Model for "C3h"

Generated on 2026-01-25 20:43:37 by MultiPie 2.0.4

General Condition

- Basis type: `lgs`
- SAMB selection:
  - Type: `[Q, G]`
  - Rank: `[0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11]`
  - Irrep.: $[A', A'', E', E'']$
  - 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.: $[A', A'', E', E'']$
  - Spin (s): `[0, 1]`
- Site-cluster selection:
  - Rank: `[0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11]`
  - Irrep.: $[A', A'', E', E'']$
- Bond-cluster selection:
  - Type: `[Q, G, M, T]`
  - Rank: `[0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11]`
  - Irrep.: $[A', A'', E', E'']$
- Max. neighbor: `10`
- Search cell range: `(-2, 3), (-2, 3), (-2, 3)`
- Toroidal priority: `false`

Group and Unit Cell

- Group: PG No. 22 C_{3h} $\bar{6}$ [hexagonal]
- Unit cell:
  $a =$ 1.00000, $b =$ 1.00000, $c =$ 1.00000, $\alpha =$ 90.0, $\beta =$ 90.0, $\gamma =$ 120.0
- Lattice vectors (conventional cell):
  $\boldsymbol{a}_1 =$ [1.00000, 0.00000, 0.00000]
  $\boldsymbol{a}_2 =$ [-0.50000, 0.86603, 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	3^{+}_{001}	3	3^{-}_{001}	4	m_{001}	5	-6^{-}_{001}
6	-6^{+}_{001}								

Harmonics

Table 2: Harmonics

#	symbol	irrep.	rank	X	multiplicity	component	symmetry
1	$\mathbb{Q}_0(A')$	A'	0	Q, T	-	-	1
2	$\mathbb{G}_1(A')$	A'	1	G, M	-	-	z
3	$\mathbb{Q}_2(A')$	A'	2	Q, T	-	-	$-\frac{x^2}{2}-\frac{y^2}{2}+z^2$
4	$\mathbb{G}_3(A')$	A'	3	G, M	-	-	$-\frac{z\left(3x^2+3y^2-2z^2\right)}{2}$
5	$\mathbb{Q}_3(A',1)$	A'	3	Q, T	1	-	$\frac{\sqrt{10}y\left(3x^2-y^2\right)}{4}$
6	$\mathbb{Q}_3(A',2)$	A'	3	Q, T	2	-	$\frac{\sqrt{10}x\left(x^2-3y^2\right)}{4}$
7	$\mathbb{G}_0(A'')$	A''	0	G, M	-	-	1
8	$\mathbb{Q}_1(A'')$	A''	1	Q, T	-	-	z

continued ...

Table 2

#	symbol	irrep.	rank	X	multiplicity	component	symmetry
9	$\mathbb{G}_2(A'')$	A''	2	G, M	-	-	$-\frac{x^2}{2} - \frac{y^2}{2} + z^2$
10	$\mathbb{G}_3(A'', 1)$	A''	3	G, M	1	-	$\frac{\sqrt{10}y(3x^2-y^2)}{4}$
11	$\mathbb{G}_3(A'', 2)$	A''	3	G, M	2	-	$\frac{\sqrt{10}x(x^2-3y^2)}{4}$
12	$\mathbb{Q}_{1,1}(E')$	E'	1	Q, T	-	1	x
13	$\mathbb{Q}_{1,2}(E')$					2	y
14	$\mathbb{G}_{2,1}(E')$	E'	2	G, M	-	1	$\sqrt{3}yz$
15	$\mathbb{G}_{2,2}(E')$					2	$-\sqrt{3}xz$
16	$\mathbb{Q}_{2,1}(E')$	E'	2	Q, T	-	1	$\frac{\sqrt{3}(x-y)(x+y)}{2}$
17	$\mathbb{Q}_{2,2}(E')$					2	$-\sqrt{3}xy$
18	$\mathbb{G}_{3,1}(E')$	E'	3	G, M	-	1	$\sqrt{15}xyz$
19	$\mathbb{G}_{3,2}(E')$					2	$\frac{\sqrt{15}z(x-y)(x+y)}{2}$
20	$\mathbb{Q}_{3,1}(E')$	E'	3	Q, T	-	1	$-\frac{\sqrt{6}x(x^2+y^2-4z^2)}{4}$
21	$\mathbb{Q}_{3,2}(E')$					2	$-\frac{\sqrt{6}y(x^2+y^2-4z^2)}{4}$
22	$\mathbb{G}_{1,1}(E'')$	E''	1	G, M	-	1	x
23	$\mathbb{G}_{1,2}(E'')$					2	y
24	$\mathbb{G}_{2,1}(E'')$	E''	2	G, M	-	1	$\frac{\sqrt{3}(x-y)(x+y)}{2}$
25	$\mathbb{G}_{2,2}(E'')$					2	$-\sqrt{3}xy$
26	$\mathbb{Q}_{2,1}(E'')$	E''	2	Q, T	-	1	$\sqrt{3}yz$
27	$\mathbb{Q}_{2,2}(E'')$					2	$-\sqrt{3}xz$
28	$\mathbb{G}_{3,1}(E'')$	E''	3	G, M	-	1	$-\frac{\sqrt{6}x(x^2+y^2-4z^2)}{4}$
29	$\mathbb{G}_{3,2}(E'')$					2	$-\frac{\sqrt{6}y(x^2+y^2-4z^2)}{4}$

continued ...

Table 2

#	symbol	irrep.	rank	X	multiplicity	component	symmetry
30	$\mathbb{Q}_{3,1}(E'')$	E''	3	Q, T	-	1	$\sqrt{15}xyz$
31	$\mathbb{Q}_{3,2}(E'')$					2	$\frac{\sqrt{15}z(x-y)(x+y)}{2}$

Basis in full matrix

Table 3: dimension = 32

#	orbital@atom(SL)	#	orbital@atom(SL)	#	orbital@atom(SL)	#	orbital@atom(SL)	#	orbital@atom(SL)
0	$\|s,\uparrow\rangle$ @H1(1)	1	$\|s,\downarrow\rangle$ @H1(1)	2	$\|s,\uparrow\rangle$ @H2(1)	3	$\|s,\downarrow\rangle$ @H2(1)	4	$\|s,\uparrow\rangle$ @H2(2)
5	$\|s,\downarrow\rangle$ @H2(2)	6	$\|s,\uparrow\rangle$ @H2(3)	7	$\|s,\downarrow\rangle$ @H2(3)	8	$\|s,\uparrow\rangle$ @O(1)	9	$\|s,\downarrow\rangle$ @O(1)
10	$\|p_x,\uparrow\rangle$ @O(1)	11	$\|p_x,\downarrow\rangle$ @O(1)	12	$\|p_y,\uparrow\rangle$ @O(1)	13	$\|p_y,\downarrow\rangle$ @O(1)	14	$\|p_z,\uparrow\rangle$ @O(1)
15	$\|p_z,\downarrow\rangle$ @O(1)	16	$\|s,\uparrow\rangle$ @O(2)	17	$\|s,\downarrow\rangle$ @O(2)	18	$\|p_x,\uparrow\rangle$ @O(2)	19	$\|p_x,\downarrow\rangle$ @O(2)
20	$\|p_y,\uparrow\rangle$ @O(2)	21	$\|p_y,\downarrow\rangle$ @O(2)	22	$\|p_z,\uparrow\rangle$ @O(2)	23	$\|p_z,\downarrow\rangle$ @O(2)	24	$\|s,\uparrow\rangle$ @O(3)
25	$\|s,\downarrow\rangle$ @O(3)	26	$\|p_x,\uparrow\rangle$ @O(3)	27	$\|p_x,\downarrow\rangle$ @O(3)	28	$\|p_y,\uparrow\rangle$ @O(3)	29	$\|p_y,\downarrow\rangle$ @O(3)
30	$\|p_z,\uparrow\rangle$ @O(3)	31	$\|p_z,\downarrow\rangle$ @O(3)						

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

184 (all 184) SAMBs

- 'H1' site-cluster : `H1`
  * bra: $\langle s,\uparrow\rvert$, $\langle s,\downarrow\rvert$
  * ket: $\lvert s,\uparrow\rangle$, $\lvert s,\downarrow\rangle$
  * wyckoff: `1o`

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

- 'H2' site-cluster : `H2`
  * bra: $\langle s,\uparrow\rvert$, $\langle s,\downarrow\rvert$
  * ket: $\lvert s,\uparrow\rangle$, $\lvert s,\downarrow\rangle$
  * wyckoff: `3b`

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

$\boxed{\text{z63}}$ $\mathbb{Q}_{1,1}^{(c)}(E') = \dfrac{\sqrt{2}\mathbb{Q}_0^{(a)}(A')\mathbb{Q}_{1,1}^{(s)}(E')}{2}$

$\boxed{\text{z64}}$ $\mathbb{Q}_{1,2}^{(c)}(E') = \dfrac{\sqrt{2}\mathbb{Q}_0^{(a)}(A')\mathbb{Q}_{1,2}^{(s)}(E')}{2}$

- '0' site-cluster : `0`
  * bra: $\langle s,\uparrow|$, $\langle s,\downarrow|$
  * ket: $|s,\uparrow\rangle$, $|s,\downarrow\rangle$
  * wyckoff: `3b`

$\boxed{\text{z3}}$ $\mathbb{Q}_0^{(c)}(A') = \mathbb{Q}_0^{(a)}(A')\mathbb{Q}_0^{(s)}(A')$

$$\boxed{\text{z65}}\quad \mathbb{Q}_{1,1}^{(c)}(E') = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A')\mathbb{Q}_{1,1}^{(s)}(E')}{2}$$

$$\boxed{\text{z66}}\quad \mathbb{Q}_{1,2}^{(c)}(E') = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A')\mathbb{Q}_{1,2}^{(s)}(E')}{2}$$

