Model for "C3h"

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]`
- 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} | | | | | |

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	-	-	$-\frac{z(3x^2+3y^2-2z^2)}{2}$
5	$\mathbb{Q}_3(A',1)$	A'	3	Q, T	1	-	$\frac{\sqrt{10}y(3x^2-y^2)}{4}$
6	$\mathbb{Q}_3(A',2)$	A'	3	Q, T	2	-	$\frac{\sqrt{10}x(x^2-3y^2)}{4}$
7	$\mathbb{G}_0(A'')$	A''	0	G, M	-	-	1
8	$\mathbb{Q}_1(A'')$	A''	1	Q, T	-	-	z
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	$\sqrt{3}yz$

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Table 2

#	symbol	irrep.	rank	X	multiplicity	component	symmetry
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	$-\frac{\sqrt{6}y(x^2+y^2-4z^2)}{4}$
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)
1	$|s,\uparrow\rangle$ @H1(1)	2	$|s,\downarrow\rangle$ @H1(1)	3	$|s,\uparrow\rangle$ @H2(1)	4	$|s,\downarrow\rangle$ @H2(1)	5	$|s,\uparrow\rangle$ @H2(2)
6	$|s,\downarrow\rangle$ @H2(2)	7	$|s,\uparrow\rangle$ @H2(3)	8	$|s,\downarrow\rangle$ @H2(3)	9	$|s,\uparrow\rangle$ @O(1)	10	$|s,\downarrow\rangle$ @O(1)
11	$|p_x,\uparrow\rangle$ @O(1)	12	$|p_x,\downarrow\rangle$ @O(1)	13	$|p_y,\uparrow\rangle$ @O(1)	14	$|p_y,\downarrow\rangle$ @O(1)	15	$|p_z,\uparrow\rangle$ @O(1)
16	$|p_z,\downarrow\rangle$ @O(1)	17	$|s,\uparrow\rangle$ @O(2)	18	$|s,\downarrow\rangle$ @O(2)	19	$|p_x,\uparrow\rangle$ @O(2)	20	$|p_x,\downarrow\rangle$ @O(2)
21	$|p_y,\uparrow\rangle$ @O(2)	22	$|p_y,\downarrow\rangle$ @O(2)	23	$|p_z,\uparrow\rangle$ @O(2)	24	$|p_z,\downarrow\rangle$ @O(2)	25	$|s,\uparrow\rangle$ @O(3)
26	$|s,\downarrow\rangle$ @O(3)	27	$|p_x,\uparrow\rangle$ @O(3)	28	$|p_x,\downarrow\rangle$ @O(3)	29	$|p_y,\uparrow\rangle$ @O(3)	30	$|p_y,\downarrow\rangle$ @O(3)
31	$|p_z,\uparrow\rangle$ @O(3)	32	$|p_z,\downarrow\rangle$ @O(3)							

Table 4: Atomic basis (orbital part only)

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

123 (all 184) SAMBs

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

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

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

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

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

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

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

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

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

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

- 'O' 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: `3b`

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

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

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

$\boxed{\text{z7}}$ $\quad \mathbb{Q}_1^{(c)}(A'') = \mathbb{Q}_1^{(a)}(A'')\mathbb{Q}_0^{(s)}(A')$

$\boxed{\text{z8}}$ $\quad \mathbb{Q}_1^{(1,0;c)}(A'') = \mathbb{Q}_1^{(1,0;a)}(A'')\mathbb{Q}_0^{(s)}(A')$

$\boxed{\text{z9}}$ $\quad \mathbb{Q}_{1,1}^{(c)}(E') = \dfrac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E')\mathbb{Q}_0^{(s)}(A')}{2}$

$\boxed{\text{z35}}$ $\quad \mathbb{Q}_{1,2}^{(c)}(E') = \dfrac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E')\mathbb{Q}_0^{(s)}(A')}{2}$

$\boxed{\text{z36}}$ $\quad \mathbb{Q}_{2,1}^{(c)}(E') = \dfrac{\mathbb{Q}_{1,1}^{(a)}(E')\mathbb{Q}_{1,1}^{(s)}(E')}{2} - \dfrac{\mathbb{Q}_{1,2}^{(a)}(E')\mathbb{Q}_{1,2}^{(s)}(E')}{2}$

$\boxed{\text{z37}}$ $\quad \mathbb{Q}_{2,2}^{(c)}(E') = -\dfrac{\mathbb{Q}_{1,1}^{(a)}(E')\mathbb{Q}_{1,2}^{(s)}(E')}{2} - \dfrac{\mathbb{Q}_{1,2}^{(a)}(E')\mathbb{Q}_{1,1}^{(s)}(E')}{2}$

$\boxed{\text{z38}}$ $\quad \mathbb{Q}_{2,1}^{(1,-1;c)}(E') = -\dfrac{\mathbb{G}_{2,1}^{(1,-1;a)}(E')\mathbb{Q}_{1,1}^{(s)}(E')}{2} + \dfrac{\mathbb{G}_{2,2}^{(1,-1;a)}(E')\mathbb{Q}_{1,2}^{(s)}(E')}{2}$

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

$\boxed{\text{z40}}$ $\quad \mathbb{Q}_{1,1}^{(1,0;c)}(E') = \dfrac{\sqrt{2}\mathbb{Q}_{1,1}^{(1,0;a)}(E')\mathbb{Q}_0^{(s)}(A')}{2}$

$\boxed{\text{z67}}$ $\quad \mathbb{Q}_{1,2}^{(1,0;c)}(E') = \dfrac{\sqrt{2}\mathbb{Q}_{1,2}^{(1,0;a)}(E')\mathbb{Q}_0^{(s)}(A')}{2}$

