

Model for “MoS2”

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General Condition

- Basis type: 1g
- SAMB selection:
 - Type: [Q, G]
 - Rank: [0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11]
 - Irrep.: [A'_1 , A'_2 , A''_1 , A''_2 , 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'_1 , A'_2 , A''_1 , A''_2 , E' , E'']
 - Spin (s): [0, 1]
- Site-cluster selection:
 - Rank: [0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11]
 - Irrep.: [A'_1 , A'_2 , A''_1 , A''_2 , 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'_1 , A'_2 , A''_1 , A''_2 , E' , E'']
- Max. neighbor: 10
- Search cell range: (-2, 3), (-2, 3), (-2, 3)
- Toroidal priority: false

Group and Unit Cell

- Group: SG No. 187 D_{3h}^1 $P\bar{6}m2$ [hexagonal]
- Associated point group: PG No. 187 D_{3h} $\bar{6}m2$ (-6m2 setting) [hexagonal]
- Unit cell:
 $a = 3.16610, b = 3.16610, c = 20.00000, \alpha = 90.0, \beta = 90.0, \gamma = 120.0$
- Lattice vectors (conventional cell):
 $a_1 = [3.16610, 0.00000, 0.00000]$
 $a_2 = [-1.58305, 2.74192, 0.00000]$
 $a_3 = [0.00000, 0.00000, 20.00000]$

Symmetry Operation

Table 1: Symmetry operation

#	SO	#	SO	#	SO	#	SO	#	SO
1	{1 0}	2	{3 ⁺ ₀₀₁ 0}	3	{3 ⁻ ₀₀₁ 0}	4	{m ₀₀₁ 0}	5	{-6 ⁻ ₀₀₁ 0}
6	{-6 ⁺ ₀₀₁ 0}	7	{m ₁₁₀ 0}	8	{m ₁₀₀ 0}	9	{m ₀₁₀ 0}	10	{2 ₁₋₁₀ 0}
11	{2 ₁₂₀ 0}	12	{2 ₂₁₀ 0}						

Harmonics

Table 2: Harmonics

#	symbol	irrep.	rank	X	multiplicity	component	symmetry
1	$\mathbb{Q}_0(A'_1)$	A'_1	0	Q, T	-	-	1
2	$\mathbb{Q}_2(A'_1)$	A'_1	2	Q, T	-	-	$-\frac{x^2}{2} - \frac{y^2}{2} + z^2$
3	$\mathbb{Q}_3(A'_1)$	A'_1	3	Q, T	-	-	$\frac{\sqrt{10}y(3x^2-y^2)}{4}$
4	$\mathbb{Q}_4(A'_1)$	A'_1	4	Q, T	-	-	$\frac{3x^4}{8} + \frac{3x^2y^2}{4} - 3x^2z^2 + \frac{3y^4}{8} - 3y^2z^2 + z^4$
5	$\mathbb{Q}_5(A'_1)$	A'_1	5	Q, T	-	-	$-\frac{\sqrt{70}y(3x^2-y^2)(x^2+y^2-8z^2)}{16}$
6	$\mathbb{G}_0(A''_1)$	A''_1	0	G, M	-	-	1
7	$\mathbb{G}_2(A''_1)$	A''_1	2	G, M	-	-	$-\frac{x^2}{2} - \frac{y^2}{2} + z^2$
8	$\mathbb{G}_3(A''_1)$	A''_1	3	G, M	-	-	$\frac{\sqrt{10}y(3x^2-y^2)}{4}$

continued ...