- '0' site-cluster : `0`
  * 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: `3b`

$$\boxed{\text{z4}}\quad \mathbb{Q}_0^{(c)}(A') = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E')\mathbb{Q}_{1,1}^{(s)}(E')}{2} + \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E')\mathbb{Q}_{1,2}^{(s)}(E')}{2}$$

$$\boxed{\text{z5}}\quad \mathbb{Q}_2^{(1,-1;c)}(A') = -\frac{\sqrt{2}\mathbb{G}_{2,1}^{(1,-1;a)}(E')\mathbb{Q}_{1,1}^{(s)}(E')}{2} - \frac{\sqrt{2}\mathbb{G}_{2,2}^{(1,-1;a)}(E')\mathbb{Q}_{1,2}^{(s)}(E')}{2}$$

$$\boxed{\text{z6}}\quad \mathbb{Q}_0^{(1,0;c)}(A') = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(1,0;a)}(E')\mathbb{Q}_{1,1}^{(s)}(E')}{2} + \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(1,0;a)}(E')\mathbb{Q}_{1,2}^{(s)}(E')}{2}$$

$$\boxed{\text{z7}}\quad \mathbb{G}_1^{(c)}(A') = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E')\mathbb{Q}_{1,2}^{(s)}(E')}{2} - \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E')\mathbb{Q}_{1,1}^{(s)}(E')}{2}$$

$$\boxed{\text{z8}}\quad \mathbb{G}_1^{(1,-1;c)}(A') = \frac{\sqrt{2}\mathbb{G}_{2,1}^{(1,-1;a)}(E')\mathbb{Q}_{1,2}^{(s)}(E')}{2} - \frac{\sqrt{2}\mathbb{G}_{2,2}^{(1,-1;a)}(E')\mathbb{Q}_{1,1}^{(s)}(E')}{2}$$

$$\boxed{\text{z9}}\quad \mathbb{G}_1^{(1,0;c)}(A') = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(1,0;a)}(E')\mathbb{Q}_{1,2}^{(s)}(E')}{2} - \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(1,0;a)}(E')\mathbb{Q}_{1,1}^{(s)}(E')}{2}$$

$\boxed{\text{z35}}$ $\mathbb{Q}_1^{(c)}(A'') = \mathbb{Q}_1^{(a)}(A'')\mathbb{Q}_0^{(s)}(A')$

$\boxed{\text{z36}}$ $\mathbb{Q}_1^{(1,0;c)}(A'') = \mathbb{Q}_1^{(1,0;a)}(A'')\mathbb{Q}_0^{(s)}(A')$

$\boxed{\text{z37}}$ $\mathbb{G}_2^{(1,-1;c)}(A'') = \mathbb{G}_2^{(1,-1;a)}(A'')\mathbb{Q}_0^{(s)}(A')$

$\boxed{\text{z38}}$ $\mathbb{G}_3^{(1,-1;c)}(A'',1) = \frac{\sqrt{2}\mathbb{G}_{2,1}^{(1,-1;a)}(E'')\mathbb{Q}_{1,2}^{(s)}(E')}{2} - \frac{\sqrt{2}\mathbb{G}_{2,2}^{(1,-1;a)}(E'')\mathbb{Q}_{1,1}^{(s)}(E')}{2}$

$\boxed{\text{z39}}$ $\mathbb{G}_3^{(1,-1;c)}(A'',2) = \frac{\sqrt{2}\mathbb{G}_{2,1}^{(1,-1;a)}(E'')\mathbb{Q}_{1,1}^{(s)}(E')}{2} + \frac{\sqrt{2}\mathbb{G}_{2,2}^{(1,-1;a)}(E'')\mathbb{Q}_{1,2}^{(s)}(E')}{2}$

$\boxed{\text{z40}}$ $\mathbb{G}_0^{(1,1;c)}(A'') = \mathbb{G}_0^{(1,1;a)}(A'')\mathbb{Q}_0^{(s)}(A')$

$\boxed{\text{z67}}$ $\mathbb{Q}_{1,1}^{(c)}(E') = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E')\mathbb{Q}_0^{(s)}(A')}{2}$

$\boxed{\text{z68}}$ $\mathbb{Q}_{1,2}^{(c)}(E') = \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E')\mathbb{Q}_0^{(s)}(A')}{2}$

$\boxed{\text{z69}}$ $\mathbb{Q}_{2,1}^{(c)}(E') = \frac{\mathbb{Q}_{1,1}^{(a)}(E')\mathbb{Q}_{1,1}^{(s)}(E')}{2} - \frac{\mathbb{Q}_{1,2}^{(a)}(E')\mathbb{Q}_{1,2}^{(s)}(E')}{2}$

$\boxed{\text{z70}}$ $\mathbb{Q}_{2,2}^{(c)}(E') = -\frac{\mathbb{Q}_{1,1}^{(a)}(E')\mathbb{Q}_{1,2}^{(s)}(E')}{2} - \frac{\mathbb{Q}_{1,2}^{(a)}(E')\mathbb{Q}_{1,1}^{(s)}(E')}{2}$

$\boxed{\text{z71}}$ $\mathbb{Q}_{2,1}^{(1,-1;c)}(E') = -\frac{\mathbb{G}_{2,1}^{(1,-1;a)}(E')\mathbb{Q}_{1,1}^{(s)}(E')}{2} + \frac{\mathbb{G}_{2,2}^{(1,-1;a)}(E')\mathbb{Q}_{1,2}^{(s)}(E')}{2}$

$\boxed{\text{z72}}$ $\mathbb{Q}_{2,2}^{(1,-1;c)}(E') = \frac{\mathbb{G}_{2,1}^{(1,-1;a)}(E')\mathbb{Q}_{1,2}^{(s)}(E')}{2} + \frac{\mathbb{G}_{2,2}^{(1,-1;a)}(E')\mathbb{Q}_{1,1}^{(s)}(E')}{2}$

$\boxed{\text{z73}}$ $\mathbb{Q}_{1,1}^{(1,0;c)}(E') = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(1,0;a)}(E')\mathbb{Q}_0^{(s)}(A')}{2}$

$\boxed{\text{z74}}$ $\mathbb{Q}_{1,2}^{(1,0;c)}(E') = \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(1,0;a)}(E')\mathbb{Q}_0^{(s)}(A')}{2}$

$\boxed{\text{z75}}$ $\mathbb{Q}_{2,1}^{(1,0;c)}(E') = \frac{\mathbb{Q}_{1,1}^{(1,0;a)}(E')\mathbb{Q}_{1,1}^{(s)}(E')}{2} - \frac{\mathbb{Q}_{1,2}^{(1,0;a)}(E')\mathbb{Q}_{1,2}^{(s)}(E')}{2}$

$\boxed{\text{z76}}$ $\mathbb{Q}_{2,2}^{(1,0;c)}(E') = -\frac{\mathbb{Q}_{1,1}^{(1,0;a)}(E')\mathbb{Q}_{1,2}^{(s)}(E')}{2} - \frac{\mathbb{Q}_{1,2}^{(1,0;a)}(E')\mathbb{Q}_{1,1}^{(s)}(E')}{2}$

$\boxed{\text{z77}}$ $\mathbb{G}_{2,1}^{(1,-1;c)}(E') = \dfrac{\sqrt{2}\mathbb{G}_{2,1}^{(1,-1;a)}(E')\mathbb{Q}_0^{(s)}(A')}{2}$

$\boxed{\text{z78}}$ $\mathbb{G}_{2,2}^{(1,-1;c)}(E') = \dfrac{\sqrt{2}\mathbb{G}_{2,2}^{(1,-1;a)}(E')\mathbb{Q}_0^{(s)}(A')}{2}$

$\boxed{\text{z129}}$ $\mathbb{Q}_{2,1}^{(c)}(E'') = \dfrac{\sqrt{2}\mathbb{Q}_1^{(a)}(A'')\mathbb{Q}_{1,2}^{(s)}(E')}{2}$

$\boxed{\text{z130}}$ $\mathbb{Q}_{2,2}^{(c)}(E'') = -\dfrac{\sqrt{2}\mathbb{Q}_1^{(a)}(A'')\mathbb{Q}_{1,1}^{(s)}(E')}{2}$

$\boxed{\text{z131}}$ $\mathbb{Q}_{2,1}^{(1,-1;c)}(E'') = \dfrac{\sqrt{10}\mathbb{G}_{2,1}^{(1,-1;a)}(E'')\mathbb{Q}_{1,1}^{(s)}(E')}{10} - \dfrac{\sqrt{10}\mathbb{G}_{2,2}^{(1,-1;a)}(E'')\mathbb{Q}_{1,2}^{(s)}(E')}{10} + \dfrac{\sqrt{30}\mathbb{G}_{2}^{(1,-1;a)}(A'')\mathbb{Q}_{1,1}^{(s)}(E')}{10}$

$\boxed{\text{z132}}$ $\mathbb{Q}_{2,2}^{(1,-1;c)}(E'') = -\dfrac{\sqrt{10}\mathbb{G}_{2,1}^{(1,-1;a)}(E'')\mathbb{Q}_{1,2}^{(s)}(E')}{10} - \dfrac{\sqrt{10}\mathbb{G}_{2,2}^{(1,-1;a)}(E'')\mathbb{Q}_{1,1}^{(s)}(E')}{10} + \dfrac{\sqrt{30}\mathbb{G}_{2}^{(1,-1;a)}(A'')\mathbb{Q}_{1,2}^{(s)}(E')}{10}$

$\boxed{\text{z133}}$ $\mathbb{Q}_{2,1}^{(1,0;c)}(E'') = \dfrac{\sqrt{2}\mathbb{Q}_1^{(1,0;a)}(A'')\mathbb{Q}_{1,2}^{(s)}(E')}{2}$

$\boxed{\text{z134}}$ $\mathbb{Q}_{2,2}^{(1,0;c)}(E'') = -\dfrac{\sqrt{2}\mathbb{Q}_1^{(1,0;a)}(A'')\mathbb{Q}_{1,1}^{(s)}(E')}{2}$

$\boxed{\text{z135}}$ $\mathbb{G}_{1,1}^{(1,-1;c)}(E'') = \dfrac{\sqrt{15}\mathbb{G}_{2,1}^{(1,-1;a)}(E'')\mathbb{Q}_{1,1}^{(s)}(E')}{10} - \dfrac{\sqrt{15}\mathbb{G}_{2,2}^{(1,-1;a)}(E'')\mathbb{Q}_{1,2}^{(s)}(E')}{10} - \dfrac{\sqrt{5}\mathbb{G}_{2}^{(1,-1;a)}(A'')\mathbb{Q}_{1,1}^{(s)}(E')}{5}$

$\boxed{\text{z136}}$ $\mathbb{G}_{1,2}^{(1,-1;c)}(E'') = -\dfrac{\sqrt{15}\mathbb{G}_{2,1}^{(1,-1;a)}(E'')\mathbb{Q}_{1,2}^{(s)}(E')}{10} - \dfrac{\sqrt{15}\mathbb{G}_{2,2}^{(1,-1;a)}(E'')\mathbb{Q}_{1,1}^{(s)}(E')}{10} - \dfrac{\sqrt{5}\mathbb{G}_{2}^{(1,-1;a)}(A'')\mathbb{Q}_{1,2}^{(s)}(E')}{5}$

$\boxed{\text{z137}}$ $\mathbb{G}_{2,1}^{(1,-1;c)}(E'') = \dfrac{\sqrt{2}\mathbb{G}_{2,1}^{(1,-1;a)}(E'')\mathbb{Q}_0^{(s)}(A')}{2}$

$\boxed{\text{z138}}$ $\mathbb{G}_{2,2}^{(1,-1;c)}(E'') = \dfrac{\sqrt{2}\mathbb{G}_{2,2}^{(1,-1;a)}(E'')\mathbb{Q}_0^{(s)}(A')}{2}$

