

Model for “C3h”

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General Condition

- Basis type: **lgs**
- SAMB selection:
 - Type: [Q, G]
 - Rank: [0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11]
 - Irrep.: [A' , 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):
 - $\mathbf{a}_1 = [1.00000, 0.00000, 0.00000]$
 - $\mathbf{a}_2 = [-0.50000, 0.86603, 0.00000]$
 - $\mathbf{a}_3 = [0.00000, 0.00000, 1.00000]$

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	-	-	$-\frac{z(3x^2+3y^2-2z^2)}{2}$
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	-	-	$-\frac{x^2}{2} - \frac{y^2}{2} + z^2$

continued ...

Table 2

#	symbol	irrep.	rank	X	multiplicity	component	symmetry
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	$-\frac{\sqrt{6}y(x^2+y^2-4z^2)}{4}$
30	$\mathbb{Q}_{3,1}(E'')$	E''	3	Q, T	-	1	$\sqrt{15}xyz$

continued ...

Table 2

#	symbol	irrep.	rank	X	multiplicity	component	symmetry
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
$ s\rangle$	1
$ p_x\rangle$	x
$ p_y\rangle$	y
$ p_z\rangle$	z

SAMB: 184 (all 184)

• H1 : 'H1' site-cluster

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

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

• H2 : 'H2' site-cluster

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

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

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

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

• 0 : '0' site-cluster

* bra: $\langle s, \uparrow |, \langle s, \downarrow |$

* ket: $|s, \uparrow\rangle, |s, \downarrow\rangle$

* wyckoff: **3b**

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

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

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

• **0 : '0' 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**

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

$$\boxed{\text{z131}} \quad \mathbb{Q}_{2,1}^{(1,-1;c)}(E'') = \frac{\sqrt{10}\mathbb{G}_{2,1}^{(1,-1;a)}(E'')\mathbb{Q}_{1,1}^{(s)}(E')}{10} - \frac{\sqrt{10}\mathbb{G}_{2,2}^{(1,-1;a)}(E'')\mathbb{Q}_{1,2}^{(s)}(E')}{10} + \frac{\sqrt{30}\mathbb{G}_2^{(1,-1;a)}(A'')\mathbb{Q}_{1,1}^{(s)}(E')}{10}$$

$$\boxed{\text{z132}} \quad \mathbb{Q}_{2,2}^{(1,-1;c)}(E'') = -\frac{\sqrt{10}\mathbb{G}_{2,1}^{(1,-1;a)}(E'')\mathbb{Q}_{1,2}^{(s)}(E')}{10} - \frac{\sqrt{10}\mathbb{G}_{2,2}^{(1,-1;a)}(E'')\mathbb{Q}_{1,1}^{(s)}(E')}{10} + \frac{\sqrt{30}\mathbb{G}_2^{(1,-1;a)}(A'')\mathbb{Q}_{1,2}^{(s)}(E')}{10}$$

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

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

$$\boxed{\text{z135}} \quad \mathbb{G}_{1,1}^{(1,-1;c)}(E'') = \frac{\sqrt{15}\mathbb{G}_{2,1}^{(1,-1;a)}(E'')\mathbb{Q}_{1,1}^{(s)}(E')}{10} - \frac{\sqrt{15}\mathbb{G}_{2,2}^{(1,-1;a)}(E'')\mathbb{Q}_{1,2}^{(s)}(E')}{10} - \frac{\sqrt{5}\mathbb{G}_2^{(1,-1;a)}(A'')\mathbb{Q}_{1,1}^{(s)}(E')}{5}$$

$$\boxed{\text{z136}} \quad \mathbb{G}_{1,2}^{(1,-1;c)}(E'') = -\frac{\sqrt{15}\mathbb{G}_{2,1}^{(1,-1;a)}(E'')\mathbb{Q}_{1,2}^{(s)}(E')}{10} - \frac{\sqrt{15}\mathbb{G}_{2,2}^{(1,-1;a)}(E'')\mathbb{Q}_{1,1}^{(s)}(E')}{10} - \frac{\sqrt{5}\mathbb{G}_2^{(1,-1;a)}(A'')\mathbb{Q}_{1,2}^{(s)}(E')}{5}$$