$\boxed{\text{z68}}$ $\quad \mathbb{Q}_{2,1}^{(1,0;c)}(E') = \dfrac{\mathbb{Q}_{1,1}^{(1,0;a)}(E')\mathbb{Q}_{1,1}^{(s)}(E')}{2} - \dfrac{\mathbb{Q}_{1,2}^{(1,0;a)}(E')\mathbb{Q}_{1,2}^{(s)}(E')}{2}$

$\boxed{\text{z69}}$ $\quad \mathbb{Q}_{2,2}^{(1,0;c)}(E') = -\dfrac{\mathbb{Q}_{1,1}^{(1,0;a)}(E')\mathbb{Q}_{1,2}^{(s)}(E')}{2} - \dfrac{\mathbb{Q}_{1,2}^{(1,0;a)}(E')\mathbb{Q}_{1,1}^{(s)}(E')}{2}$

$\boxed{\text{z70}}$ $\quad \mathbb{Q}_{2,1}^{(c)}(E'') = \dfrac{\sqrt{2}\mathbb{Q}_{1}^{(a)}(A'')\mathbb{Q}_{1,2}^{(s)}(E')}{2}$

$\boxed{\text{z71}}$ $\quad \mathbb{Q}_{2,2}^{(c)}(E'') = -\dfrac{\sqrt{2}\mathbb{Q}_{1}^{(a)}(A'')\mathbb{Q}_{1,1}^{(s)}(E')}{2}$

$\boxed{\text{z72}}$ $\quad \mathbb{Q}_{2,1}^{(1,-1;c)}(E'') = \dfrac{\sqrt{10}\mathbb{G}_{2,1}^{(1,-1;a)}(E'')\mathbb{Q}_{1,1}^{(s)}(E')}{10} - \dfrac{\sqrt{10}\mathbb{G}_{2,2}^{(1,-1;a)}(E'')\mathbb{Q}_{1,2}^{(s)}(E')}{10} + \dfrac{\sqrt{30}\mathbb{G}_{2}^{(1,-1;a)}(A'')\mathbb{Q}_{1,1}^{(s)}(E')}{10}$

$\boxed{\text{z73}}$ $\quad \mathbb{Q}_{2,2}^{(1,-1;c)}(E'') = -\dfrac{\sqrt{10}\mathbb{G}_{2,1}^{(1,-1;a)}(E'')\mathbb{Q}_{1,2}^{(s)}(E')}{10} - \dfrac{\sqrt{10}\mathbb{G}_{2,2}^{(1,-1;a)}(E'')\mathbb{Q}_{1,1}^{(s)}(E')}{10} + \dfrac{\sqrt{30}\mathbb{G}_{2}^{(1,-1;a)}(A'')\mathbb{Q}_{1,2}^{(s)}(E')}{10}$

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

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

$\boxed{\text{z76}}$ $\quad \mathbb{G}_{1}^{(c)}(A') = \dfrac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E')\mathbb{Q}_{1,2}^{(s)}(E')}{2} - \dfrac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E')\mathbb{Q}_{1,1}^{(s)}(E')}{2}$

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

$\boxed{\text{z78}}$ $\quad \mathbb{G}_{1}^{(1,0;c)}(A') = \dfrac{\sqrt{2}\mathbb{Q}_{1,1}^{(1,0;a)}(E')\mathbb{Q}_{1,2}^{(s)}(E')}{2} - \dfrac{\sqrt{2}\mathbb{Q}_{1,2}^{(1,0;a)}(E')\mathbb{Q}_{1,1}^{(s)}(E')}{2}$

$\boxed{\text{z129}}$ $\quad \mathbb{G}_{2}^{(1,-1;c)}(A'') = \mathbb{G}_{2}^{(1,-1;a)}(A'')\mathbb{Q}_{0}^{(s)}(A')$

$\boxed{\text{z130}}$ $\quad \mathbb{G}_{3}^{(1,-1;c)}(A'',1) = \dfrac{\sqrt{2}\mathbb{G}_{2,1}^{(1,-1;a)}(E'')\mathbb{Q}_{1,2}^{(s)}(E')}{2} - \dfrac{\sqrt{2}\mathbb{G}_{2,2}^{(1,-1;a)}(E'')\mathbb{Q}_{1,1}^{(s)}(E')}{2}$

$\boxed{\text{z131}}$ $\quad \mathbb{G}_{3}^{(1,-1;c)}(A'',2) = \dfrac{\sqrt{2}\mathbb{G}_{2,1}^{(1,-1;a)}(E'')\mathbb{Q}_{1,1}^{(s)}(E')}{2} + \dfrac{\sqrt{2}\mathbb{G}_{2,2}^{(1,-1;a)}(E'')\mathbb{Q}_{1,2}^{(s)}(E')}{2}$

$\boxed{\text{z132}}$ $\quad \mathbb{G}_0^{(1,1;c)}(A'') = \mathbb{G}_0^{(1,1;a)}(A'')\mathbb{Q}_0^{(s)}(A')$

$\boxed{\text{z133}}$ $\quad \mathbb{G}_{2,1}^{(1,-1;c)}(E') = \dfrac{\sqrt{2}\mathbb{G}_{2,1}^{(1,-1;a)}(E')\mathbb{Q}_0^{(s)}(A')}{2}$

$\boxed{\text{z134}}$ $\quad \mathbb{G}_{2,2}^{(1,-1;c)}(E') = \dfrac{\sqrt{2}\mathbb{G}_{2,2}^{(1,-1;a)}(E')\mathbb{Q}_0^{(s)}(A')}{2}$