$\boxed{\text{z139}}$ $\mathbb{G}_{1,1}^{(1,1;c)}(E'') = \dfrac{\sqrt{2}\mathbb{G}_0^{(1,1;a)}(A'')\mathbb{Q}_{1,1}^{(s)}(E')}{2}$

$\boxed{\text{z140}}$ $\mathbb{G}_{1,2}^{(1,1;c)}(E'') = \dfrac{\sqrt{2}\mathbb{G}_0^{(1,1;a)}(A'')\mathbb{Q}_{1,2}^{(s)}(E')}{2}$

- '`0`' site-cluster : `0`
  * 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: `3b`

$$\boxed{\text{z10}}\quad \mathbb{Q}_0^{(c)}(A') = \mathbb{Q}_0^{(a)}(A')\mathbb{Q}_0^{(s)}(A')$$

$$\boxed{\text{z11}}\quad \mathbb{Q}_2^{(c)}(A') = \mathbb{Q}_2^{(a)}(A')\mathbb{Q}_0^{(s)}(A')$$

$$\boxed{\text{z12}}\quad \mathbb{Q}_3^{(c)}(A',1) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E')\mathbb{Q}_{1,2}^{(s)}(E')}{2} - \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E')\mathbb{Q}_{1,1}^{(s)}(E')}{2}$$

$$\boxed{\text{z13}}\quad \mathbb{Q}_3^{(c)}(A',2) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E')\mathbb{Q}_{1,1}^{(s)}(E')}{2} + \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E')\mathbb{Q}_{1,2}^{(s)}(E')}{2}$$

$$\boxed{\text{z14}}\quad \mathbb{Q}_2^{(1,-1;c)}(A') = \mathbb{Q}_2^{(1,-1;a)}(A')\mathbb{Q}_0^{(s)}(A')$$

$$\boxed{\text{z15}}\quad \mathbb{Q}_3^{(1,-1;c)}(A',1) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(1,-1;a)}(E')\mathbb{Q}_{1,2}^{(s)}(E')}{2} - \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(1,-1;a)}(E')\mathbb{Q}_{1,1}^{(s)}(E')}{2}$$

$$\boxed{\text{z16}}\quad \mathbb{Q}_3^{(1,-1;c)}(A',2) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(1,-1;a)}(E')\mathbb{Q}_{1,1}^{(s)}(E')}{2} + \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(1,-1;a)}(E')\mathbb{Q}_{1,2}^{(s)}(E')}{2}$$

$$\boxed{\text{z17}}\quad \mathbb{Q}_0^{(1,1;c)}(A') = \mathbb{Q}_0^{(1,1;a)}(A')\mathbb{Q}_0^{(s)}(A')$$

$$\boxed{\text{z18}}\quad \mathbb{G}_1^{(1,0;c)}(A') = \mathbb{G}_1^{(1,0;a)}(A')\mathbb{Q}_0^{(s)}(A')$$

$$\boxed{\text{z41}}\quad \mathbb{Q}_1^{(c)}(A'') = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E'')\mathbb{Q}_{1,2}^{(s)}(E')}{2} - \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E'')\mathbb{Q}_{1,1}^{(s)}(E')}{2}$$

$$\boxed{\text{z42}}\quad \mathbb{Q}_1^{(1,-1;c)}(A'') = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(1,-1;a)}(E'')\mathbb{Q}_{1,2}^{(s)}(E')}{2} - \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(1,-1;a)}(E'')\mathbb{Q}_{1,1}^{(s)}(E')}{2}$$

$$\boxed{\text{z43}}\quad \mathbb{Q}_1^{(1,0;c)}(A'') = \frac{\sqrt{2}\mathbb{G}_{1,1}^{(1,0;a)}(E'')\mathbb{Q}_{1,2}^{(s)}(E')}{2} - \frac{\sqrt{2}\mathbb{G}_{1,2}^{(1,0;a)}(E'')\mathbb{Q}_{1,1}^{(s)}(E')}{2}$$

$$\boxed{\text{z44}}\quad \mathbb{G}_2^{(c)}(A'') = -\frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E'')\mathbb{Q}_{1,1}^{(s)}(E')}{2} - \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E'')\mathbb{Q}_{1,2}^{(s)}(E')}{2}$$

$\boxed{\text{z45}}$ $$\mathbb{G}_{2}^{(1,-1;c)}(A'') = -\frac{\sqrt{2}\mathbb{Q}_{2,1}^{(1,-1;a)}(E'')\mathbb{Q}_{1,1}^{(s)}(E')}{2} - \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(1,-1;a)}(E'')\mathbb{Q}_{1,2}^{(s)}(E')}{2}$$

$\boxed{\text{z46}}$ $$\mathbb{G}_{0}^{(1,0;c)}(A'') = \frac{\sqrt{2}\mathbb{G}_{1,1}^{(1,0;a)}(E'')\mathbb{Q}_{1,1}^{(s)}(E')}{2} + \frac{\sqrt{2}\mathbb{G}_{1,2}^{(1,0;a)}(E'')\mathbb{Q}_{1,2}^{(s)}(E')}{2}$$

$\boxed{\text{z79}}$ $$\mathbb{Q}_{1,1}^{(c)}(E', a) = \frac{\sqrt{2}\mathbb{Q}_{0}^{(a)}(A')\mathbb{Q}_{1,1}^{(s)}(E')}{2}$$

$\boxed{\text{z80}}$ $$\mathbb{Q}_{1,2}^{(c)}(E', a) = \frac{\sqrt{2}\mathbb{Q}_{0}^{(a)}(A')\mathbb{Q}_{1,2}^{(s)}(E')}{2}$$

$\boxed{\text{z81}}$ $$\mathbb{Q}_{1,1}^{(c)}(E', b) = \frac{\sqrt{42}\mathbb{Q}_{2,1}^{(a)}(E')\mathbb{Q}_{1,1}^{(s)}(E')}{14} - \frac{\sqrt{42}\mathbb{Q}_{2,2}^{(a)}(E')\mathbb{Q}_{1,2}^{(s)}(E')}{14} - \frac{\sqrt{14}\mathbb{Q}_{2}^{(a)}(A')\mathbb{Q}_{1,1}^{(s)}(E')}{14}$$

$\boxed{\text{z82}}$ $$\mathbb{Q}_{1,2}^{(c)}(E', b) = -\frac{\sqrt{42}\mathbb{Q}_{2,1}^{(a)}(E')\mathbb{Q}_{1,2}^{(s)}(E')}{14} - \frac{\sqrt{42}\mathbb{Q}_{2,2}^{(a)}(E')\mathbb{Q}_{1,1}^{(s)}(E')}{14} - \frac{\sqrt{14}\mathbb{Q}_{2}^{(a)}(A')\mathbb{Q}_{1,2}^{(s)}(E')}{14}$$

$\boxed{\text{z83}}$ $$\mathbb{Q}_{2,1}^{(c)}(E') = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E')\mathbb{Q}_{0}^{(s)}(A')}{2}$$

$\boxed{\text{z84}}$ $$\mathbb{Q}_{2,2}^{(c)}(E') = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E')\mathbb{Q}_{0}^{(s)}(A')}{2}$$

$\boxed{\text{z85}}$ $$\mathbb{Q}_{3,1}^{(c)}(E') = \frac{\sqrt{7}\mathbb{Q}_{2,1}^{(a)}(E')\mathbb{Q}_{1,1}^{(s)}(E')}{14} - \frac{\sqrt{7}\mathbb{Q}_{2,2}^{(a)}(E')\mathbb{Q}_{1,2}^{(s)}(E')}{14} + \frac{\sqrt{21}\mathbb{Q}_{2}^{(a)}(A')\mathbb{Q}_{1,1}^{(s)}(E')}{7}$$

$\boxed{\text{z86}}$ $$\mathbb{Q}_{3,2}^{(c)}(E') = -\frac{\sqrt{7}\mathbb{Q}_{2,1}^{(a)}(E')\mathbb{Q}_{1,2}^{(s)}(E')}{14} - \frac{\sqrt{7}\mathbb{Q}_{2,2}^{(a)}(E')\mathbb{Q}_{1,1}^{(s)}(E')}{14} + \frac{\sqrt{21}\mathbb{Q}_{2}^{(a)}(A')\mathbb{Q}_{1,2}^{(s)}(E')}{7}$$

$\boxed{\text{z87}}$ $$\mathbb{Q}_{1,1}^{(1,-1;c)}(E') = \frac{\sqrt{42}\mathbb{Q}_{2,1}^{(1,-1;a)}(E')\mathbb{Q}_{1,1}^{(s)}(E')}{14} - \frac{\sqrt{42}\mathbb{Q}_{2,2}^{(1,-1;a)}(E')\mathbb{Q}_{1,2}^{(s)}(E')}{14} - \frac{\sqrt{14}\mathbb{Q}_{2}^{(1,-1;a)}(A')\mathbb{Q}_{1,1}^{(s)}(E')}{14}$$

$\boxed{\text{z88}}$ $$\mathbb{Q}_{1,2}^{(1,-1;c)}(E') = -\frac{\sqrt{42}\mathbb{Q}_{2,1}^{(1,-1;a)}(E')\mathbb{Q}_{1,2}^{(s)}(E')}{14} - \frac{\sqrt{42}\mathbb{Q}_{2,2}^{(1,-1;a)}(E')\mathbb{Q}_{1,1}^{(s)}(E')}{14} - \frac{\sqrt{14}\mathbb{Q}_{2}^{(1,-1;a)}(A')\mathbb{Q}_{1,2}^{(s)}(E')}{14}$$

$\boxed{\text{z89}}$ $$\mathbb{Q}_{2,1}^{(1,-1;c)}(E') = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(1,-1;a)}(E')\mathbb{Q}_{0}^{(s)}(A')}{2}$$

