

#	symbol	irrep.	rank	X	multiplicity	component	symmetry
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	$\frac{x(2x^2-3y^2-3z^2)}{2}$
15	$\mathbb{G}_{3,2}(T_1)$					2	$-\frac{y(3x^2-2y^2+3z^2)}{2}$
16	$\mathbb{G}_{3,3}(T_1)$					3	$-\frac{z(3x^2+3y^2-2z^2)}{2}$
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	$\frac{\sqrt{15}z(x-y)(x+y)}{2}$

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Basis in full matrix

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Table 3: dimension = 16

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

Table 4: Atomic basis (orbital part only)

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

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— SAMB: 11 (all 11) —

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

z1	$\mathbb{Q}_0^{(c)}(A_1) = \mathbb{Q}_0^{(a)}(A_1)\mathbb{Q}_0^{(s)}(A_1)$
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- C : 'C' site-cluster

\* 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

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

- C : 'C' site-cluster

\* 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

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

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

- H : 'H' site-cluster

\* bra:  $\langle s, \uparrow |, \langle s, \downarrow |$   
 \* ket:  $|s, \uparrow \rangle, |s, \downarrow \rangle$   
 \* wyckoff: 4a

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

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

\* bra:  $\langle s, \uparrow |, \langle s, \downarrow |$   
 \* ket:  $|s, \uparrow \rangle, |s, \downarrow \rangle$   
 \* wyckoff: 4a@4a

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

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

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

\* 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

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

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

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

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

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### — Atomic SAMB —

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

$$\boxed{x16} \quad \mathbb{G}_0^{(1,1;a)}(A_2) = \begin{bmatrix} 0 & \frac{\sqrt{3}i}{6} & 0 & \frac{\sqrt{3}}{6} & \frac{\sqrt{3}i}{6} & 0 \\ \frac{\sqrt{3}i}{6} & 0 & -\frac{\sqrt{3}}{6} & 0 & 0 & -\frac{\sqrt{3}i}{6} \end{bmatrix}$$

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

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

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

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

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

$$\boxed{x22} \quad \mathbb{M}_0^{(1,1;a)}(A_2) = \begin{bmatrix} 0 & \frac{\sqrt{3}}{6} & 0 & -\frac{\sqrt{3}i}{6} & \frac{\sqrt{3}}{6} & 0 \\ \frac{\sqrt{3}}{6} & 0 & \frac{\sqrt{3}i}{6} & 0 & 0 & -\frac{\sqrt{3}}{6} \end{bmatrix}$$

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

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

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

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

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

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

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

$$\boxed{x29} \quad \mathbb{Q}_0^{(a)}(A_1) = \begin{bmatrix} \frac{\sqrt{6}}{6} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{6}}{6} & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{6}}{6} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{6}}{6} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{6}}{6} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{6}}{6} \end{bmatrix}$$

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

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

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

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

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

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

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

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

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

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

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

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

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

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

$$\boxed{x44} \quad M_{1,1}^{(a)}(T_1) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{i}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{i}{2} \\ 0 & 0 & \frac{i}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{i}{2} & 0 & 0 \end{bmatrix}$$

$$\boxed{x45} \quad M_{1,2}^{(a)}(T_1) = \begin{bmatrix} 0 & 0 & 0 & 0 & \frac{i}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{i}{2} \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ -\frac{i}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{i}{2} & 0 & 0 & 0 & 0 \end{bmatrix}$$

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

$$\boxed{x47} \quad M_3^{(1,-1;a)}(A_2) = \begin{bmatrix} 0 & 0 & \frac{\sqrt{3}}{6} & 0 & 0 & -\frac{\sqrt{3}i}{6} \\ 0 & 0 & 0 & -\frac{\sqrt{3}}{6} & \frac{\sqrt{3}i}{6} & 0 \\ \frac{\sqrt{3}}{6} & 0 & 0 & 0 & 0 & \frac{\sqrt{3}}{6} \\ 0 & -\frac{\sqrt{3}}{6} & 0 & 0 & \frac{\sqrt{3}}{6} & 0 \\ 0 & -\frac{\sqrt{3}i}{6} & 0 & \frac{\sqrt{3}}{6} & 0 & 0 \\ \frac{\sqrt{3}i}{6} & 0 & \frac{\sqrt{3}}{6} & 0 & 0 & 0 \end{bmatrix}$$

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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### — Cluster SAMB —

- Site cluster

\*\* Wyckoff: 1o

$$\boxed{y1} \quad \mathbb{Q}_0^{(s)}(A_1) = [1]$$

\*\* Wyckoff: 4a

$$\boxed{y2} \quad \mathbb{Q}_0^{(s)}(A_1) = \left[ \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \right]$$

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

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

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

- Bond cluster

\*\* Wyckoff: 4a@4a

$$\boxed{y6} \quad \mathbb{Q}_0^{(s)}(A_1) = \left[ \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \right]$$

$$\boxed{y7} \quad \mathbb{T}_0^{(s)}(A_1) = \left[ \frac{i}{2}, \frac{i}{2}, \frac{i}{2}, \frac{i}{2} \right]$$

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

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

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

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

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

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

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— Site and Bond —————

Table 5: Orbital of each site

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

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**— Site in Unit Cell —**

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

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

SL	position ( $s$ )	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 ( $s$ )	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]

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**— Bond in Unit Cell —**

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Bonds in (conventional) cell (no plus set): tail, head = (SL, plus set), (N)D = (non)directional (listed up to 5th neighbor at most)

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

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