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

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

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

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

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

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

- 'O' 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: 3b

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

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

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

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

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

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

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

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

$\boxed{\text{z18}}$ $\mathbb{Q}_1^{(c)}(A'') = \dfrac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E'')\mathbb{Q}_{1,2}^{(s)}(E')}{2} - \dfrac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E'')\mathbb{Q}_{1,1}^{(s)}(E')}{2}$

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

$\boxed{\text{z42}}$ $\mathbb{Q}_1^{(1,0;c)}(A'') = \dfrac{\sqrt{2}\mathbb{G}_{1,1}^{(1,0;a)}(E'')\mathbb{Q}_{1,2}^{(s)}(E')}{2} - \dfrac{\sqrt{2}\mathbb{G}_{1,2}^{(1,0;a)}(E'')\mathbb{Q}_{1,1}^{(s)}(E')}{2}$

$\boxed{\text{z43}}$ $\mathbb{Q}_{1,1}^{(c)}(E',a) = \dfrac{\sqrt{2}\mathbb{Q}_0^{(a)}(A')\mathbb{Q}_{1,1}^{(s)}(E')}{2}$

$\boxed{\text{z44}}$ $\mathbb{Q}_{1,2}^{(c)}(E',a) = \dfrac{\sqrt{2}\mathbb{Q}_0^{(a)}(A')\mathbb{Q}_{1,2}^{(s)}(E')}{2}$

$\boxed{\text{z45}}$ $\mathbb{Q}_{1,1}^{(c)}(E',b) = \dfrac{\sqrt{42}\mathbb{Q}_{2,1}^{(a)}(E')\mathbb{Q}_{1,1}^{(s)}(E')}{14} - \dfrac{\sqrt{42}\mathbb{Q}_{2,2}^{(a)}(E')\mathbb{Q}_{1,2}^{(s)}(E')}{14} - \dfrac{\sqrt{14}\mathbb{Q}_2^{(a)}(A')\mathbb{Q}_{1,1}^{(s)}(E')}{14}$

$\boxed{\text{z46}}$ $\mathbb{Q}_{1,2}^{(c)}(E',b) = -\dfrac{\sqrt{42}\mathbb{Q}_{2,1}^{(a)}(E')\mathbb{Q}_{1,2}^{(s)}(E')}{14} - \dfrac{\sqrt{42}\mathbb{Q}_{2,2}^{(a)}(E')\mathbb{Q}_{1,1}^{(s)}(E')}{14} - \dfrac{\sqrt{14}\mathbb{Q}_2^{(a)}(A')\mathbb{Q}_{1,2}^{(s)}(E')}{14}$

$\boxed{\text{z79}}$ $\mathbb{Q}_{2,1}^{(c)}(E') = \dfrac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E')\mathbb{Q}_0^{(s)}(A')}{2}$

$\boxed{\text{z80}}$ $\mathbb{Q}_{2,2}^{(c)}(E') = \dfrac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E')\mathbb{Q}_0^{(s)}(A')}{2}$

$\boxed{\text{z81}}$ $\mathbb{Q}_{3,1}^{(c)}(E') = \dfrac{\sqrt{7}\mathbb{Q}_{2,1}^{(a)}(E')\mathbb{Q}_{1,1}^{(s)}(E')}{14} - \dfrac{\sqrt{7}\mathbb{Q}_{2,2}^{(a)}(E')\mathbb{Q}_{1,2}^{(s)}(E')}{14} + \dfrac{\sqrt{21}\mathbb{Q}_2^{(a)}(A')\mathbb{Q}_{1,1}^{(s)}(E')}{7}$

z82 $\mathbb{Q}_{3,2}^{(c)}(E') = -\dfrac{\sqrt{7}\mathbb{Q}_{2,1}^{(a)}(E')\mathbb{Q}_{1,2}^{(s)}(E')}{14} - \dfrac{\sqrt{7}\mathbb{Q}_{2,2}^{(a)}(E')\mathbb{Q}_{1,1}^{(s)}(E')}{14} + \dfrac{\sqrt{21}\mathbb{Q}_{2}^{(a)}(A')\mathbb{Q}_{1,2}^{(s)}(E')}{7}$

z83 $\mathbb{Q}_{1,1}^{(1,-1;c)}(E') = \dfrac{\sqrt{42}\mathbb{Q}_{2,1}^{(1,-1;a)}(E')\mathbb{Q}_{1,1}^{(s)}(E')}{14} - \dfrac{\sqrt{42}\mathbb{Q}_{2,2}^{(1,-1;a)}(E')\mathbb{Q}_{1,2}^{(s)}(E')}{14} - \dfrac{\sqrt{14}\mathbb{Q}_{2}^{(1,-1;a)}(A')\mathbb{Q}_{1,1}^{(s)}(E')}{14}$

z84 $\mathbb{Q}_{1,2}^{(1,-1;c)}(E') = -\dfrac{\sqrt{42}\mathbb{Q}_{2,1}^{(1,-1;a)}(E')\mathbb{Q}_{1,2}^{(s)}(E')}{14} - \dfrac{\sqrt{42}\mathbb{Q}_{2,2}^{(1,-1;a)}(E')\mathbb{Q}_{1,1}^{(s)}(E')}{14} - \dfrac{\sqrt{14}\mathbb{Q}_{2}^{(1,-1;a)}(A')\mathbb{Q}_{1,2}^{(s)}(E')}{14}$

z85 $\mathbb{Q}_{2,1}^{(1,-1;c)}(E') = \dfrac{\sqrt{2}\mathbb{Q}_{2,1}^{(1,-1;a)}(E')\mathbb{Q}_{0}^{(s)}(A')}{2}$