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

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

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

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

- 0 : '0' 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**

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

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

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

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

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

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

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

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

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

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

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

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

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

$$\boxed{\text{z45}} \quad \mathbb{G}_2^{(1,-1;c)}(A'') = -\frac{\sqrt{2}\mathbb{Q}_{2,1}^{(1,-1;a)}(E'')\mathbb{Q}_{1,1}^{(s)}(E')}{2} - \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(1,-1;a)}(E'')\mathbb{Q}_{1,2}^{(s)}(E')}{2}$$

$$\boxed{\text{z46}} \quad \mathbb{G}_0^{(1,0;c)}(A'') = \frac{\sqrt{2}\mathbb{G}_{1,1}^{(1,0;a)}(E'')\mathbb{Q}_{1,1}^{(s)}(E')}{2} + \frac{\sqrt{2}\mathbb{G}_{1,2}^{(1,0;a)}(E'')\mathbb{Q}_{1,2}^{(s)}(E')}{2}$$

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

$$\boxed{\text{z80}} \quad \mathbb{Q}_{1,2}^{(c)}(E', a) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A')\mathbb{Q}_{1,2}^{(s)}(E')}{2}$$

$$\boxed{\text{z81}} \quad \mathbb{Q}_{1,1}^{(c)}(E', b) = \frac{\sqrt{42}\mathbb{Q}_{2,1}^{(a)}(E')\mathbb{Q}_{1,1}^{(s)}(E')}{14} - \frac{\sqrt{42}\mathbb{Q}_{2,2}^{(a)}(E')\mathbb{Q}_{1,2}^{(s)}(E')}{14} - \frac{\sqrt{14}\mathbb{Q}_2^{(a)}(A')\mathbb{Q}_{1,1}^{(s)}(E')}{14}$$

$$\boxed{\text{z82}} \quad \mathbb{Q}_{1,2}^{(c)}(E', b) = -\frac{\sqrt{42}\mathbb{Q}_{2,1}^{(a)}(E')\mathbb{Q}_{1,2}^{(s)}(E')}{14} - \frac{\sqrt{42}\mathbb{Q}_{2,2}^{(a)}(E')\mathbb{Q}_{1,1}^{(s)}(E')}{14} - \frac{\sqrt{14}\mathbb{Q}_2^{(a)}(A')\mathbb{Q}_{1,2}^{(s)}(E')}{14}$$

$$\boxed{\text{z83}} \quad \mathbb{Q}_{2,1}^{(c)}(E') = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E')\mathbb{Q}_0^{(s)}(A')}{2}$$

$$\boxed{\text{z84}} \quad \mathbb{Q}_{2,2}^{(c)}(E') = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E')\mathbb{Q}_0^{(s)}(A')}{2}$$

$$\boxed{\text{z85}} \quad \mathbb{Q}_{3,1}^{(c)}(E') = \frac{\sqrt{7}\mathbb{Q}_{2,1}^{(a)}(E')\mathbb{Q}_{1,1}^{(s)}(E')}{14} - \frac{\sqrt{7}\mathbb{Q}_{2,2}^{(a)}(E')\mathbb{Q}_{1,2}^{(s)}(E')}{14} + \frac{\sqrt{21}\mathbb{Q}_2^{(a)}(A')\mathbb{Q}_{1,1}^{(s)}(E')}{7}$$

$$\boxed{\text{z86}} \quad \mathbb{Q}_{3,2}^{(c)}(E') = -\frac{\sqrt{7}\mathbb{Q}_{2,1}^{(a)}(E')\mathbb{Q}_{1,2}^{(s)}(E')}{14} - \frac{\sqrt{7}\mathbb{Q}_{2,2}^{(a)}(E')\mathbb{Q}_{1,1}^{(s)}(E')}{14} + \frac{\sqrt{21}\mathbb{Q}_2^{(a)}(A')\mathbb{Q}_{1,2}^{(s)}(E')}{7}$$