$\boxed{\text{z90}}$ $$\mathbb{Q}_{2,2}^{(1,-1;c)}(E') = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(1,-1;a)}(E')\mathbb{Q}_{0}^{(s)}(A')}{2}$$

$$\boxed{\text{z91}}\quad \mathbb{Q}_{3,1}^{(1,-1;c)}(E') = \frac{\sqrt{7}\mathbb{Q}_{2,1}^{(1,-1;a)}(E')\mathbb{Q}_{1,1}^{(s)}(E')}{14} - \frac{\sqrt{7}\mathbb{Q}_{2,2}^{(1,-1;a)}(E')\mathbb{Q}_{1,2}^{(s)}(E')}{14} + \frac{\sqrt{21}\mathbb{Q}_{2}^{(1,-1;a)}(A')\mathbb{Q}_{1,1}^{(s)}(E')}{7}$$

$$\boxed{\text{z92}}\quad \mathbb{Q}_{3,2}^{(1,-1;c)}(E') = -\frac{\sqrt{7}\mathbb{Q}_{2,1}^{(1,-1;a)}(E')\mathbb{Q}_{1,2}^{(s)}(E')}{14} - \frac{\sqrt{7}\mathbb{Q}_{2,2}^{(1,-1;a)}(E')\mathbb{Q}_{1,1}^{(s)}(E')}{14} + \frac{\sqrt{21}\mathbb{Q}_{2}^{(1,-1;a)}(A')\mathbb{Q}_{1,2}^{(s)}(E')}{7}$$

$$\boxed{\text{z93}}\quad \mathbb{Q}_{1,1}^{(1,0;c)}(E') = -\frac{\sqrt{2}\mathbb{G}_{1}^{(1,0;a)}(A')\mathbb{Q}_{1,2}^{(s)}(E')}{2}$$

$$\boxed{\text{z94}}\quad \mathbb{Q}_{1,2}^{(1,0;c)}(E') = \frac{\sqrt{2}\mathbb{G}_{1}^{(1,0;a)}(A')\mathbb{Q}_{1,1}^{(s)}(E')}{2}$$

$$\boxed{\text{z95}}\quad \mathbb{Q}_{1,1}^{(1,1;c)}(E') = \frac{\sqrt{2}\mathbb{Q}_{0}^{(1,1;a)}(A')\mathbb{Q}_{1,1}^{(s)}(E')}{2}$$

$$\boxed{\text{z96}}\quad \mathbb{Q}_{1,2}^{(1,1;c)}(E') = \frac{\sqrt{2}\mathbb{Q}_{0}^{(1,1;a)}(A')\mathbb{Q}_{1,2}^{(s)}(E')}{2}$$

$$\boxed{\text{z141}}\quad \mathbb{Q}_{2,1}^{(c)}(E'') = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E'')\mathbb{Q}_{0}^{(s)}(A')}{2}$$

$$\boxed{\text{z142}}\quad \mathbb{Q}_{2,2}^{(c)}(E'') = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E'')\mathbb{Q}_{0}^{(s)}(A')}{2}$$

$$\boxed{\text{z143}}\quad \mathbb{Q}_{3,1}^{(c)}(E'') = \frac{\mathbb{Q}_{2,1}^{(a)}(E'')\mathbb{Q}_{1,1}^{(s)}(E')}{2} - \frac{\mathbb{Q}_{2,2}^{(a)}(E'')\mathbb{Q}_{1,2}^{(s)}(E')}{2}$$

$$\boxed{\text{z144}}\quad \mathbb{Q}_{3,2}^{(c)}(E'') = -\frac{\mathbb{Q}_{2,1}^{(a)}(E'')\mathbb{Q}_{1,2}^{(s)}(E')}{2} - \frac{\mathbb{Q}_{2,2}^{(a)}(E'')\mathbb{Q}_{1,1}^{(s)}(E')}{2}$$

$$\boxed{\text{z145}}\quad \mathbb{Q}_{2,1}^{(1,-1;c)}(E'') = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(1,-1;a)}(E'')\mathbb{Q}_{0}^{(s)}(A')}{2}$$

$$\boxed{\text{z146}}\quad \mathbb{Q}_{2,2}^{(1,-1;c)}(E'') = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(1,-1;a)}(E'')\mathbb{Q}_{0}^{(s)}(A')}{2}$$

$$\boxed{\text{z147}}\quad \mathbb{Q}_{3,1}^{(1,-1;c)}(E'') = \frac{\mathbb{Q}_{2,1}^{(1,-1;a)}(E'')\mathbb{Q}_{1,1}^{(s)}(E')}{2} - \frac{\mathbb{Q}_{2,2}^{(1,-1;a)}(E'')\mathbb{Q}_{1,2}^{(s)}(E')}{2}$$

$$\boxed{\text{z148}}\quad \mathbb{Q}_{3,2}^{(1,-1;c)}(E'') = -\frac{\mathbb{Q}_{2,1}^{(1,-1;a)}(E'')\mathbb{Q}_{1,2}^{(s)}(E')}{2} - \frac{\mathbb{Q}_{2,2}^{(1,-1;a)}(E'')\mathbb{Q}_{1,1}^{(s)}(E')}{2}$$

$\boxed{\text{z149}}$ $$\mathbb{G}_{1,1}^{(1,0;c)}(E'') = \frac{\sqrt{2}\mathbb{G}_{1,1}^{(1,0;a)}(E'')\mathbb{Q}_{0}^{(s)}(A')}{2}$$

$\boxed{\text{z150}}$ $$\mathbb{G}_{1,2}^{(1,0;c)}(E'') = \frac{\sqrt{2}\mathbb{G}_{1,2}^{(1,0;a)}(E'')\mathbb{Q}_{0}^{(s)}(A')}{2}$$

$\boxed{\text{z151}}$ $$\mathbb{G}_{2,1}^{(1,0;c)}(E'') = \frac{\mathbb{G}_{1,1}^{(1,0;a)}(E'')\mathbb{Q}_{1,1}^{(s)}(E')}{2} - \frac{\mathbb{G}_{1,2}^{(1,0;a)}(E'')\mathbb{Q}_{1,2}^{(s)}(E')}{2}$$

$\boxed{\text{z152}}$ $$\mathbb{G}_{2,2}^{(1,0;c)}(E'') = -\frac{\mathbb{G}_{1,1}^{(1,0;a)}(E'')\mathbb{Q}_{1,2}^{(s)}(E')}{2} - \frac{\mathbb{G}_{1,2}^{(1,0;a)}(E'')\mathbb{Q}_{1,1}^{(s)}(E')}{2}$$

- 'H1'-'O' bond-cluster : `O;H1_001_1`
  - * bra: $\langle s,\uparrow|$, $\langle s,\downarrow|$
  - * ket: $|s,\uparrow\rangle$, $|s,\downarrow\rangle$
  - * wyckoff: `3a@3b`

$\boxed{\text{z19}}$ $$\mathbb{Q}_{0}^{(c)}(A') = \mathbb{Q}_{0}^{(a)}(A')\mathbb{Q}_{0}^{(b)}(A')$$

$\boxed{\text{z20}}$ $$\mathbb{G}_{1}^{(1,-1;c)}(A') = \mathbb{M}_{1}^{(1,-1;a)}(A')\mathbb{T}_{0}^{(b)}(A')$$

$\boxed{\text{z47}}$ $$\mathbb{Q}_{1}^{(1,-1;c)}(A'') = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E'')\mathbb{T}_{1,2}^{(b)}(E')}{2} - \frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E'')\mathbb{T}_{1,1}^{(b)}(E')}{2}$$

$\boxed{\text{z48}}$ $$\mathbb{G}_{0}^{(1,-1;c)}(A'') = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E'')\mathbb{T}_{1,1}^{(b)}(E')}{2} + \frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E'')\mathbb{T}_{1,2}^{(b)}(E')}{2}$$

$\boxed{\text{z97}}$ $$\mathbb{Q}_{1,1}^{(c)}(E') = \frac{\sqrt{2}\mathbb{Q}_{0}^{(a)}(A')\mathbb{Q}_{1,1}^{(b)}(E')}{2}$$

$\boxed{\text{z98}}$ $$\mathbb{Q}_{1,2}^{(c)}(E') = \frac{\sqrt{2}\mathbb{Q}_{0}^{(a)}(A')\mathbb{Q}_{1,2}^{(b)}(E')}{2}$$

$\boxed{\text{z99}}$ $$\mathbb{Q}_{1,1}^{(1,-1;c)}(E') = -\frac{\sqrt{2}\mathbb{M}_{1}^{(1,-1;a)}(A')\mathbb{T}_{1,2}^{(b)}(E')}{2}$$

$\boxed{\text{z100}}$ $$\mathbb{Q}_{1,2}^{(1,-1;c)}(E') = \frac{\sqrt{2}\mathbb{M}_{1}^{(1,-1;a)}(A')\mathbb{T}_{1,1}^{(b)}(E')}{2}$$

$\boxed{\text{z153}}$ $\mathbb{G}_{1,1}^{(1,-1;c)}(E'') = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E'')\mathbb{T}_{0}^{(b)}(A')}{2}$

$\boxed{\text{z154}}$ $\mathbb{G}_{1,2}^{(1,-1;c)}(E'') = \frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E'')\mathbb{T}_{0}^{(b)}(A')}{2}$

$\boxed{\text{z155}}$ $\mathbb{G}_{2,1}^{(1,-1;c)}(E'') = \frac{\mathbb{M}_{1,1}^{(1,-1;a)}(E'')\mathbb{T}_{1,1}^{(b)}(E')}{2} - \frac{\mathbb{M}_{1,2}^{(1,-1;a)}(E'')\mathbb{T}_{1,2}^{(b)}(E')}{2}$

$\boxed{\text{z156}}$ $\mathbb{G}_{2,2}^{(1,-1;c)}(E'') = -\frac{\mathbb{M}_{1,1}^{(1,-1;a)}(E'')\mathbb{T}_{1,2}^{(b)}(E')}{2} - \frac{\mathbb{M}_{1,2}^{(1,-1;a)}(E'')\mathbb{T}_{1,1}^{(b)}(E')}{2}$

- 'H1'-'O' bond-cluster : `O;H1_001_1`
  * 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: `3a@3b`

$\boxed{\text{z21}}$ $\mathbb{Q}_{0}^{(c)}(A') = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{2} + \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{2}$

$\boxed{\text{z22}}$ $\mathbb{Q}_{2}^{(1,-1;c)}(A') = -\frac{\sqrt{2}\mathbb{G}_{2,1}^{(1,-1;a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{2} - \frac{\sqrt{2}\mathbb{G}_{2,2}^{(1,-1;a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{2}$

$\boxed{\text{z23}}$ $\mathbb{Q}_{0}^{(1,0;c)}(A') = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(1,0;a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{2} + \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(1,0;a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{2}$

$\boxed{\text{z24}}$ $\mathbb{G}_{1}^{(c)}(A') = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{2} - \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{2}$

$\boxed{\text{z25}}$ $\mathbb{G}_{1}^{(1,-1;c)}(A') = \frac{\sqrt{2}\mathbb{G}_{2,1}^{(1,-1;a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{2} - \frac{\sqrt{2}\mathbb{G}_{2,2}^{(1,-1;a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{2}$

$\boxed{\text{z26}}$ $\mathbb{G}_{1}^{(1,0;c)}(A') = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(1,0;a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{2} - \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(1,0;a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{2}$

$\boxed{\text{z49}}$ $\mathbb{Q}_{1}^{(c)}(A'') = \mathbb{Q}_{1}^{(a)}(A'')\mathbb{Q}_{0}^{(b)}(A')$