z86 $\mathbb{Q}_{2,2}^{(1,-1;c)}(E') = \dfrac{\sqrt{2}\mathbb{Q}_{2,2}^{(1,-1;a)}(E')\mathbb{Q}_{0}^{(s)}(A')}{2}$

z87 $\mathbb{Q}_{3,1}^{(1,-1;c)}(E') = \dfrac{\sqrt{7}\mathbb{Q}_{2,1}^{(1,-1;a)}(E')\mathbb{Q}_{1,1}^{(s)}(E')}{14} - \dfrac{\sqrt{7}\mathbb{Q}_{2,2}^{(1,-1;a)}(E')\mathbb{Q}_{1,2}^{(s)}(E')}{14} + \dfrac{\sqrt{21}\mathbb{Q}_{2}^{(1,-1;a)}(A')\mathbb{Q}_{1,1}^{(s)}(E')}{7}$

z88 $\mathbb{Q}_{3,2}^{(1,-1;c)}(E') = -\dfrac{\sqrt{7}\mathbb{Q}_{2,1}^{(1,-1;a)}(E')\mathbb{Q}_{1,2}^{(s)}(E')}{14} - \dfrac{\sqrt{7}\mathbb{Q}_{2,2}^{(1,-1;a)}(E')\mathbb{Q}_{1,1}^{(s)}(E')}{14} + \dfrac{\sqrt{21}\mathbb{Q}_{2}^{(1,-1;a)}(A')\mathbb{Q}_{1,2}^{(s)}(E')}{7}$

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

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

z91 $\mathbb{Q}_{1,1}^{(1,1;c)}(E') = \dfrac{\sqrt{2}\mathbb{Q}_{0}^{(1,1;a)}(A')\mathbb{Q}_{1,1}^{(s)}(E')}{2}$

z92 $\mathbb{Q}_{1,2}^{(1,1;c)}(E') = \dfrac{\sqrt{2}\mathbb{Q}_{0}^{(1,1;a)}(A')\mathbb{Q}_{1,2}^{(s)}(E')}{2}$

z93 $\mathbb{Q}_{2,1}^{(c)}(E'') = \dfrac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E'')\mathbb{Q}_{0}^{(s)}(A')}{2}$

z94 $\mathbb{Q}_{2,2}^{(c)}(E'') = \dfrac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E'')\mathbb{Q}_{0}^{(s)}(A')}{2}$

z95 $\mathbb{Q}_{3,1}^{(c)}(E'') = \dfrac{\mathbb{Q}_{2,1}^{(a)}(E'')\mathbb{Q}_{1,1}^{(s)}(E')}{2} - \dfrac{\mathbb{Q}_{2,2}^{(a)}(E'')\mathbb{Q}_{1,2}^{(s)}(E')}{2}$

$\boxed{\text{z96}}$ $\quad \mathbb{Q}_{3,2}^{(c)}(E'') = -\dfrac{\mathbb{Q}_{2,1}^{(a)}(E'')\mathbb{Q}_{1,2}^{(s)}(E')}{2} - \dfrac{\mathbb{Q}_{2,2}^{(a)}(E'')\mathbb{Q}_{1,1}^{(s)}(E')}{2}$

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

$\boxed{\text{z142}}$ $\quad \mathbb{Q}_{2,2}^{(1,-1;c)}(E'') = \dfrac{\sqrt{2}\mathbb{Q}_{2,2}^{(1,-1;a)}(E'')\mathbb{Q}_{0}^{(s)}(A')}{2}$

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

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

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

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

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

$\boxed{\text{z148}}$ $\quad \mathbb{G}_{0}^{(1,0;c)}(A'') = \dfrac{\sqrt{2}\mathbb{G}_{1,1}^{(1,0;a)}(E'')\mathbb{Q}_{1,1}^{(s)}(E')}{2} + \dfrac{\sqrt{2}\mathbb{G}_{1,2}^{(1,0;a)}(E'')\mathbb{Q}_{1,2}^{(s)}(E')}{2}$

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

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

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

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

- 'H1'-'O' bond-cluster

* bra: $\langle s, \uparrow |$, $\langle s, \downarrow |$
* ket: $|s, \uparrow \rangle$, $|s, \downarrow \rangle$
* wyckoff: `3a@3b`

z19 $\quad \mathbb{Q}_0^{(c)}(A') = \mathbb{Q}_0^{(a)}(A')\mathbb{Q}_0^{(b)}(A')$

z20 $\quad \mathbb{Q}_1^{(1,-1;c)}(A'') = \dfrac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E'')\mathbb{T}_{1,2}^{(b)}(E')}{2} - \dfrac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E'')\mathbb{T}_{1,1}^{(b)}(E')}{2}$

z47 $\quad \mathbb{Q}_{1,1}^{(c)}(E') = \dfrac{\sqrt{2}\mathbb{Q}_0^{(a)}(A')\mathbb{Q}_{1,1}^{(b)}(E')}{2}$

z48 $\quad \mathbb{Q}_{1,2}^{(c)}(E') = \dfrac{\sqrt{2}\mathbb{Q}_0^{(a)}(A')\mathbb{Q}_{1,2}^{(b)}(E')}{2}$

z97 $\quad \mathbb{Q}_{1,1}^{(1,-1;c)}(E') = -\dfrac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(A')\mathbb{T}_{1,2}^{(b)}(E')}{2}$

z98 $\quad \mathbb{Q}_{1,2}^{(1,-1;c)}(E') = \dfrac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(A')\mathbb{T}_{1,1}^{(b)}(E')}{2}$

z99 $\quad \mathbb{G}_1^{(1,-1;c)}(A') = \mathbb{M}_1^{(1,-1;a)}(A')\mathbb{T}_0^{(b)}(A')$

z100 $\quad \mathbb{G}_0^{(1,-1;c)}(A'') = \dfrac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E'')\mathbb{T}_{1,1}^{(b)}(E')}{2} + \dfrac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E'')\mathbb{T}_{1,2}^{(b)}(E')}{2}$

z153 $\quad \mathbb{G}_{1,1}^{(1,-1;c)}(E'') = \dfrac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E'')\mathbb{T}_0^{(b)}(A')}{2}$

z154 $\quad \mathbb{G}_{1,2}^{(1,-1;c)}(E'') = \dfrac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E'')\mathbb{T}_0^{(b)}(A')}{2}$