$$\boxed{\text{z87}} \quad \mathbb{Q}_{1,1}^{(1,-1;c)}(E') = \frac{\sqrt{42}\mathbb{Q}_{2,1}^{(1,-1;a)}(E')\mathbb{Q}_{1,1}^{(s)}(E')}{14} - \frac{\sqrt{42}\mathbb{Q}_{2,2}^{(1,-1;a)}(E')\mathbb{Q}_{1,2}^{(s)}(E')}{14} - \frac{\sqrt{14}\mathbb{Q}_2^{(1,-1;a)}(A')\mathbb{Q}_{1,1}^{(s)}(E')}{14}$$

$$\boxed{\text{z88}} \quad \mathbb{Q}_{1,2}^{(1,-1;c)}(E') = -\frac{\sqrt{42}\mathbb{Q}_{2,1}^{(1,-1;a)}(E')\mathbb{Q}_{1,2}^{(s)}(E')}{14} - \frac{\sqrt{42}\mathbb{Q}_{2,2}^{(1,-1;a)}(E')\mathbb{Q}_{1,1}^{(s)}(E')}{14} - \frac{\sqrt{14}\mathbb{Q}_2^{(1,-1;a)}(A')\mathbb{Q}_{1,2}^{(s)}(E')}{14}$$

$$\boxed{\text{z89}} \quad \mathbb{Q}_{2,1}^{(1,-1;c)}(E') = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(1,-1;a)}(E')\mathbb{Q}_0^{(s)}(A')}{2}$$

$$\boxed{\text{z90}} \quad \mathbb{Q}_{2,2}^{(1,-1;c)}(E') = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(1,-1;a)}(E')\mathbb{Q}_0^{(s)}(A')}{2}$$

$$\boxed{\text{z91}} \quad \mathbb{Q}_{3,1}^{(1,-1;c)}(E') = \frac{\sqrt{7}\mathbb{Q}_{2,1}^{(1,-1;a)}(E')\mathbb{Q}_{1,1}^{(s)}(E')}{14} - \frac{\sqrt{7}\mathbb{Q}_{2,2}^{(1,-1;a)}(E')\mathbb{Q}_{1,2}^{(s)}(E')}{14} + \frac{\sqrt{21}\mathbb{Q}_2^{(1,-1;a)}(A')\mathbb{Q}_{1,1}^{(s)}(E')}{7}$$

$$\boxed{\text{z92}} \quad \mathbb{Q}_{3,2}^{(1,-1;c)}(E') = -\frac{\sqrt{7}\mathbb{Q}_{2,1}^{(1,-1;a)}(E')\mathbb{Q}_{1,2}^{(s)}(E')}{14} - \frac{\sqrt{7}\mathbb{Q}_{2,2}^{(1,-1;a)}(E')\mathbb{Q}_{1,1}^{(s)}(E')}{14} + \frac{\sqrt{21}\mathbb{Q}_2^{(1,-1;a)}(A')\mathbb{Q}_{1,2}^{(s)}(E')}{7}$$

$$\boxed{\text{z93}} \quad \mathbb{Q}_{1,1}^{(1,0;c)}(E') = -\frac{\sqrt{2}\mathbb{G}_1^{(1,0;a)}(A')\mathbb{Q}_{1,2}^{(s)}(E')}{2}$$

$$\boxed{\text{z94}} \quad \mathbb{Q}_{1,2}^{(1,0;c)}(E') = \frac{\sqrt{2}\mathbb{G}_1^{(1,0;a)}(A')\mathbb{Q}_{1,1}^{(s)}(E')}{2}$$

$$\boxed{\text{z95}} \quad \mathbb{Q}_{1,1}^{(1,1;c)}(E') = \frac{\sqrt{2}\mathbb{Q}_0^{(1,1;a)}(A')\mathbb{Q}_{1,1}^{(s)}(E')}{2}$$