$\boxed{\text{z50}}$ $\mathbb{Q}_{1}^{(1,0;c)}(A'') = \mathbb{Q}_{1}^{(1,0;a)}(A'')\mathbb{Q}_{0}^{(b)}(A')$

$$\boxed{\text{z51}}\quad \mathbb{G}_2^{(1,-1;c)}(A'') = \mathbb{G}_2^{(1,-1;a)}(A'')\mathbb{Q}_0^{(b)}(A')$$

$$\boxed{\text{z52}}\quad \mathbb{G}_3^{(1,-1;c)}(A'',1) = \frac{\sqrt{2}\mathbb{G}_{2,1}^{(1,-1;a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{2} - \frac{\sqrt{2}\mathbb{G}_{2,2}^{(1,-1;a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{2}$$

$$\boxed{\text{z53}}\quad \mathbb{G}_3^{(1,-1;c)}(A'',2) = \frac{\sqrt{2}\mathbb{G}_{2,1}^{(1,-1;a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{2} + \frac{\sqrt{2}\mathbb{G}_{2,2}^{(1,-1;a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{2}$$

$$\boxed{\text{z54}}\quad \mathbb{G}_0^{(1,1;c)}(A'') = \mathbb{G}_0^{(1,1;a)}(A'')\mathbb{Q}_0^{(b)}(A')$$

$$\boxed{\text{z101}}\quad \mathbb{Q}_{1,1}^{(c)}(E') = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E')\mathbb{Q}_0^{(b)}(A')}{2}$$

$$\boxed{\text{z102}}\quad \mathbb{Q}_{1,2}^{(c)}(E') = \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E')\mathbb{Q}_0^{(b)}(A')}{2}$$

$$\boxed{\text{z103}}\quad \mathbb{Q}_{2,1}^{(c)}(E') = \frac{\mathbb{Q}_{1,1}^{(a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{2} - \frac{\mathbb{Q}_{1,2}^{(a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{2}$$

$$\boxed{\text{z104}}\quad \mathbb{Q}_{2,2}^{(c)}(E') = -\frac{\mathbb{Q}_{1,1}^{(a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{2} - \frac{\mathbb{Q}_{1,2}^{(a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{2}$$

$$\boxed{\text{z105}}\quad \mathbb{Q}_{2,1}^{(1,-1;c)}(E') = -\frac{\mathbb{G}_{2,1}^{(1,-1;a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{2} + \frac{\mathbb{G}_{2,2}^{(1,-1;a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{2}$$

$$\boxed{\text{z106}}\quad \mathbb{Q}_{2,2}^{(1,-1;c)}(E') = \frac{\mathbb{G}_{2,1}^{(1,-1;a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{2} + \frac{\mathbb{G}_{2,2}^{(1,-1;a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{2}$$

$$\boxed{\text{z107}}\quad \mathbb{Q}_{1,1}^{(1,0;c)}(E') = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(1,0;a)}(E')\mathbb{Q}_0^{(b)}(A')}{2}$$

$$\boxed{\text{z108}}\quad \mathbb{Q}_{1,2}^{(1,0;c)}(E') = \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(1,0;a)}(E')\mathbb{Q}_0^{(b)}(A')}{2}$$

$$\boxed{\text{z109}}\quad \mathbb{Q}_{2,1}^{(1,0;c)}(E') = \frac{\mathbb{Q}_{1,1}^{(1,0;a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{2} - \frac{\mathbb{Q}_{1,2}^{(1,0;a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{2}$$

$$\boxed{\text{z110}}\quad \mathbb{Q}_{2,2}^{(1,0;c)}(E') = -\frac{\mathbb{Q}_{1,1}^{(1,0;a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{2} - \frac{\mathbb{Q}_{1,2}^{(1,0;a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{2}$$

$\boxed{\text{z111}}$ $$\mathbb{G}_{2,1}^{(1,-1;c)}(E') = \frac{\sqrt{2}\mathbb{G}_{2,1}^{(1,-1;a)}(E')\mathbb{Q}_{0}^{(b)}(A')}{2}$$

$\boxed{\text{z112}}$ $$\mathbb{G}_{2,2}^{(1,-1;c)}(E') = \frac{\sqrt{2}\mathbb{G}_{2,2}^{(1,-1;a)}(E')\mathbb{Q}_{0}^{(b)}(A')}{2}$$

$\boxed{\text{z157}}$ $$\mathbb{Q}_{2,1}^{(c)}(E'') = \frac{\sqrt{2}\mathbb{Q}_{1}^{(a)}(A'')\mathbb{Q}_{1,2}^{(b)}(E')}{2}$$

$\boxed{\text{z158}}$ $$\mathbb{Q}_{2,2}^{(c)}(E'') = -\frac{\sqrt{2}\mathbb{Q}_{1}^{(a)}(A'')\mathbb{Q}_{1,1}^{(b)}(E')}{2}$$

$\boxed{\text{z159}}$ $$\mathbb{Q}_{2,1}^{(1,-1;c)}(E'') = \frac{\sqrt{10}\mathbb{G}_{2,1}^{(1,-1;a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{10} - \frac{\sqrt{10}\mathbb{G}_{2,2}^{(1,-1;a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{10} + \frac{\sqrt{30}\mathbb{G}_{2}^{(1,-1;a)}(A'')\mathbb{Q}_{1,1}^{(b)}(E')}{10}$$

$\boxed{\text{z160}}$ $$\mathbb{Q}_{2,2}^{(1,-1;c)}(E'') = -\frac{\sqrt{10}\mathbb{G}_{2,1}^{(1,-1;a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{10} - \frac{\sqrt{10}\mathbb{G}_{2,2}^{(1,-1;a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{10} + \frac{\sqrt{30}\mathbb{G}_{2}^{(1,-1;a)}(A'')\mathbb{Q}_{1,2}^{(b)}(E')}{10}$$

$\boxed{\text{z161}}$ $$\mathbb{Q}_{2,1}^{(1,0;c)}(E'') = \frac{\sqrt{2}\mathbb{Q}_{1}^{(1,0;a)}(A'')\mathbb{Q}_{1,2}^{(b)}(E')}{2}$$

$\boxed{\text{z162}}$ $$\mathbb{Q}_{2,2}^{(1,0;c)}(E'') = -\frac{\sqrt{2}\mathbb{Q}_{1}^{(1,0;a)}(A'')\mathbb{Q}_{1,1}^{(b)}(E')}{2}$$

$\boxed{\text{z163}}$ $$\mathbb{G}_{1,1}^{(1,-1;c)}(E'') = \frac{\sqrt{15}\mathbb{G}_{2,1}^{(1,-1;a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{10} - \frac{\sqrt{15}\mathbb{G}_{2,2}^{(1,-1;a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{10} - \frac{\sqrt{5}\mathbb{G}_{2}^{(1,-1;a)}(A'')\mathbb{Q}_{1,1}^{(b)}(E')}{5}$$

$\boxed{\text{z164}}$ $$\mathbb{G}_{1,2}^{(1,-1;c)}(E'') = -\frac{\sqrt{15}\mathbb{G}_{2,1}^{(1,-1;a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{10} - \frac{\sqrt{15}\mathbb{G}_{2,2}^{(1,-1;a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{10} - \frac{\sqrt{5}\mathbb{G}_{2}^{(1,-1;a)}(A'')\mathbb{Q}_{1,2}^{(b)}(E')}{5}$$

$\boxed{\text{z165}}$ $$\mathbb{G}_{2,1}^{(1,-1;c)}(E'') = \frac{\sqrt{2}\mathbb{G}_{2,1}^{(1,-1;a)}(E'')\mathbb{Q}_{0}^{(b)}(A')}{2}$$

$\boxed{\text{z166}}$ $$\mathbb{G}_{2,2}^{(1,-1;c)}(E'') = \frac{\sqrt{2}\mathbb{G}_{2,2}^{(1,-1;a)}(E'')\mathbb{Q}_{0}^{(b)}(A')}{2}$$

$\boxed{\text{z167}}$ $$\mathbb{G}_{1,1}^{(1,1;c)}(E'') = \frac{\sqrt{2}\mathbb{G}_{0}^{(1,1;a)}(A'')\mathbb{Q}_{1,1}^{(b)}(E')}{2}$$

$\boxed{\text{z168}}$ $$\mathbb{G}_{1,2}^{(1,1;c)}(E'') = \frac{\sqrt{2}\mathbb{G}_{0}^{(1,1;a)}(A'')\mathbb{Q}_{1,2}^{(b)}(E')}{2}$$

- 'H2'-'O' bond-cluster : `O;H2_001_1`
  * bra: $\langle s,\uparrow|$, $\langle s,\downarrow|$
  * ket: $|s,\uparrow\rangle$, $|s,\downarrow\rangle$
  * wyckoff: `3a@3b`

$\boxed{\text{z27}}$ $\mathbb{Q}_0^{(c)}(A') = \mathbb{Q}_0^{(a)}(A')\mathbb{Q}_0^{(b)}(A')$

$\boxed{\text{z28}}$ $\mathbb{G}_1^{(1,-1;c)}(A') = \mathbb{M}_1^{(1,-1;a)}(A')\mathbb{T}_0^{(b)}(A')$

$\boxed{\text{z55}}$ $\mathbb{Q}_1^{(1,-1;c)}(A'') = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E'')\mathbb{T}_{1,2}^{(b)}(E')}{2} - \frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E'')\mathbb{T}_{1,1}^{(b)}(E')}{2}$

$\boxed{\text{z56}}$ $\mathbb{G}_0^{(1,-1;c)}(A'') = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E'')\mathbb{T}_{1,1}^{(b)}(E')}{2} + \frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E'')\mathbb{T}_{1,2}^{(b)}(E')}{2}$

$\boxed{\text{z113}}$ $\mathbb{Q}_{1,1}^{(c)}(E') = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A')\mathbb{Q}_{1,1}^{(b)}(E')}{2}$

$\boxed{\text{z114}}$ $\mathbb{Q}_{1,2}^{(c)}(E') = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A')\mathbb{Q}_{1,2}^{(b)}(E')}{2}$

$\boxed{\text{z115}}$ $\mathbb{Q}_{1,1}^{(1,-1;c)}(E') = -\frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(A')\mathbb{T}_{1,2}^{(b)}(E')}{2}$

$\boxed{\text{z116}}$ $\mathbb{Q}_{1,2}^{(1,-1;c)}(E') = \frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(A')\mathbb{T}_{1,1}^{(b)}(E')}{2}$

$\boxed{\text{z169}}$ $\mathbb{G}_{1,1}^{(1,-1;c)}(E'') = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E'')\mathbb{T}_0^{(b)}(A')}{2}$

$\boxed{\text{z170}}$ $\mathbb{G}_{1,2}^{(1,-1;c)}(E'') = \frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E'')\mathbb{T}_0^{(b)}(A')}{2}$

$\boxed{\text{z171}}$ $\mathbb{G}_{2,1}^{(1,-1;c)}(E'') = \frac{\mathbb{M}_{1,1}^{(1,-1;a)}(E'')\mathbb{T}_{1,1}^{(b)}(E')}{2} - \frac{\mathbb{M}_{1,2}^{(1,-1;a)}(E'')\mathbb{T}_{1,2}^{(b)}(E')}{2}$