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

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

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

$\boxed{\text{z21}}$ $\quad \mathbb{Q}_0^{(c)}(A') = \dfrac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{2} + \dfrac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{2}$

$\boxed{\text{z22}}$ $\quad \mathbb{Q}_2^{(1,-1;c)}(A') = -\dfrac{\sqrt{2}\mathbb{G}_{2,1}^{(1,-1;a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{2} - \dfrac{\sqrt{2}\mathbb{G}_{2,2}^{(1,-1;a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{2}$

$\boxed{\text{z23}}$ $\quad \mathbb{Q}_0^{(1,0;c)}(A') = \dfrac{\sqrt{2}\mathbb{Q}_{1,1}^{(1,0;a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{2} + \dfrac{\sqrt{2}\mathbb{Q}_{1,2}^{(1,0;a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{2}$

$\boxed{\text{z24}}$ $\quad \mathbb{Q}_1^{(c)}(A'') = \mathbb{Q}_1^{(a)}(A'')\mathbb{Q}_0^{(b)}(A')$

$\boxed{\text{z25}}$ $\quad \mathbb{Q}_1^{(1,0;c)}(A'') = \mathbb{Q}_1^{(1,0;a)}(A'')\mathbb{Q}_0^{(b)}(A')$

$\boxed{\text{z26}}$ $\quad \mathbb{Q}_{1,1}^{(c)}(E') = \dfrac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E')\mathbb{Q}_0^{(b)}(A')}{2}$

$\boxed{\text{z49}}$ $\quad \mathbb{Q}_{1,2}^{(c)}(E') = \dfrac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E')\mathbb{Q}_0^{(b)}(A')}{2}$

$\boxed{\text{z50}}$ $\quad \mathbb{Q}_{2,1}^{(c)}(E') = \dfrac{\mathbb{Q}_{1,1}^{(a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{2} - \dfrac{\mathbb{Q}_{1,2}^{(a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{2}$

$\boxed{\text{z51}}$ $\quad \mathbb{Q}_{2,2}^{(c)}(E') = -\dfrac{\mathbb{Q}_{1,1}^{(a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{2} - \dfrac{\mathbb{Q}_{1,2}^{(a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{2}$

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

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

$\boxed{\text{z54}}$ $\quad \mathbb{Q}_{1,1}^{(1,0;c)}(E') = \dfrac{\sqrt{2}\mathbb{Q}_{1,1}^{(1,0;a)}(E')\mathbb{Q}_0^{(b)}(A')}{2}$

$\boxed{\text{z101}}$ $\quad \mathbb{Q}_{1,2}^{(1,0;c)}(E') = \dfrac{\sqrt{2}\mathbb{Q}_{1,2}^{(1,0;a)}(E')\mathbb{Q}_0^{(b)}(A')}{2}$

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$$\boxed{\text{z102}} \quad \mathbb{Q}_{2,1}^{(1,0;c)}(E') = \frac{\mathbb{Q}_{1,1}^{(1,0;a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{2} - \frac{\mathbb{Q}_{1,2}^{(1,0;a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{2}$$

$$\boxed{\text{z103}} \quad \mathbb{Q}_{2,2}^{(1,0;c)}(E') = -\frac{\mathbb{Q}_{1,1}^{(1,0;a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{2} - \frac{\mathbb{Q}_{1,2}^{(1,0;a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{2}$$

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

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

$$\boxed{\text{z106}} \quad \mathbb{Q}_{2,1}^{(1,-1;c)}(E'') = \frac{\sqrt{10}\mathbb{G}_{2,1}^{(1,-1;a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{10} - \frac{\sqrt{10}\mathbb{G}_{2,2}^{(1,-1;a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{10} + \frac{\sqrt{30}\mathbb{G}_{2}^{(1,-1;a)}(A'')\mathbb{Q}_{1,1}^{(b)}(E')}{10}$$

$$\boxed{\text{z107}} \quad \mathbb{Q}_{2,2}^{(1,-1;c)}(E'') = -\frac{\sqrt{10}\mathbb{G}_{2,1}^{(1,-1;a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{10} - \frac{\sqrt{10}\mathbb{G}_{2,2}^{(1,-1;a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{10} + \frac{\sqrt{30}\mathbb{G}_{2}^{(1,-1;a)}(A'')\mathbb{Q}_{1,2}^{(b)}(E')}{10}$$

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

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

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

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

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

$$\boxed{\text{z157}} \quad \mathbb{G}_{2}^{(1,-1;c)}(A'') = \mathbb{G}_{2}^{(1,-1;a)}(A'')\mathbb{Q}_{0}^{(b)}(A')$$

$$\boxed{\text{z158}} \quad \mathbb{G}_{3}^{(1,-1;c)}(A'',1) = \frac{\sqrt{2}\mathbb{G}_{2,1}^{(1,-1;a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{2} - \frac{\sqrt{2}\mathbb{G}_{2,2}^{(1,-1;a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{2}$$

$$\boxed{\text{z159}} \quad \mathbb{G}_{3}^{(1,-1;c)}(A'',2) = \frac{\sqrt{2}\mathbb{G}_{2,1}^{(1,-1;a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{2} + \frac{\sqrt{2}\mathbb{G}_{2,2}^{(1,-1;a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{2}$$