$$\boxed{\text{z96}} \quad \mathbb{Q}_{1,2}^{(1,1;c)}(E') = \frac{\sqrt{2}\mathbb{Q}_0^{(1,1;a)}(A')\mathbb{Q}_{1,2}^{(s)}(E')}{2}$$

$$\boxed{\text{z141}} \quad \mathbb{Q}_{2,1}^{(c)}(E'') = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E'')\mathbb{Q}_0^{(s)}(A')}{2}$$

$$\boxed{\text{z142}} \quad \mathbb{Q}_{2,2}^{(c)}(E'') = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E'')\mathbb{Q}_0^{(s)}(A')}{2}$$

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

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

$$\boxed{\text{z145}} \quad \mathbb{Q}_{2,1}^{(1,-1;c)}(E'') = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(1,-1;a)}(E'')\mathbb{Q}_0^{(s)}(A')}{2}$$

$$\boxed{\text{z146}} \quad \mathbb{Q}_{2,2}^{(1,-1;c)}(E'') = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(1,-1;a)}(E'')\mathbb{Q}_0^{(s)}(A')}{2}$$

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

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

$$\boxed{\text{z149}} \quad \mathbb{G}_{1,1}^{(1,0;c)}(E'') = \frac{\sqrt{2}\mathbb{G}_{1,1}^{(1,0;a)}(E'')\mathbb{Q}_0^{(s)}(A')}{2}$$

$$\boxed{\text{z150}} \quad \mathbb{G}_{1,2}^{(1,0;c)}(E'') = \frac{\sqrt{2}\mathbb{G}_{1,2}^{(1,0;a)}(E'')\mathbb{Q}_0^{(s)}(A')}{2}$$

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

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

• **0;H1_001_1 : 'H1'-'O' bond-cluster**

* bra: $\langle s, \uparrow |, \langle s, \downarrow |$

* ket: $|s, \uparrow \rangle, |s, \downarrow \rangle$

* wyckoff: **3a03b**

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

$$\boxed{\text{z20}} \quad \mathbb{G}_1^{(1,-1;c)}(A') = \mathbb{M}_1^{(1,-1;a)}(A')\mathbb{T}_0^{(b)}(A')$$

$$\boxed{\text{z47}} \quad \mathbb{Q}_1^{(1,-1;c)}(A'') = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E'')\mathbb{T}_{1,2}^{(b)}(E')}{2} - \frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E'')\mathbb{T}_{1,1}^{(b)}(E')}{2}$$

$$\boxed{\text{z48}} \quad \mathbb{G}_0^{(1,-1;c)}(A'') = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E'')\mathbb{T}_{1,1}^{(b)}(E')}{2} + \frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E'')\mathbb{T}_{1,2}^{(b)}(E')}{2}$$

$$\boxed{\text{z97}} \quad \mathbb{Q}_{1,1}^{(c)}(E') = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A')\mathbb{Q}_{1,1}^{(b)}(E')}{2}$$

$$\boxed{\text{z98}} \quad \mathbb{Q}_{1,2}^{(c)}(E') = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A')\mathbb{Q}_{1,2}^{(b)}(E')}{2}$$

$$\boxed{\text{z99}} \quad \mathbb{Q}_{1,1}^{(1,-1;c)}(E') = -\frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(A')\mathbb{T}_{1,2}^{(b)}(E')}{2}$$

$$\boxed{\text{z100}} \quad \mathbb{Q}_{1,2}^{(1,-1;c)}(E') = \frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(A')\mathbb{T}_{1,1}^{(b)}(E')}{2}$$

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

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

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

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

• **0;H1_001_1 : 'H1'-'0' 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**