$\boxed{\text{z172}}$ $\mathbb{G}_{2,2}^{(1,-1;c)}(E'') = -\frac{\mathbb{M}_{1,1}^{(1,-1;a)}(E'')\mathbb{T}_{1,2}^{(b)}(E')}{2} - \frac{\mathbb{M}_{1,2}^{(1,-1;a)}(E'')\mathbb{T}_{1,1}^{(b)}(E')}{2}$

- 'H2'-'O' bond-cluster : `O;H2_001_1`

* 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: `3a@3b`

$\boxed{\text{z29}}$ $$\mathbb{Q}_0^{(c)}(A') = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{2} + \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{2}$$

$\boxed{\text{z30}}$ $$\mathbb{Q}_2^{(1,-1;c)}(A') = -\frac{\sqrt{2}\mathbb{G}_{2,1}^{(1,-1;a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{2} - \frac{\sqrt{2}\mathbb{G}_{2,2}^{(1,-1;a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{2}$$

$\boxed{\text{z31}}$ $$\mathbb{Q}_0^{(1,0;c)}(A') = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(1,0;a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{2} + \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(1,0;a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{2}$$

$\boxed{\text{z32}}$ $$\mathbb{G}_1^{(c)}(A') = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{2} - \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{2}$$

$\boxed{\text{z33}}$ $$\mathbb{G}_1^{(1,-1;c)}(A') = \frac{\sqrt{2}\mathbb{G}_{2,1}^{(1,-1;a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{2} - \frac{\sqrt{2}\mathbb{G}_{2,2}^{(1,-1;a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{2}$$

$\boxed{\text{z34}}$ $$\mathbb{G}_1^{(1,0;c)}(A') = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(1,0;a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{2} - \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(1,0;a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{2}$$

$\boxed{\text{z57}}$ $$\mathbb{Q}_1^{(c)}(A'') = \mathbb{Q}_1^{(a)}(A'')\mathbb{Q}_0^{(b)}(A')$$

$\boxed{\text{z58}}$ $$\mathbb{Q}_1^{(1,0;c)}(A'') = \mathbb{Q}_1^{(1,0;a)}(A'')\mathbb{Q}_0^{(b)}(A')$$

$\boxed{\text{z59}}$ $$\mathbb{G}_2^{(1,-1;c)}(A'') = \mathbb{G}_2^{(1,-1;a)}(A'')\mathbb{Q}_0^{(b)}(A')$$

$\boxed{\text{z60}}$ $$\mathbb{G}_3^{(1,-1;c)}(A'',1) = \frac{\sqrt{2}\mathbb{G}_{2,1}^{(1,-1;a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{2} - \frac{\sqrt{2}\mathbb{G}_{2,2}^{(1,-1;a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{2}$$

$\boxed{\text{z61}}$ $$\mathbb{G}_3^{(1,-1;c)}(A'',2) = \frac{\sqrt{2}\mathbb{G}_{2,1}^{(1,-1;a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{2} + \frac{\sqrt{2}\mathbb{G}_{2,2}^{(1,-1;a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{2}$$

$\boxed{\text{z62}}$ $$\mathbb{G}_0^{(1,1;c)}(A'') = \mathbb{G}_0^{(1,1;a)}(A'')\mathbb{Q}_0^{(b)}(A')$$

$\boxed{\text{z117}}$ $$\mathbb{Q}_{1,1}^{(c)}(E') = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E')\mathbb{Q}_0^{(b)}(A')}{2}$$

$\boxed{\text{z118}}$ $\mathbb{Q}_{1,2}^{(c)}(E') = \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E')\mathbb{Q}_{0}^{(b)}(A')}{2}$

$\boxed{\text{z119}}$ $\mathbb{Q}_{2,1}^{(c)}(E') = \frac{\mathbb{Q}_{1,1}^{(a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{2} - \frac{\mathbb{Q}_{1,2}^{(a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{2}$

$\boxed{\text{z120}}$ $\mathbb{Q}_{2,2}^{(c)}(E') = -\frac{\mathbb{Q}_{1,1}^{(a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{2} - \frac{\mathbb{Q}_{1,2}^{(a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{2}$

$\boxed{\text{z121}}$ $\mathbb{Q}_{2,1}^{(1,-1;c)}(E') = -\frac{\mathbb{G}_{2,1}^{(1,-1;a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{2} + \frac{\mathbb{G}_{2,2}^{(1,-1;a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{2}$

$\boxed{\text{z122}}$ $\mathbb{Q}_{2,2}^{(1,-1;c)}(E') = \frac{\mathbb{G}_{2,1}^{(1,-1;a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{2} + \frac{\mathbb{G}_{2,2}^{(1,-1;a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{2}$

$\boxed{\text{z123}}$ $\mathbb{Q}_{1,1}^{(1,0;c)}(E') = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(1,0;a)}(E')\mathbb{Q}_{0}^{(b)}(A')}{2}$

$\boxed{\text{z124}}$ $\mathbb{Q}_{1,2}^{(1,0;c)}(E') = \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(1,0;a)}(E')\mathbb{Q}_{0}^{(b)}(A')}{2}$

$\boxed{\text{z125}}$ $\mathbb{Q}_{2,1}^{(1,0;c)}(E') = \frac{\mathbb{Q}_{1,1}^{(1,0;a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{2} - \frac{\mathbb{Q}_{1,2}^{(1,0;a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{2}$

$\boxed{\text{z126}}$ $\mathbb{Q}_{2,2}^{(1,0;c)}(E') = -\frac{\mathbb{Q}_{1,1}^{(1,0;a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{2} - \frac{\mathbb{Q}_{1,2}^{(1,0;a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{2}$

$\boxed{\text{z127}}$ $\mathbb{G}_{2,1}^{(1,-1;c)}(E') = \frac{\sqrt{2}\mathbb{G}_{2,1}^{(1,-1;a)}(E')\mathbb{Q}_{0}^{(b)}(A')}{2}$

$\boxed{\text{z128}}$ $\mathbb{G}_{2,2}^{(1,-1;c)}(E') = \frac{\sqrt{2}\mathbb{G}_{2,2}^{(1,-1;a)}(E')\mathbb{Q}_{0}^{(b)}(A')}{2}$

$\boxed{\text{z173}}$ $\mathbb{Q}_{2,1}^{(c)}(E'') = \frac{\sqrt{2}\mathbb{Q}_{1}^{(a)}(A'')\mathbb{Q}_{1,2}^{(b)}(E')}{2}$

$\boxed{\text{z174}}$ $\mathbb{Q}_{2,2}^{(c)}(E'') = -\frac{\sqrt{2}\mathbb{Q}_{1}^{(a)}(A'')\mathbb{Q}_{1,1}^{(b)}(E')}{2}$

$\boxed{\text{z175}}$ $\mathbb{Q}_{2,1}^{(1,-1;c)}(E'') = \frac{\sqrt{10}\mathbb{G}_{2,1}^{(1,-1;a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{10} - \frac{\sqrt{10}\mathbb{G}_{2,2}^{(1,-1;a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{10} + \frac{\sqrt{30}\mathbb{G}_{2}^{(1,-1;a)}(A'')\mathbb{Q}_{1,1}^{(b)}(E')}{10}$

$\boxed{\text{z176}}$ $$\mathbb{Q}_{2,2}^{(1,-1;c)}(E'') = -\frac{\sqrt{10}\mathbb{G}_{2,1}^{(1,-1;a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{10} - \frac{\sqrt{10}\mathbb{G}_{2,2}^{(1,-1;a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{10} + \frac{\sqrt{30}\mathbb{G}_{2}^{(1,-1;a)}(A'')\mathbb{Q}_{1,2}^{(b)}(E')}{10}$$

$\boxed{\text{z177}}$ $$\mathbb{Q}_{2,1}^{(1,0;c)}(E'') = \frac{\sqrt{2}\mathbb{Q}_{1}^{(1,0;a)}(A'')\mathbb{Q}_{1,2}^{(b)}(E')}{2}$$

$\boxed{\text{z178}}$ $$\mathbb{Q}_{2,2}^{(1,0;c)}(E'') = -\frac{\sqrt{2}\mathbb{Q}_{1}^{(1,0;a)}(A'')\mathbb{Q}_{1,1}^{(b)}(E')}{2}$$

$\boxed{\text{z179}}$ $$\mathbb{G}_{1,1}^{(1,-1;c)}(E'') = \frac{\sqrt{15}\mathbb{G}_{2,1}^{(1,-1;a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{10} - \frac{\sqrt{15}\mathbb{G}_{2,2}^{(1,-1;a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{10} - \frac{\sqrt{5}\mathbb{G}_{2}^{(1,-1;a)}(A'')\mathbb{Q}_{1,1}^{(b)}(E')}{5}$$

$\boxed{\text{z180}}$ $$\mathbb{G}_{1,2}^{(1,-1;c)}(E'') = -\frac{\sqrt{15}\mathbb{G}_{2,1}^{(1,-1;a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{10} - \frac{\sqrt{15}\mathbb{G}_{2,2}^{(1,-1;a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{10} - \frac{\sqrt{5}\mathbb{G}_{2}^{(1,-1;a)}(A'')\mathbb{Q}_{1,2}^{(b)}(E')}{5}$$

$\boxed{\text{z181}}$ $$\mathbb{G}_{2,1}^{(1,-1;c)}(E'') = \frac{\sqrt{2}\mathbb{G}_{2,1}^{(1,-1;a)}(E'')\mathbb{Q}_{0}^{(b)}(A')}{2}$$

$\boxed{\text{z182}}$ $$\mathbb{G}_{2,2}^{(1,-1;c)}(E'') = \frac{\sqrt{2}\mathbb{G}_{2,2}^{(1,-1;a)}(E'')\mathbb{Q}_{0}^{(b)}(A')}{2}$$

$\boxed{\text{z183}}$ $$\mathbb{G}_{1,1}^{(1,1;c)}(E'') = \frac{\sqrt{2}\mathbb{G}_{0}^{(1,1;a)}(A'')\mathbb{Q}_{1,1}^{(b)}(E')}{2}$$

$\boxed{\text{z184}}$ $$\mathbb{G}_{1,2}^{(1,1;c)}(E'') = \frac{\sqrt{2}\mathbb{G}_{0}^{(1,1;a)}(A'')\mathbb{Q}_{1,2}^{(b)}(E')}{2}$$

Atomic SAMB

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

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

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

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

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

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

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

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

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

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

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

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

$\boxed{\text{x11}}$ $\mathbb{G}_{2}^{(1,-1;a)}(A'') = \begin{bmatrix} 0 & -\frac{\sqrt{6}i}{12} & 0 & -\frac{\sqrt{6}}{12} & \frac{\sqrt{6}i}{6} & 0 \\ -\frac{\sqrt{6}i}{12} & 0 & \frac{\sqrt{6}}{12} & 0 & 0 & -\frac{\sqrt{6}i}{6} \end{bmatrix}$