Table 2

#	symbol	irrep.	rank	X	multiplicity	component	symmetry
9	$\mathbb{G}_4(A''_1)$	A''_1	4	G, M	-	-	$\frac{3x^4}{8} + \frac{3x^2y^2}{4} - 3x^2z^2 + \frac{3y^4}{8} - 3y^2z^2 + z^4$
10	$\mathbb{Q}_4(A''_1)$	A''_1	4	Q, T	-	-	$\frac{\sqrt{70}xz(x^2-3y^2)}{4}$
11	$\mathbb{G}_1(A'_2)$	A'_2	1	G, M	-	-	z
12	$\mathbb{G}_3(A'_2)$	A'_2	3	G, M	-	-	$-\frac{z(3x^2+3y^2-2z^2)}{2}$
13	$\mathbb{Q}_3(A'_2)$	A'_2	3	Q, T	-	-	$\frac{\sqrt{10}x(x^2-3y^2)}{4}$
14	$\mathbb{Q}_5(A'_2)$	A'_2	5	Q, T	-	-	$-\frac{\sqrt{70}x(x^2-3y^2)(x^2+y^2-8z^2)}{16}$
15	$\mathbb{Q}_1(A''_2)$	A''_2	1	Q, T	-	-	z
16	$\mathbb{G}_3(A''_2)$	A''_2	3	G, M	-	-	$\frac{\sqrt{10}x(x^2-3y^2)}{4}$
17	$\mathbb{Q}_3(A''_2)$	A''_2	3	Q, T	-	-	$-\frac{z(3x^2+3y^2-2z^2)}{2}$
18	$\mathbb{Q}_4(A''_2)$	A''_2	4	Q, T	-	-	$\frac{\sqrt{70}yz(3x^2-y^2)}{4}$
19	$\mathbb{Q}_{1,1}(E')$	E'	1	Q, T	-	1	x
20	$\mathbb{Q}_{1,2}(E')$					2	y
21	$\mathbb{G}_{2,1}(E')$	E'	2	G, M	-	1	$\sqrt{3}yz$
22	$\mathbb{G}_{2,2}(E')$					2	$-\sqrt{3}xz$
23	$\mathbb{Q}_{2,1}(E')$	E'	2	Q, T	-	1	$\sqrt{3}xy$
24	$\mathbb{Q}_{2,2}(E')$					2	$\frac{\sqrt{3}(x-y)(x+y)}{2}$
25	$\mathbb{G}_{3,1}(E')$	E'	3	G, M	-	1	$-\frac{\sqrt{15}z(x-y)(x+y)}{2}$
26	$\mathbb{G}_{3,2}(E')$					2	$\sqrt{15}xyz$
27	$\mathbb{Q}_{3,1}(E')$	E'	3	Q, T	-	1	$-\frac{\sqrt{6}x(x^2+y^2-4z^2)}{4}$
28	$\mathbb{Q}_{3,2}(E')$					2	$-\frac{\sqrt{6}y(x^2+y^2-4z^2)}{4}$
29	$\mathbb{Q}_{4,1}(E', 1)$	E'	4	Q, T	1	1	$-\frac{\sqrt{35}xy(x-y)(x+y)}{2}$

continued ...