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

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

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

$$\boxed{\text{z24}} \quad \mathbb{G}_1^{(c)}(A') = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{2} - \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{2}$$

$$\boxed{\text{z25}} \quad \mathbb{G}_1^{(1,-1;c)}(A') = \frac{\sqrt{2}\mathbb{G}_{2,1}^{(1,-1;a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{2} - \frac{\sqrt{2}\mathbb{G}_{2,2}^{(1,-1;a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{2}$$

$$\boxed{\text{z26}} \quad \mathbb{G}_1^{(1,0;c)}(A') = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(1,0;a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{2} - \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(1,0;a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{2}$$

$$\boxed{\text{z49}} \quad \mathbb{Q}_1^{(c)}(A'') = \mathbb{Q}_1^{(a)}(A'')\mathbb{Q}_0^{(b)}(A')$$

$$\boxed{\text{z50}} \quad \mathbb{Q}_1^{(1,0;c)}(A'') = \mathbb{Q}_1^{(1,0;a)}(A'')\mathbb{Q}_0^{(b)}(A')$$

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

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

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

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

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

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

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

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

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

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

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

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

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

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

$$\boxed{\text{z111}} \quad \mathbb{G}_{2,1}^{(1,-1;c)}(E') = \frac{\sqrt{2}\mathbb{G}_{2,1}^{(1,-1;a)}(E')\mathbb{Q}_0^{(b)}(A')}{2}$$

$$\boxed{\text{z112}} \quad \mathbb{G}_{2,2}^{(1,-1;c)}(E') = \frac{\sqrt{2}\mathbb{G}_{2,2}^{(1,-1;a)}(E')\mathbb{Q}_0^{(b)}(A')}{2}$$

$$\boxed{\text{z157}} \quad \mathbb{Q}_{2,1}^{(c)}(E'') = \frac{\sqrt{2}\mathbb{Q}_1^{(a)}(A'')\mathbb{Q}_{1,2}^{(b)}(E')}{2}$$

$$\boxed{\text{z158}} \quad \mathbb{Q}_{2,2}^{(c)}(E'') = -\frac{\sqrt{2}\mathbb{Q}_1^{(a)}(A'')\mathbb{Q}_{1,1}^{(b)}(E')}{2}$$

$$\boxed{\text{z159}} \quad \mathbb{Q}_{2,1}^{(1,-1;c)}(E'') = \frac{\sqrt{10}\mathbb{G}_{2,1}^{(1,-1;a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{10} - \frac{\sqrt{10}\mathbb{G}_{2,2}^{(1,-1;a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{10} + \frac{\sqrt{30}\mathbb{G}_2^{(1,-1;a)}(A'')\mathbb{Q}_{1,1}^{(b)}(E')}{10}$$

$$\boxed{\text{z160}} \quad \mathbb{Q}_{2,2}^{(1,-1;c)}(E'') = -\frac{\sqrt{10}\mathbb{G}_{2,1}^{(1,-1;a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{10} - \frac{\sqrt{10}\mathbb{G}_{2,2}^{(1,-1;a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{10} + \frac{\sqrt{30}\mathbb{G}_2^{(1,-1;a)}(A'')\mathbb{Q}_{1,2}^{(b)}(E')}{10}$$

$$\boxed{\text{z161}} \quad \mathbb{Q}_{2,1}^{(1,0;c)}(E'') = \frac{\sqrt{2}\mathbb{Q}_1^{(1,0;a)}(A'')\mathbb{Q}_{1,2}^{(b)}(E')}{2}$$

$$\boxed{\text{z162}} \quad \mathbb{Q}_{2,2}^{(1,0;c)}(E'') = -\frac{\sqrt{2}\mathbb{Q}_1^{(1,0;a)}(A'')\mathbb{Q}_{1,1}^{(b)}(E')}{2}$$

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

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

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

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

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

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

• 0;H2_001_1 : 'H2'-'0' bond-cluster

* bra: $\langle s, \uparrow |, \langle s, \downarrow |$

* ket: $|s, \uparrow\rangle, |s, \downarrow\rangle$

* wyckoff: **3a03b**

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

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

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

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

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

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

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

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

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

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

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

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

• **0;H2_001_1** : '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: 3a03b

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

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

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

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

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

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

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

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

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

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

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

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

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

$$\boxed{\text{z118}} \quad \mathbb{Q}_{1,2}^{(c)}(E') = \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E')\mathbb{Q}_0^{(b)}(A')}{2}$$