$\boxed{\text{z160}}$ $\mathbb{G}_0^{(1,1;c)}(A'') = \mathbb{G}_0^{(1,1;a)}(A'')\mathbb{Q}_0^{(b)}(A')$

$\boxed{\text{z161}}$ $\mathbb{G}_{2,1}^{(1,-1;c)}(E') = \dfrac{\sqrt{2}\mathbb{G}_{2,1}^{(1,-1;a)}(E')\mathbb{Q}_0^{(b)}(A')}{2}$

$\boxed{\text{z162}}$ $\mathbb{G}_{2,2}^{(1,-1;c)}(E') = \dfrac{\sqrt{2}\mathbb{G}_{2,2}^{(1,-1;a)}(E')\mathbb{Q}_0^{(b)}(A')}{2}$

$\boxed{\text{z163}}$ $\mathbb{G}_{1,1}^{(1,-1;c)}(E'') = \dfrac{\sqrt{15}\mathbb{G}_{2,1}^{(1,-1;a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{10} - \dfrac{\sqrt{15}\mathbb{G}_{2,2}^{(1,-1;a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{10} - \dfrac{\sqrt{5}\mathbb{G}_2^{(1,-1;a)}(A'')\mathbb{Q}_{1,1}^{(b)}(E')}{5}$

$\boxed{\text{z164}}$ $\mathbb{G}_{1,2}^{(1,-1;c)}(E'') = -\dfrac{\sqrt{15}\mathbb{G}_{2,1}^{(1,-1;a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{10} - \dfrac{\sqrt{15}\mathbb{G}_{2,2}^{(1,-1;a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{10} - \dfrac{\sqrt{5}\mathbb{G}_2^{(1,-1;a)}(A'')\mathbb{Q}_{1,2}^{(b)}(E')}{5}$

$\boxed{\text{z165}}$ $\mathbb{G}_{2,1}^{(1,-1;c)}(E'') = \dfrac{\sqrt{2}\mathbb{G}_{2,1}^{(1,-1;a)}(E'')\mathbb{Q}_0^{(b)}(A')}{2}$

$\boxed{\text{z166}}$ $\mathbb{G}_{2,2}^{(1,-1;c)}(E'') = \dfrac{\sqrt{2}\mathbb{G}_{2,2}^{(1,-1;a)}(E'')\mathbb{Q}_0^{(b)}(A')}{2}$

$\boxed{\text{z167}}$ $\mathbb{G}_{1,1}^{(1,1;c)}(E'') = \dfrac{\sqrt{2}\mathbb{G}_0^{(1,1;a)}(A'')\mathbb{Q}_{1,1}^{(b)}(E')}{2}$

$\boxed{\text{z168}}$ $\mathbb{G}_{1,2}^{(1,1;c)}(E'') = \dfrac{\sqrt{2}\mathbb{G}_0^{(1,1;a)}(A'')\mathbb{Q}_{1,2}^{(b)}(E')}{2}$

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

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

$\boxed{\text{z28}}$ $\mathbb{Q}_1^{(1,-1;c)}(A'') = \dfrac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E'')\mathbb{T}_{1,2}^{(b)}(E')}{2} - \dfrac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E'')\mathbb{T}_{1,1}^{(b)}(E')}{2}$

$\boxed{\text{z55}}$ $\mathbb{Q}_{1,1}^{(c)}(E') = \dfrac{\sqrt{2}\mathbb{Q}_0^{(a)}(A')\mathbb{Q}_{1,1}^{(b)}(E')}{2}$

$\boxed{\text{z56}}$ $\mathbb{Q}_{1,2}^{(c)}(E') = \dfrac{\sqrt{2}\mathbb{Q}_0^{(a)}(A')\mathbb{Q}_{1,2}^{(b)}(E')}{2}$

$\boxed{\text{z113}}$ $\mathbb{Q}_{1,1}^{(1,-1;c)}(E') = -\dfrac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(A')\mathbb{T}_{1,2}^{(b)}(E')}{2}$

$\boxed{\text{z114}}$ $\mathbb{Q}_{1,2}^{(1,-1;c)}(E') = \dfrac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(A')\mathbb{T}_{1,1}^{(b)}(E')}{2}$

$\boxed{\text{z115}}$ $\mathbb{G}_1^{(1,-1;c)}(A') = \mathbb{M}_1^{(1,-1;a)}(A')\mathbb{T}_0^{(b)}(A')$

$\boxed{\text{z116}}$ $\mathbb{G}_0^{(1,-1;c)}(A'') = \dfrac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E'')\mathbb{T}_{1,1}^{(b)}(E')}{2} + \dfrac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E'')\mathbb{T}_{1,2}^{(b)}(E')}{2}$

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

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

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

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

- 'H2'-'O' bond-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: `3a@3b`

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

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

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

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$$\boxed{\text{z32}} \quad \mathbb{Q}_1^{(c)}(A'') = \mathbb{Q}_1^{(a)}(A'')\mathbb{Q}_0^{(b)}(A')$$

$$\boxed{\text{z33}} \quad \mathbb{Q}_1^{(1,0;c)}(A'') = \mathbb{Q}_1^{(1,0;a)}(A'')\mathbb{Q}_0^{(b)}(A')$$

$$\boxed{\text{z34}} \quad \mathbb{Q}_{1,1}^{(c)}(E') = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E')\mathbb{Q}_0^{(b)}(A')}{2}$$