Table 2

#	symbol	irrep.	rank	X	multiplicity	component	symmetry
30	$\mathbb{Q}_{4,2}(E', 1)$					2	$\frac{\sqrt{35}(x^2 - 2xy - y^2)(x^2 + 2xy - y^2)}{8}$
31	$\mathbb{Q}_{4,1}(E', 2)$	E'	4	Q, T	2	1	$-\frac{\sqrt{5}xy(x^2 + y^2 - 6z^2)}{2}$
32	$\mathbb{Q}_{4,2}(E', 2)$					2	$-\frac{\sqrt{5}(x-y)(x+y)(x^2 + y^2 - 6z^2)}{4}$
33	$\mathbb{Q}_{5,1}(E', 1)$	E'	5	Q, T	1	1	$\frac{3\sqrt{14}x(x^4 - 10x^2y^2 + 5y^4)}{16}$
34	$\mathbb{Q}_{5,2}(E', 1)$					2	$-\frac{3\sqrt{14}y(5x^4 - 10x^2y^2 + y^4)}{16}$
35	$\mathbb{Q}_{5,1}(E', 2)$	E'	5	Q, T	2	1	$\frac{\sqrt{15}x(x^4 + 2x^2y^2 - 12x^2z^2 + y^4 - 12y^2z^2 + 8z^4)}{8}$
36	$\mathbb{Q}_{5,2}(E', 2)$					2	$\frac{\sqrt{15}y(x^4 + 2x^2y^2 - 12x^2z^2 + y^4 - 12y^2z^2 + 8z^4)}{8}$
37	$\mathbb{G}_{1,1}(E'')$	E''	1	G, M	-	1	x
38	$\mathbb{G}_{1,2}(E'')$					2	y
39	$\mathbb{G}_{2,1}(E'')$	E''	2	G, M	-	1	$\sqrt{3}xy$
40	$\mathbb{G}_{2,2}(E'')$					2	$\frac{\sqrt{3}(x-y)(x+y)}{2}$
41	$\mathbb{Q}_{2,1}(E'')$	E''	2	Q, T	-	1	$\sqrt{3}yz$
42	$\mathbb{Q}_{2,2}(E'')$					2	$-\sqrt{3}xz$
43	$\mathbb{G}_{3,1}(E'')$	E''	3	G, M	-	1	$-\frac{\sqrt{6}x(x^2 + y^2 - 4z^2)}{4}$
44	$\mathbb{G}_{3,2}(E'')$					2	$-\frac{\sqrt{6}y(x^2 + y^2 - 4z^2)}{4}$
45	$\mathbb{Q}_{3,1}(E'')$	E''	3	Q, T	-	1	$-\frac{\sqrt{15}z(x-y)(x+y)}{2}$
46	$\mathbb{Q}_{3,2}(E'')$					2	$\sqrt{15}xyz$
47	$\mathbb{G}_{4,1}(E'', 1)$	E''	4	G, M	1	1	$-\frac{\sqrt{35}xy(x-y)(x+y)}{2}$
48	$\mathbb{G}_{4,2}(E'', 1)$					2	$\frac{\sqrt{35}(x^2 - 2xy - y^2)(x^2 + 2xy - y^2)}{8}$
49	$\mathbb{Q}_{4,1}(E'')$	E''	4	Q, T	-	1	$-\frac{\sqrt{10}yz(3x^2 + 3y^2 - 4z^2)}{4}$
50	$\mathbb{Q}_{4,2}(E'')$					2	$\frac{\sqrt{10}xz(3x^2 + 3y^2 - 4z^2)}{4}$

continued ...

Table 2

#	symbol	irrep.	rank	X	multiplicity	component	symmetry
51	$\mathbb{Q}_{5,1}(E'', 1)$	E''	5	Q, T	1	1	$-\frac{3\sqrt{35}z(x^2-2xy-y^2)(x^2+2xy-y^2)}{8}$
52	$\mathbb{Q}_{5,2}(E'', 1)$					2	$-\frac{3\sqrt{35}xyz(x-y)(x+y)}{2}$
53	$\mathbb{Q}_{5,1}(E'', 2)$	E''	5	Q, T	2	1	$\frac{\sqrt{105}z(x-y)(x+y)(x^2+y^2-2z^2)}{4}$
54	$\mathbb{Q}_{5,2}(E'', 2)$					2	$-\frac{\sqrt{105}xyz(x^2+y^2-2z^2)}{2}$

Basis in full matrix

Table 3: dimension = 11

#	orbital@atom(SL)	#	orbital@atom(SL)	#	orbital@atom(SL)	#	orbital@atom(SL)	#	orbital@atom(SL)
0	$ d_v\rangle @Mo(1)$	1	$ d_{xy}\rangle @Mo(1)$	2	$ d_{xz}\rangle @Mo(1)$	3	$ d_{yz}\rangle @Mo(1)$	4	$ d_u\rangle @Mo(1)$
5	$ p_x\rangle @S(1)$	6	$ p_y\rangle @S(1)$	7	$ p_z\rangle @S(1)$	8	$ p_x\rangle @S(2)$	9	$ p_y\rangle @S(2)$
10	$ p_z\rangle @S(2)$								

Table 4: Atomic basis (orbital part only)

orbital	definition
$ p_x\rangle$	x
$ p_y\rangle$	y

continued ...