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

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

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

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

$$\boxed{\text{z123}} \quad \mathbb{Q}_{1,1}^{(1,0;c)}(E') = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(1,0;a)}(E')\mathbb{Q}_0^{(b)}(A')}{2}$$

$$\boxed{\text{z124}} \quad \mathbb{Q}_{1,2}^{(1,0;c)}(E') = \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(1,0;a)}(E')\mathbb{Q}_0^{(b)}(A')}{2}$$

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

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

$$\boxed{\text{z127}} \quad \mathbb{G}_{2,1}^{(1,-1;c)}(E') = \frac{\sqrt{2}\mathbb{G}_{2,1}^{(1,-1;a)}(E')\mathbb{Q}_0^{(b)}(A')}{2}$$

$$\boxed{\text{z128}} \quad \mathbb{G}_{2,2}^{(1,-1;c)}(E') = \frac{\sqrt{2}\mathbb{G}_{2,2}^{(1,-1;a)}(E')\mathbb{Q}_0^{(b)}(A')}{2}$$

$$\boxed{\text{z173}} \quad \mathbb{Q}_{2,1}^{(c)}(E'') = \frac{\sqrt{2}\mathbb{Q}_1^{(a)}(A'')\mathbb{Q}_{1,2}^{(b)}(E')}{2}$$

$$\boxed{\text{z174}} \quad \mathbb{Q}_{2,2}^{(c)}(E'') = -\frac{\sqrt{2}\mathbb{Q}_1^{(a)}(A'')\mathbb{Q}_{1,1}^{(b)}(E')}{2}$$

$$\boxed{\text{z175}} \quad \mathbb{Q}_{2,1}^{(1,-1;c)}(E'') = \frac{\sqrt{10}\mathbb{G}_{2,1}^{(1,-1;a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{10} - \frac{\sqrt{10}\mathbb{G}_{2,2}^{(1,-1;a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{10} + \frac{\sqrt{30}\mathbb{G}_2^{(1,-1;a)}(A'')\mathbb{Q}_{1,1}^{(b)}(E')}{10}$$

$$\boxed{\text{z176}} \quad \mathbb{Q}_{2,2}^{(1,-1;c)}(E'') = -\frac{\sqrt{10}\mathbb{G}_{2,1}^{(1,-1;a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{10} - \frac{\sqrt{10}\mathbb{G}_{2,2}^{(1,-1;a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{10} + \frac{\sqrt{30}\mathbb{G}_2^{(1,-1;a)}(A'')\mathbb{Q}_{1,2}^{(b)}(E')}{10}$$

$$\boxed{\text{z177}} \quad \mathbb{Q}_{2,1}^{(1,0;c)}(E'') = \frac{\sqrt{2}\mathbb{Q}_1^{(1,0;a)}(A'')\mathbb{Q}_{1,2}^{(b)}(E')}{2}$$

$$\boxed{\text{z178}} \quad \mathbb{Q}_{2,2}^{(1,0;c)}(E'') = -\frac{\sqrt{2}\mathbb{Q}_1^{(1,0;a)}(A'')\mathbb{Q}_{1,1}^{(b)}(E')}{2}$$

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

$$\boxed{\text{z180}} \quad \mathbb{G}_{1,2}^{(1,-1;c)}(E'') = -\frac{\sqrt{15}\mathbb{G}_{2,1}^{(1,-1;a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{10} - \frac{\sqrt{15}\mathbb{G}_{2,2}^{(1,-1;a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{10} - \frac{\sqrt{5}\mathbb{G}_2^{(1,-1;a)}(A'')\mathbb{Q}_{1,2}^{(b)}(E')}{5}$$

$$\boxed{\text{z181}} \quad \mathbb{G}_{2,1}^{(1,-1;c)}(E'') = \frac{\sqrt{2}\mathbb{G}_{2,1}^{(1,-1;a)}(E'')\mathbb{Q}_0^{(b)}(A')}{2}$$