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

$$\boxed{\text{z58}} \quad \mathbb{Q}_{2,1}^{(c)}(E') = \frac{\mathbb{Q}_{1,1}^{(a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{2} - \frac{\mathbb{Q}_{1,2}^{(a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{2}$$

$$\boxed{\text{z59}} \quad \mathbb{Q}_{2,2}^{(c)}(E') = -\frac{\mathbb{Q}_{1,1}^{(a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{2} - \frac{\mathbb{Q}_{1,2}^{(a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{2}$$

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

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

$$\boxed{\text{z62}} \quad \mathbb{Q}_{1,1}^{(1,0;c)}(E') = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(1,0;a)}(E')\mathbb{Q}_0^{(b)}(A')}{2}$$

$$\boxed{\text{z117}} \quad \mathbb{Q}_{1,2}^{(1,0;c)}(E') = \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(1,0;a)}(E')\mathbb{Q}_0^{(b)}(A')}{2}$$

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

$$\boxed{\text{z119}} \quad \mathbb{Q}_{2,2}^{(1,0;c)}(E') = -\frac{\mathbb{Q}_{1,1}^{(1,0;a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{2} - \frac{\mathbb{Q}_{1,2}^{(1,0;a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{2}$$

$$\boxed{\text{z120}} \quad \mathbb{Q}_{2,1}^{(c)}(E'') = \frac{\sqrt{2}\mathbb{Q}_1^{(a)}(A'')\mathbb{Q}_{1,2}^{(b)}(E')}{2}$$

$$\boxed{\text{z121}} \quad \mathbb{Q}_{2,2}^{(c)}(E'') = -\frac{\sqrt{2}\mathbb{Q}_1^{(a)}(A'')\mathbb{Q}_{1,1}^{(b)}(E')}{2}$$

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$\boxed{\text{z122}}$ $\mathbb{Q}_{2,1}^{(1,-1;c)}(E'') = \dfrac{\sqrt{10}\mathbb{G}_{2,1}^{(1,-1;a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{10} - \dfrac{\sqrt{10}\mathbb{G}_{2,2}^{(1,-1;a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{10} + \dfrac{\sqrt{30}\mathbb{G}_2^{(1,-1;a)}(A'')\mathbb{Q}_{1,1}^{(b)}(E')}{10}$

$\boxed{\text{z123}}$ $\mathbb{Q}_{2,2}^{(1,-1;c)}(E'') = -\dfrac{\sqrt{10}\mathbb{G}_{2,1}^{(1,-1;a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{10} - \dfrac{\sqrt{10}\mathbb{G}_{2,2}^{(1,-1;a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{10} + \dfrac{\sqrt{30}\mathbb{G}_2^{(1,-1;a)}(A'')\mathbb{Q}_{1,2}^{(b)}(E')}{10}$

$\boxed{\text{z124}}$ $\mathbb{Q}_{2,1}^{(1,0;c)}(E'') = \dfrac{\sqrt{2}\mathbb{Q}_1^{(1,0;a)}(A'')\mathbb{Q}_{1,2}^{(b)}(E')}{2}$

$\boxed{\text{z125}}$ $\mathbb{Q}_{2,2}^{(1,0;c)}(E'') = -\dfrac{\sqrt{2}\mathbb{Q}_1^{(1,0;a)}(A'')\mathbb{Q}_{1,1}^{(b)}(E')}{2}$

$\boxed{\text{z126}}$ $\mathbb{G}_1^{(c)}(A') = \dfrac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{2} - \dfrac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{2}$

$\boxed{\text{z127}}$ $\mathbb{G}_1^{(1,-1;c)}(A') = \dfrac{\sqrt{2}\mathbb{G}_{2,1}^{(1,-1;a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{2} - \dfrac{\sqrt{2}\mathbb{G}_{2,2}^{(1,-1;a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{2}$

$\boxed{\text{z128}}$ $\mathbb{G}_1^{(1,0;c)}(A') = \dfrac{\sqrt{2}\mathbb{Q}_{1,1}^{(1,0;a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{2} - \dfrac{\sqrt{2}\mathbb{Q}_{1,2}^{(1,0;a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{2}$

$\boxed{\text{z173}}$ $\mathbb{G}_2^{(1,-1;c)}(A'') = \mathbb{G}_2^{(1,-1;a)}(A'')\mathbb{Q}_0^{(b)}(A')$

$\boxed{\text{z174}}$ $\mathbb{G}_3^{(1,-1;c)}(A'',1) = \dfrac{\sqrt{2}\mathbb{G}_{2,1}^{(1,-1;a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{2} - \dfrac{\sqrt{2}\mathbb{G}_{2,2}^{(1,-1;a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{2}$

$\boxed{\text{z175}}$ $\mathbb{G}_3^{(1,-1;c)}(A'',2) = \dfrac{\sqrt{2}\mathbb{G}_{2,1}^{(1,-1;a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{2} + \dfrac{\sqrt{2}\mathbb{G}_{2,2}^{(1,-1;a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{2}$

$\boxed{\text{z176}}$ $\mathbb{G}_0^{(1,1;c)}(A'') = \mathbb{G}_0^{(1,1;a)}(A'')\mathbb{Q}_0^{(b)}(A')$

$\boxed{\text{z177}}$ $\mathbb{G}_{2,1}^{(1,-1;c)}(E') = \dfrac{\sqrt{2}\mathbb{G}_{2,1}^{(1,-1;a)}(E')\mathbb{Q}_0^{(b)}(A')}{2}$

$\boxed{\text{z178}}$ $\mathbb{G}_{2,2}^{(1,-1;c)}(E') = \dfrac{\sqrt{2}\mathbb{G}_{2,2}^{(1,-1;a)}(E')\mathbb{Q}_0^{(b)}(A')}{2}$