Table 4

orbital	definition
$ p_z\rangle$	z
$ d_v\rangle$	$\frac{\sqrt{3}(x^2-y^2)}{2}$
$ d_{xy}\rangle$	$\sqrt{3}xy$
$ d_{xz}\rangle$	$\sqrt{3}xz$
$ d_{yz}\rangle$	$\sqrt{3}yz$
$ d_u\rangle$	$-\frac{x^2}{2} - \frac{y^2}{2} + z^2$

— SAMB: 246 (all 246) —

- Mo : 'Mo' site-cluster

* bra: $\langle d_v |, \langle d_{xy} |, \langle d_{xz} |, \langle d_{yz} |, \langle d_u |$

* ket: $|d_v \rangle, |d_{xy} \rangle, |d_{xz} \rangle, |d_{yz} \rangle, |d_u \rangle$

* wyckoff: 1a

[z1] $\mathbb{Q}_0^{(c)}(A'_1) = \mathbb{Q}_0^{(a)}(A'_1)\mathbb{Q}_0^{(s)}(A'_1)$

[z2] $\mathbb{Q}_2^{(c)}(A'_1) = \mathbb{Q}_2^{(a)}(A'_1)\mathbb{Q}_0^{(s)}(A'_1)$

[z3] $\mathbb{Q}_4^{(c)}(A'_1) = \mathbb{Q}_4^{(a)}(A'_1)\mathbb{Q}_0^{(s)}(A'_1)$

[z43] $\mathbb{Q}_4^{(c)}(A''_1) = \mathbb{Q}_4^{(a)}(A''_1)\mathbb{Q}_0^{(s)}(A'_1)$

[z60] $\mathbb{Q}_4^{(c)}(A''_2) = \mathbb{Q}_4^{(a)}(A''_2)\mathbb{Q}_0^{(s)}(A'_1)$

[z83] $\mathbb{Q}_{2,1}^{(c)}(E') = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E')\mathbb{Q}_0^{(s)}(A'_1)}{2}$

[z84] $\mathbb{Q}_{2,2}^{(c)}(E') = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E')\mathbb{Q}_0^{(s)}(A'_1)}{2}$

$$\boxed{\text{z85}} \quad \mathbb{Q}_{4,1}^{(c)}(E', 1) = \frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E', 1)\mathbb{Q}_0^{(s)}(A'_1)}{2}$$

$$\boxed{\text{z86}} \quad \mathbb{Q}_{4,2}^{(c)}(E', 1) = \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E', 1)\mathbb{Q}_0^{(s)}(A'_1)}{2}$$

$$\boxed{\text{z87}} \quad \mathbb{Q}_{4,1}^{(c)}(E', 2) = \frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E', 2)\mathbb{Q}_0^{(s)}(A'_1)}{2}$$

$$\boxed{\text{z88}} \quad \mathbb{Q}_{4,2}^{(c)}(E', 2) = \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E', 2)\mathbb{Q}_0^{(s)}(A'_1)}{2}$$

$$\boxed{\text{z167}} \quad \mathbb{Q}_{2,1}^{(c)}(E'') = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E'')\mathbb{Q}_0^{(s)}(A'_1)}{2}$$

$$\boxed{\text{z168}} \quad \mathbb{Q}_{2,2}^{(c)}(E'') = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E'')\mathbb{Q}_0^{(s)}(A'_1)}{2}$$

$$\boxed{\text{z169}} \quad \mathbb{Q}_{4,1}^{(c)}(E'') = \frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E'')\mathbb{Q}_0^{(s)}(A'_1)}{2}$$

$$\boxed{\text{z170}} \quad \mathbb{Q}_{4,2}^{(c)}(E'') = \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E'')\mathbb{Q}_0^{(s)}(A'_1)}{2}$$