$$\boxed{\text{z182}} \quad \mathbb{G}_{2,2}^{(1,-1;c)}(E'') = \frac{\sqrt{2}\mathbb{G}_{2,2}^{(1,-1;a)}(E'')\mathbb{Q}_0^{(b)}(A')}{2}$$

$$\boxed{\text{z183}} \quad \mathbb{G}_{1,1}^{(1,1;c)}(E'') = \frac{\sqrt{2}\mathbb{G}_0^{(1,1;a)}(A'')\mathbb{Q}_{1,1}^{(b)}(E')}{2}$$

$$\boxed{\text{z184}} \quad \mathbb{G}_{1,2}^{(1,1;c)}(E'') = \frac{\sqrt{2}\mathbb{G}_0^{(1,1;a)}(A'')\mathbb{Q}_{1,2}^{(b)}(E')}{2}$$

Atomic SAMB

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

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

$$\boxed{\text{x2}} \quad \mathbb{M}_1^{(1,-1;a)}(A') = \begin{bmatrix} \frac{\sqrt{2}}{2} & 0 \\ 0 & -\frac{\sqrt{2}}{2} \end{bmatrix}$$

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

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

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

$$\boxed{\text{x5}} \quad \mathbb{Q}_1^{(a)}(A'') = \begin{bmatrix} 0 & 0 & 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{2} \end{bmatrix}$$

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

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

$$\boxed{\text{x8}} \quad \mathbb{Q}_1^{(1,0;a)}(A'') = \begin{bmatrix} 0 & -\frac{\sqrt{2}}{4} & 0 & \frac{\sqrt{2}i}{4} & 0 & 0 \\ \frac{\sqrt{2}}{4} & 0 & \frac{\sqrt{2}i}{4} & 0 & 0 & 0 \end{bmatrix}$$

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

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

$$\boxed{\text{x11}} \quad \mathbb{G}_2^{(1,-1;a)}(A'') = \begin{bmatrix} 0 & -\frac{\sqrt{6}i}{12} & 0 & -\frac{\sqrt{6}}{12} & \frac{\sqrt{6}i}{6} & 0 \\ -\frac{\sqrt{6}i}{12} & 0 & \frac{\sqrt{6}}{12} & 0 & 0 & -\frac{\sqrt{6}i}{6} \end{bmatrix}$$

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

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

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

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

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

$$\boxed{\text{x17}} \quad \mathbb{M}_2^{(1,-1;a)}(A'') = \begin{bmatrix} 0 & -\frac{\sqrt{6}}{12} & 0 & \frac{\sqrt{6}i}{12} & \frac{\sqrt{6}}{6} & 0 \\ -\frac{\sqrt{6}}{12} & 0 & -\frac{\sqrt{6}i}{12} & 0 & 0 & -\frac{\sqrt{6}}{6} \end{bmatrix}$$

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

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

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

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

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

$$\boxed{\text{x23}} \quad \mathbb{T}_1^{(a)}(A'') = \begin{bmatrix} 0 & 0 & 0 & 0 & \frac{i}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{i}{2} \end{bmatrix}$$

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

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

$$\boxed{\text{x26}} \quad \mathbb{T}_1^{(1,0;a)}(A'') = \begin{bmatrix} 0 & \frac{\sqrt{2}i}{4} & 0 & \frac{\sqrt{2}}{4} & 0 & 0 \\ -\frac{\sqrt{2}i}{4} & 0 & \frac{\sqrt{2}}{4} & 0 & 0 & 0 \end{bmatrix}$$