$\boxed{\text{x12}}$ $\mathbb{G}_{2,1}^{(1,-1;a)}(E') = \begin{bmatrix} 0 & 0 & \frac{\sqrt{2}i}{4} & 0 & 0 & \frac{\sqrt{2}}{4} \\ 0 & 0 & 0 & -\frac{\sqrt{2}i}{4} & -\frac{\sqrt{2}}{4} & 0 \end{bmatrix}$

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

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

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

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

$\boxed{\text{x17}}$ $\mathbb{M}_{2}^{(1,-1;a)}(A'') = \begin{bmatrix} 0 & -\frac{\sqrt{6}}{12} & 0 & \frac{\sqrt{6}i}{12} & \frac{\sqrt{6}}{6} & 0 \\ -\frac{\sqrt{6}}{12} & 0 & -\frac{\sqrt{6}i}{12} & 0 & 0 & -\frac{\sqrt{6}}{6} \end{bmatrix}$

$\boxed{\text{x18}}$ $\mathbb{M}_{2,1}^{(1,-1;a)}(E') = \begin{bmatrix} 0 & 0 & \frac{\sqrt{2}}{4} & 0 & 0 & -\frac{\sqrt{2}i}{4} \\ 0 & 0 & 0 & -\frac{\sqrt{2}}{4} & \frac{\sqrt{2}i}{4} & 0 \end{bmatrix}$

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

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

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

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

$\boxed{\text{x23}}$ $\mathbb{T}_{1}^{(a)}(A'') = \begin{bmatrix} 0 & 0 & 0 & 0 & \frac{i}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{i}{2} \end{bmatrix}$

$\boxed{\text{x24}}$ $\mathbb{T}_{1,1}^{(a)}(E') = \begin{bmatrix} \frac{i}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{i}{2} & 0 & 0 & 0 & 0 \end{bmatrix}$

$\boxed{\text{x25}}$ $\mathbb{T}_{1,2}^{(a)}(E') = \begin{bmatrix} 0 & 0 & \frac{i}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{i}{2} & 0 & 0 \end{bmatrix}$

$\boxed{\text{x26}}$ $\mathbb{T}_{1}^{(1,0;a)}(A'') = \begin{bmatrix} 0 & \frac{\sqrt{2}i}{4} & 0 & \frac{\sqrt{2}}{4} & 0 & 0 \\ -\frac{\sqrt{2}i}{4} & 0 & \frac{\sqrt{2}}{4} & 0 & 0 & 0 \end{bmatrix}$

$\boxed{\text{x27}}$ $\mathbb{T}_{1,1}^{(1,0;a)}(E') = \begin{bmatrix} 0 & 0 & -\frac{\sqrt{2}}{4} & 0 & 0 & -\frac{\sqrt{2}i}{4} \\ 0 & 0 & 0 & \frac{\sqrt{2}}{4} & \frac{\sqrt{2}i}{4} & 0 \end{bmatrix}$

$\boxed{\text{x28}}$ $\mathbb{T}_{1,2}^{(1,0;a)}(E') = \begin{bmatrix} \frac{\sqrt{2}}{4} & 0 & 0 & 0 & 0 & -\frac{\sqrt{2}}{4} \\ 0 & -\frac{\sqrt{2}}{4} & 0 & 0 & -\frac{\sqrt{2}}{4} & 0 \end{bmatrix}$

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

$\boxed{\text{x48}}$ $$\mathbb{M}_{3}^{(1,-1;a)}(A') = \begin{bmatrix} -\frac{\sqrt{5}}{10} & 0 & 0 & 0 & 0 & -\frac{\sqrt{5}}{10} \\ 0 & \frac{\sqrt{5}}{10} & 0 & 0 & -\frac{\sqrt{5}}{10} & 0 \\ 0 & 0 & -\frac{\sqrt{5}}{10} & 0 & 0 & \frac{\sqrt{5}i}{10} \\ 0 & 0 & 0 & \frac{\sqrt{5}}{10} & -\frac{\sqrt{5}i}{10} & 0 \\ 0 & -\frac{\sqrt{5}}{10} & 0 & \frac{\sqrt{5}i}{10} & \frac{\sqrt{5}}{5} & 0 \\ -\frac{\sqrt{5}}{10} & 0 & -\frac{\sqrt{5}i}{10} & 0 & 0 & -\frac{\sqrt{5}}{5} \end{bmatrix}$$

$\boxed{\text{x49}}$ $$\mathbb{M}_{3}^{(1,-1;a)}(A'',1) = \begin{bmatrix} 0 & -\frac{\sqrt{2}i}{4} & 0 & \frac{\sqrt{2}}{4} & 0 & 0 \\ \frac{\sqrt{2}i}{4} & 0 & \frac{\sqrt{2}}{4} & 0 & 0 & 0 \\ 0 & \frac{\sqrt{2}}{4} & 0 & \frac{\sqrt{2}i}{4} & 0 & 0 \\ \frac{\sqrt{2}}{4} & 0 & -\frac{\sqrt{2}i}{4} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$\boxed{\text{x50}}$ $$\mathbb{M}_{3}^{(1,-1;a)}(A'',2) = \begin{bmatrix} 0 & \frac{\sqrt{2}}{4} & 0 & \frac{\sqrt{2}i}{4} & 0 & 0 \\ \frac{\sqrt{2}}{4} & 0 & -\frac{\sqrt{2}i}{4} & 0 & 0 & 0 \\ 0 & \frac{\sqrt{2}i}{4} & 0 & -\frac{\sqrt{2}}{4} & 0 & 0 \\ -\frac{\sqrt{2}i}{4} & 0 & -\frac{\sqrt{2}}{4} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$\boxed{\text{x51}}$ $$\mathbb{M}_{3,1}^{(1,-1;a)}(E') = \begin{bmatrix} 0 & 0 & \frac{\sqrt{3}}{6} & 0 & 0 & -\frac{\sqrt{3}i}{6} \\ 0 & 0 & 0 & -\frac{\sqrt{3}}{6} & \frac{\sqrt{3}i}{6} & 0 \\ \frac{\sqrt{3}}{6} & 0 & 0 & 0 & 0 & \frac{\sqrt{3}}{6} \\ 0 & -\frac{\sqrt{3}}{6} & 0 & 0 & \frac{\sqrt{3}}{6} & 0 \\ 0 & -\frac{\sqrt{3}i}{6} & 0 & \frac{\sqrt{3}}{6} & 0 & 0 \\ \frac{\sqrt{3}i}{6} & 0 & \frac{\sqrt{3}}{6} & 0 & 0 & 0 \end{bmatrix}$$

$\boxed{\text{x52}}$ $$\mathbb{M}_{3,2}^{(1,-1;a)}(E') = \begin{bmatrix} \frac{\sqrt{3}}{6} & 0 & 0 & 0 & 0 & \frac{\sqrt{3}}{6} \\ 0 & -\frac{\sqrt{3}}{6} & 0 & 0 & \frac{\sqrt{3}}{6} & 0 \\ 0 & 0 & -\frac{\sqrt{3}}{6} & 0 & 0 & \frac{\sqrt{3}i}{6} \\ 0 & 0 & 0 & \frac{\sqrt{3}}{6} & -\frac{\sqrt{3}i}{6} & 0 \\ 0 & \frac{\sqrt{3}}{6} & 0 & \frac{\sqrt{3}i}{6} & 0 & 0 \\ \frac{\sqrt{3}}{6} & 0 & -\frac{\sqrt{3}i}{6} & 0 & 0 & 0 \end{bmatrix}$$

$\boxed{\text{x53}}$ $$\mathbb{M}_{1,1}^{(1,-1;a)}(E'') = \begin{bmatrix} 0 & \frac{\sqrt{6}}{6} & 0 & 0 & 0 & 0 \\ \frac{\sqrt{6}}{6} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{6}}{6} & 0 & 0 \\ 0 & 0 & \frac{\sqrt{6}}{6} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{6}}{6} \\ 0 & 0 & 0 & 0 & \frac{\sqrt{6}}{6} & 0 \end{bmatrix}$$

$\boxed{\text{x54}}$ $$\mathbb{M}_{1,2}^{(1,-1;a)}(E'') = \begin{bmatrix} 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 \\ \frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 \\ 0 & 0 & \frac{\sqrt{6}i}{6} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{6}i}{6} \\ 0 & 0 & 0 & 0 & \frac{\sqrt{6}i}{6} & 0 \end{bmatrix}$$

$$\boxed{\text{x55}} \quad \mathbb{M}_{3,1}^{(1,-1;a)}(E'') = \begin{bmatrix} 0 & -\frac{\sqrt{30}}{20} & 0 & \frac{\sqrt{30}i}{60} & \frac{\sqrt{30}}{15} & 0 \\ -\frac{\sqrt{30}}{20} & 0 & -\frac{\sqrt{30}i}{60} & 0 & 0 & -\frac{\sqrt{30}}{15} \\ 0 & \frac{\sqrt{30}i}{60} & 0 & -\frac{\sqrt{30}}{60} & 0 & 0 \\ -\frac{\sqrt{30}i}{60} & 0 & -\frac{\sqrt{30}}{60} & 0 & 0 & 0 \\ \frac{\sqrt{30}}{15} & 0 & 0 & 0 & 0 & \frac{\sqrt{30}}{15} \\ 0 & -\frac{\sqrt{30}}{15} & 0 & 0 & \frac{\sqrt{30}}{15} & 0 \end{bmatrix}$$

$$\boxed{\text{x56}} \quad \mathbb{M}_{3,2}^{(1,-1;a)}(E'') = \begin{bmatrix} 0 & \frac{\sqrt{30}i}{60} & 0 & -\frac{\sqrt{30}}{60} & 0 & 0 \\ -\frac{\sqrt{30}i}{60} & 0 & -\frac{\sqrt{30}}{60} & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{30}}{60} & 0 & \frac{\sqrt{30}i}{20} & \frac{\sqrt{30}}{15} & 0 \\ -\frac{\sqrt{30}}{60} & 0 & -\frac{\sqrt{30}i}{20} & 0 & 0 & -\frac{\sqrt{30}}{15} \\ 0 & 0 & \frac{\sqrt{30}}{15} & 0 & 0 & -\frac{\sqrt{30}i}{15} \\ 0 & 0 & 0 & -\frac{\sqrt{30}}{15} & \frac{\sqrt{30}i}{15} & 0 \end{bmatrix}$$