$\boxed{\text{z179}}$ $\mathbb{G}_{1,1}^{(1,-1;c)}(E'') = \dfrac{\sqrt{15}\mathbb{G}_{2,1}^{(1,-1;a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{10} - \dfrac{\sqrt{15}\mathbb{G}_{2,2}^{(1,-1;a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{10} - \dfrac{\sqrt{5}\mathbb{G}_2^{(1,-1;a)}(A'')\mathbb{Q}_{1,1}^{(b)}(E')}{5}$

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

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

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

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

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

—— **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: $|p_x,\uparrow\rangle\,,\ |p_x,\downarrow\rangle\,,\ |p_y,\uparrow\rangle\,,\ |p_y,\downarrow\rangle\,,\ |p_z,\uparrow\rangle\,,\ |p_z,\downarrow\rangle$

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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$$\boxed{\text{x30}} \quad \mathbb{Q}_2^{(a)}(A') = \begin{bmatrix} -\frac{\sqrt{3}}{6} & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{3}}{6} & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{3}}{6} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{3}}{6} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{3}}{3} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{3}}{3} \end{bmatrix}$$

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

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

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

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

$$\boxed{\text{x35}} \quad \mathbb{Q}_2^{(1,-1;a)}(A') = \begin{bmatrix} 0 & 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 & -\frac{\sqrt{6}}{12} \\ 0 & 0 & 0 & \frac{\sqrt{6}i}{6} & \frac{\sqrt{6}}{12} & 0 \\ \frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 & \frac{\sqrt{6}i}{12} \\ 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 & \frac{\sqrt{6}i}{12} & 0 \\ 0 & \frac{\sqrt{6}}{12} & 0 & -\frac{\sqrt{6}i}{12} & 0 & 0 \\ -\frac{\sqrt{6}}{12} & 0 & -\frac{\sqrt{6}i}{12} & 0 & 0 & 0 \end{bmatrix}$$

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

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

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

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

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

$$\boxed{\text{x41}} \quad \mathbb{G}_1^{(1,0;a)}(A') = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{2}i}{4} \\ 0 & 0 & 0 & 0 & \frac{\sqrt{2}i}{4} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{2}}{4} \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{2}}{4} & 0 \\ 0 & -\frac{\sqrt{2}i}{4} & 0 & -\frac{\sqrt{2}}{4} & 0 & 0 \\ -\frac{\sqrt{2}i}{4} & 0 & \frac{\sqrt{2}}{4} & 0 & 0 & 0 \end{bmatrix}$$

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

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

$$\boxed{\text{x44}} \quad \mathbb{M}_1^{(a)}(A') = \begin{bmatrix} 0 & 0 & -\frac{i}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{i}{2} & 0 & 0 \\ \frac{i}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{i}{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

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

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

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

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

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

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

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

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$$\boxed{\text{x57}} \quad \mathbb{M}_1^{(1,1;a)}(A') = \begin{bmatrix} -\frac{\sqrt{30}}{30} & 0 & 0 & 0 & 0 & \frac{\sqrt{30}}{20} \\ 0 & \frac{\sqrt{30}}{30} & 0 & 0 & \frac{\sqrt{30}}{20} & 0 \\ 0 & 0 & -\frac{\sqrt{30}}{30} & 0 & 0 & -\frac{\sqrt{30}i}{20} \\ 0 & 0 & 0 & \frac{\sqrt{30}}{30} & \frac{\sqrt{30}i}{20} & 0 \\ 0 & \frac{\sqrt{30}}{20} & 0 & -\frac{\sqrt{30}i}{20} & \frac{\sqrt{30}}{15} & 0 \\ \frac{\sqrt{30}}{20} & 0 & \frac{\sqrt{30}i}{20} & 0 & 0 & -\frac{\sqrt{30}}{15} \end{bmatrix}$$

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

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

$$\boxed{\text{x60}} \quad \mathbb{T}_2^{(1,0;a)}(A') = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{2}i}{4} \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{2}i}{4} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{2}}{4} \\ 0 & 0 & 0 & 0 & \frac{\sqrt{2}}{4} & 0 \\ 0 & \frac{\sqrt{2}i}{4} & 0 & \frac{\sqrt{2}}{4} & 0 & 0 \\ -\frac{\sqrt{2}i}{4} & 0 & \frac{\sqrt{2}}{4} & 0 & 0 & 0 \end{bmatrix}$$

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

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

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

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

Cluster SAMB

- Site cluster

** Wyckoff: 1o

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

** Wyckoff: 3b

$\boxed{\text{y2}} \quad \mathbb{Q}^{(s)}_0(A') = \left[\frac{\sqrt{3}}{3}, \frac{\sqrt{3}}{3}, \frac{\sqrt{3}}{3} \right]$

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

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

- Bond cluster

** Wyckoff: `3a@3b`

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

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

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

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

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

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

━━ **Site and Bond** ━━

Table 5: Orbital of each site

#	site	orbital
1	H1	$\lvert s, \uparrow \rangle, \lvert s, \downarrow \rangle$

continued …

Table 5

#	site	orbital
2	H2	$\lvert s,\uparrow\rangle$, $\lvert s,\downarrow\rangle$
3	O	$\lvert s,\uparrow\rangle$, $\lvert s,\downarrow\rangle$, $\lvert p_x,\uparrow\rangle$, $\lvert p_x,\downarrow\rangle$, $\lvert p_y,\uparrow\rangle$, $\lvert p_y,\downarrow\rangle$, $\lvert p_z,\uparrow\rangle$, $\lvert p_z,\downarrow\rangle$

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 (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]

— **Bond in Unit Cell** —

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

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

SL	vector (v)	center (c)	mapping	head	tail	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, $|v|=$ 0.16667 (cartesian)

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