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

$$\boxed{\text{x47}} \quad \mathbb{M}_1^{(1,-1;a)}(A') = \begin{bmatrix} \frac{\sqrt{6}}{6} & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{6}}{6} & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{6}}{6} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{6}}{6} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{6}}{6} & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{6}}{6} \end{bmatrix}$$

$$\boxed{\text{x48}} \quad \mathbb{M}_3^{(1,-1;a)}(A') = \begin{bmatrix} -\frac{\sqrt{5}}{10} & 0 & 0 & 0 & 0 & -\frac{\sqrt{5}}{10} \\ 0 & \frac{\sqrt{5}}{10} & 0 & 0 & -\frac{\sqrt{5}}{10} & 0 \\ 0 & 0 & -\frac{\sqrt{5}}{10} & 0 & 0 & \frac{\sqrt{5}i}{10} \\ 0 & 0 & 0 & \frac{\sqrt{5}}{10} & -\frac{\sqrt{5}i}{10} & 0 \\ 0 & -\frac{\sqrt{5}}{10} & 0 & \frac{\sqrt{5}i}{10} & \frac{\sqrt{5}}{5} & 0 \\ -\frac{\sqrt{5}}{10} & 0 & -\frac{\sqrt{5}i}{10} & 0 & 0 & -\frac{\sqrt{5}}{5} \end{bmatrix}$$

$$\boxed{\text{x49}} \quad \mathbb{M}_3^{(1,-1;a)}(A'', 1) = \begin{bmatrix} 0 & -\frac{\sqrt{2}i}{4} & 0 & \frac{\sqrt{2}}{4} & 0 & 0 \\ \frac{\sqrt{2}i}{4} & 0 & \frac{\sqrt{2}}{4} & 0 & 0 & 0 \\ 0 & \frac{\sqrt{2}}{4} & 0 & \frac{\sqrt{2}i}{4} & 0 & 0 \\ \frac{\sqrt{2}}{4} & 0 & -\frac{\sqrt{2}i}{4} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x50}} \quad \mathbb{M}_3^{(1,-1;a)}(A'', 2) = \begin{bmatrix} 0 & \frac{\sqrt{2}}{4} & 0 & \frac{\sqrt{2}i}{4} & 0 & 0 \\ \frac{\sqrt{2}}{4} & 0 & -\frac{\sqrt{2}i}{4} & 0 & 0 & 0 \\ 0 & \frac{\sqrt{2}i}{4} & 0 & -\frac{\sqrt{2}}{4} & 0 & 0 \\ -\frac{\sqrt{2}i}{4} & 0 & -\frac{\sqrt{2}}{4} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Cluster SAMB

- Site cluster

** Wyckoff: 1o

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

** Wyckoff: 3b

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

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

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

- Bond cluster

** Wyckoff: 3a@3b

$$\boxed{\text{y5}} \quad \mathbb{Q}_0^{(s)}(A') = \left[\frac{\sqrt{3}}{3}, \frac{\sqrt{3}}{3}, \frac{\sqrt{3}}{3} \right]$$

$$\boxed{\text{y6}} \quad \mathbb{T}_0^{(s)}(A') = \left[\frac{\sqrt{3}i}{3}, \frac{\sqrt{3}i}{3}, \frac{\sqrt{3}i}{3} \right]$$

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

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

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

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

Site and Bond

Table 5: Orbital of each site

#	site	orbital
1	H1	$ s, \uparrow\rangle, s, \downarrow\rangle$
2	H2	$ s, \uparrow\rangle, s, \downarrow\rangle$
3	0	$ s, \uparrow\rangle, s, \downarrow\rangle, p_x, \uparrow\rangle, p_x, \downarrow\rangle, p_y, \uparrow\rangle, p_y, \downarrow\rangle, p_z, \uparrow\rangle, p_z, \downarrow\rangle$

Table 6: Neighbor and bra-ket of each bond

#	head	tail	neighbor	head (bra)	tail (ket)
1	H1	0	[1]	[s]	[s,p]
2	H2	0	[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 (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 (\mathbf{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, $|\mathbf{v}|=0.33333$ (cartesian)

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

SL	vector (\mathbf{v})	center (\mathbf{c})	mapping	head	tail	\mathbf{R} (primitive)
1	[0.16667, 0.16667, 0.00000]	[0.41667, 0.08333, 0.00000]	[1,4]	(1,1)	(1,1)	[0,0,0]

continued ...

Table 11

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