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

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

$$\boxed{\text{x59}} \quad \mathbb{M}_{1,2}^{(1,1;a)}(E'') = \begin{bmatrix} 0 & \frac{\sqrt{30}i}{30} & 0 & \frac{\sqrt{30}}{20} & 0 & 0 \\ -\frac{\sqrt{30}i}{30} & 0 & \frac{\sqrt{30}}{20} & 0 & 0 & 0 \\ 0 & \frac{\sqrt{30}}{20} & 0 & -\frac{\sqrt{30}i}{15} & \frac{\sqrt{30}}{20} & 0 \\ \frac{\sqrt{30}}{20} & 0 & \frac{\sqrt{30}i}{15} & 0 & 0 & -\frac{\sqrt{30}}{20} \\ 0 & 0 & \frac{\sqrt{30}}{20} & 0 & 0 & \frac{\sqrt{30}i}{30} \\ 0 & 0 & 0 & -\frac{\sqrt{30}}{20} & -\frac{\sqrt{30}i}{30} & 0 \end{bmatrix}$$

$\boxed{\text{x60}}$ $$\mathbb{T}_{2}^{(1,0;a)}(A') = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{2}i}{4} \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{2}i}{4} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{2}}{4} \\ 0 & 0 & 0 & 0 & \frac{\sqrt{2}}{4} & 0 \\ 0 & \frac{\sqrt{2}i}{4} & 0 & \frac{\sqrt{2}}{4} & 0 & 0 \\ -\frac{\sqrt{2}i}{4} & 0 & \frac{\sqrt{2}}{4} & 0 & 0 & 0 \end{bmatrix}$$

$\boxed{\text{x61}}$ $$\mathbb{T}_{2,1}^{(1,0;a)}(E') = \begin{bmatrix} 0 & 0 & -\frac{\sqrt{6}}{6} & 0 & 0 & -\frac{\sqrt{6}i}{12} \\ 0 & 0 & 0 & \frac{\sqrt{6}}{6} & \frac{\sqrt{6}i}{12} & 0 \\ -\frac{\sqrt{6}}{6} & 0 & 0 & 0 & 0 & \frac{\sqrt{6}}{12} \\ 0 & \frac{\sqrt{6}}{6} & 0 & 0 & \frac{\sqrt{6}}{12} & 0 \\ 0 & -\frac{\sqrt{6}i}{12} & 0 & \frac{\sqrt{6}}{12} & 0 & 0 \\ \frac{\sqrt{6}i}{12} & 0 & \frac{\sqrt{6}}{12} & 0 & 0 & 0 \end{bmatrix}$$

$\boxed{\text{x62}}$ $$\mathbb{T}_{2,2}^{(1,0;a)}(E') = \begin{bmatrix} -\frac{\sqrt{6}}{6} & 0 & 0 & 0 & 0 & \frac{\sqrt{6}}{12} \\ 0 & \frac{\sqrt{6}}{6} & 0 & 0 & \frac{\sqrt{6}}{12} & 0 \\ 0 & 0 & \frac{\sqrt{6}}{6} & 0 & 0 & \frac{\sqrt{6}i}{12} \\ 0 & 0 & 0 & -\frac{\sqrt{6}}{6} & -\frac{\sqrt{6}i}{12} & 0 \\ 0 & \frac{\sqrt{6}}{12} & 0 & \frac{\sqrt{6}i}{12} & 0 & 0 \\ \frac{\sqrt{6}}{12} & 0 & -\frac{\sqrt{6}i}{12} & 0 & 0 & 0 \end{bmatrix}$$

$\boxed{\text{x63}}$ $$\mathbb{T}_{2,1}^{(1,0;a)}(E'') = \begin{bmatrix} 0 & 0 & 0 & \frac{\sqrt{6}i}{12} & \frac{\sqrt{6}}{12} & 0 \\ 0 & 0 & -\frac{\sqrt{6}i}{12} & 0 & 0 & -\frac{\sqrt{6}}{12} \\ 0 & \frac{\sqrt{6}i}{12} & 0 & \frac{\sqrt{6}}{6} & 0 & 0 \\ -\frac{\sqrt{6}i}{12} & 0 & \frac{\sqrt{6}}{6} & 0 & 0 & 0 \\ \frac{\sqrt{6}}{12} & 0 & 0 & 0 & 0 & -\frac{\sqrt{6}}{6} \\ 0 & -\frac{\sqrt{6}}{12} & 0 & 0 & -\frac{\sqrt{6}}{6} & 0 \end{bmatrix}$$

$\boxed{\text{x64}}$ $$\mathbb{T}_{2,2}^{(1,0;a)}(E'') = \begin{bmatrix} 0 & -\frac{\sqrt{6}i}{6} & 0 & -\frac{\sqrt{6}}{12} & 0 & 0 \\ \frac{\sqrt{6}i}{6} & 0 & -\frac{\sqrt{6}}{12} & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{6}}{12} & 0 & 0 & \frac{\sqrt{6}}{12} & 0 \\ -\frac{\sqrt{6}}{12} & 0 & 0 & 0 & 0 & -\frac{\sqrt{6}}{12} \\ 0 & 0 & \frac{\sqrt{6}}{12} & 0 & 0 & \frac{\sqrt{6}i}{6} \\ 0 & 0 & 0 & -\frac{\sqrt{6}}{12} & -\frac{\sqrt{6}i}{6} & 0 \end{bmatrix}$$

Cluster SAMB

- Site cluster

** Wyckoff: `1o`

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

** Wyckoff: `3b`

$\boxed{\text{y2}}$ $\mathbb{Q}_{0}^{(s)}(A') = \left[\frac{\sqrt{3}}{3}, \frac{\sqrt{3}}{3}, \frac{\sqrt{3}}{3}\right]$

$\boxed{\text{y3}}$ $\mathbb{Q}_{1,1}^{(s)}(E') = \left[\frac{5\sqrt{42}}{42}, -\frac{2\sqrt{42}}{21}, -\frac{\sqrt{42}}{42}\right]$

$\boxed{\text{y4}}$ $\mathbb{Q}_{1,2}^{(s)}(E') = \left[\frac{\sqrt{14}}{14}, \frac{\sqrt{14}}{7}, -\frac{3\sqrt{14}}{14}\right]$

- Bond cluster

** Wyckoff: `3a@3b`

$\boxed{\text{y5}}$ $\mathbb{Q}_{0}^{(s)}(A') = \left[\frac{\sqrt{3}}{3}, \frac{\sqrt{3}}{3}, \frac{\sqrt{3}}{3}\right]$

$\boxed{\text{y6}}$ $\mathbb{T}_{0}^{(s)}(A') = \left[\frac{\sqrt{3}i}{3}, \frac{\sqrt{3}i}{3}, \frac{\sqrt{3}i}{3}\right]$

$\boxed{\text{y7}}$ $\mathbb{Q}_{1,1}^{(s)}(E') = \left[\frac{5\sqrt{42}}{42}, -\frac{2\sqrt{42}}{21}, -\frac{\sqrt{42}}{42}\right]$

$\boxed{\text{y8}}$ $\mathbb{Q}_{1,2}^{(s)}(E') = \left[\frac{\sqrt{14}}{14}, \frac{\sqrt{14}}{7}, -\frac{3\sqrt{14}}{14}\right]$

$\boxed{\text{y9}}$ $\mathbb{T}_{1,1}^{(s)}(E') = \left[\frac{5\sqrt{42}i}{42}, -\frac{2\sqrt{42}i}{21}, -\frac{\sqrt{42}i}{42}\right]$

$\boxed{\text{y10}}$ $\mathbb{T}_{1,2}^{(s)}(E') = \left[\frac{\sqrt{14}i}{14}, \frac{\sqrt{14}i}{7}, -\frac{3\sqrt{14}i}{14}\right]$

Site and Bond

Table 5: Orbital of each site

#	site	orbital
1	`H1`	$\vert s,\uparrow\rangle$, $\vert s,\downarrow\rangle$
2	`H2`	$\vert s,\uparrow\rangle$, $\vert s,\downarrow\rangle$
3	`O`	$\vert s,\uparrow\rangle$, $\vert s,\downarrow\rangle$, $\vert p_x,\uparrow\rangle$, $\vert p_x,\downarrow\rangle$, $\vert p_y,\uparrow\rangle$, $\vert p_y,\downarrow\rangle$, $\vert p_z,\uparrow\rangle$, $\vert p_z,\downarrow\rangle$

Table 6: Neighbor and bra-ket of each bond

#	head	tail	neighbor	head (bra)	tail (ket)
1	`H1`	`O`	`[1]`	`[s]`	`[s,p]`
2	`H2`	`O`	`[1]`	`[s]`	`[s,p]`

Site in Unit Cell

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

Table 7: 'H1' (#1) site cluster (1o), -6..

SL	position ($\boldsymbol{s}$)	mapping
1	[0.00000, 0.00000, 0.00000]	[1,2,3,4,5,6]

Table 8: 'H2' (#2) site cluster (3b), m..

SL	position ($\boldsymbol{s}$)	mapping
1	[0.50000, 0.16667, 0.00000]	[1,4]
2	[-0.16667, 0.33333, 0.00000]	[2,5]
3	[-0.33333,-0.50000, 0.00000]	[3,6]

Table 9: 'O' (#3) site cluster (3b), m..

SL	position ($\boldsymbol{s}$)	mapping
1	[0.33333, 0.00000, 0.00000]	[1,4]
2	[0.00000, 0.33333, 0.00000]	[2,5]
3	[-0.33333,-0.33333, 0.00000]	[3,6]

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

Table 10: 1-th 'H1'-'O' [1] (#1) bond cluster (3a@3b), D, $|\boldsymbol{v}|$= 0.33333 (cartesian)

SL	vector ($\boldsymbol{v}$)	center ($\boldsymbol{c}$)	mapping	head	tail	$\boldsymbol{R}$ (primitive)
1	[-0.33333, 0.00000, 0.00000]	[0.16667, 0.00000, 0.00000]	[1,4]	(1,1)	(1,1)	[0,0,0]
2	[0.00000,-0.33333, 0.00000]	[0.00000, 0.16667, 0.00000]	[2,5]	(1,1)	(2,1)	[0,0,0]
3	[0.33333, 0.33333, 0.00000]	[-0.16667,-0.16667, 0.00000]	[3,6]	(1,1)	(3,1)	[0,0,0]

Table 11: 1-th 'H2'-'O' [1] (#2) bond cluster (3a@3b), D, $|\boldsymbol{v}|$= 0.16667 (cartesian)

SL	vector ($\boldsymbol{v}$)	center ($\boldsymbol{c}$)	mapping	head	tail	$\boldsymbol{R}$ (primitive)
1	[0.16667, 0.16667, 0.00000]	[0.41667, 0.08333, 0.00000]	[1,4]	(1,1)	(1,1)	[0,0,0]
2	[-0.16667, 0.00000, 0.00000]	[-0.08333, 0.33333, 0.00000]	[2,5]	(2,1)	(2,1)	[0,0,0]
3	[0.00000,-0.16667, 0.00000]	[-0.33333,-0.41667, 0.00000]	[3,6]	(3,1)	(3,1)	[0,0,0]