- **S** : 'S' site-cluster

- * bra: $\langle p_x |, \langle p_y |, \langle p_z |$

- * ket: $|p_x\rangle, |p_y\rangle, |p_z\rangle$

- * wyckoff: **2i**

$$\boxed{\text{z4}} \quad \mathbb{Q}_0^{(c)}(A'_1) = \mathbb{Q}_0^{(a)}(A'_1)\mathbb{Q}_0^{(s)}(A'_1)$$

$$\boxed{\text{z5}} \quad \mathbb{Q}_2^{(c)}(A'_1) = \mathbb{Q}_2^{(a)}(A'_1)\mathbb{Q}_0^{(s)}(A'_1)$$

$$\boxed{\text{z61}} \quad \mathbb{Q}_1^{(c)}(A''_2, a) = \mathbb{Q}_0^{(a)}(A'_1)\mathbb{Q}_1^{(s)}(A''_2)$$

$$\boxed{\text{z62}} \quad \mathbb{Q}_1^{(c)}(A''_2, b) = \mathbb{Q}_2^{(a)}(A'_1)\mathbb{Q}_1^{(s)}(A''_2)$$

$$\boxed{\text{z89}} \quad \mathbb{Q}_{1,1}^{(c)}(E') = -\frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E'')\mathbb{Q}_1^{(s)}(A''_2)}{2}$$

$$\boxed{z90} \quad \mathbb{Q}_{1,2}^{(c)}(E') = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E'')\mathbb{Q}_1^{(s)}(A_2'')}{2}$$

$$\boxed{z91} \quad \mathbb{Q}_{2,1}^{(c)}(E') = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E')\mathbb{Q}_0^{(s)}(A_1')}{2}$$

$$\boxed{z92} \quad \mathbb{Q}_{2,2}^{(c)}(E') = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E')\mathbb{Q}_0^{(s)}(A_1')}{2}$$

$$\boxed{z171} \quad \mathbb{Q}_{2,1}^{(c)}(E'') = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E'')\mathbb{Q}_0^{(s)}(A_1')}{2}$$

$$\boxed{z172} \quad \mathbb{Q}_{2,2}^{(c)}(E'') = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E'')\mathbb{Q}_0^{(s)}(A_1')}{2}$$

$$\boxed{z173} \quad \mathbb{Q}_{3,1}^{(c)}(E'') = -\frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E')\mathbb{Q}_1^{(s)}(A_2'')}{2}$$

$$\boxed{z174} \quad \mathbb{Q}_{3,2}^{(c)}(E'') = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E')\mathbb{Q}_1^{(s)}(A_2'')}{2}$$

• Mo;Mo_001_1 : 'Mo'-'Mo' bond-cluster

* bra: $\langle d_v |, \langle d_{xy} |, \langle d_{xz} |, \langle d_{yz} |, \langle d_u |$

* ket: $|d_v \rangle, |d_{xy} \rangle, |d_{xz} \rangle, |d_{yz} \rangle, |d_u \rangle$

* wyckoff: 3b@3j

$$\boxed{z6} \quad \mathbb{Q}_0^{(c)}(A'_1, a) = \mathbb{Q}_0^{(a)}(A'_1)\mathbb{Q}_0^{(b)}(A'_1)$$

$$\boxed{z7} \quad \mathbb{Q}_0^{(c)}(A'_1, b) = \mathbb{M}_1^{(a)}(A'_2)\mathbb{M}_1^{(b)}(A'_2)$$

$$\boxed{z8} \quad \mathbb{Q}_2^{(c)}(A'_1, a) = \mathbb{Q}_2^{(a)}(A'_1)\mathbb{Q}_0^{(b)}(A'_1)$$

$$\boxed{z9} \quad \mathbb{Q}_2^{(c)}(A'_1, b) = \mathbb{M}_3^{(a)}(A'_2)\mathbb{M}_1^{(b)}(A'_2)$$

$$\boxed{z10} \quad \mathbb{Q}_3^{(c)}(A'_1, a) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{2} + \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{2}$$

$$\boxed{z11} \quad \mathbb{Q}_3^{(c)}(A'_1, b) = -\frac{\sqrt{406}\mathbb{Q}_{4,1}^{(a)}(E', 1)\mathbb{Q}_{1,1}^{(b)}(E')}{29} - \frac{\sqrt{58}\mathbb{Q}_{4,1}^{(a)}(E', 2)\mathbb{Q}_{1,1}^{(b)}(E')}{58} - \frac{\sqrt{406}\mathbb{Q}_{4,2}^{(a)}(E', 1)\mathbb{Q}_{1,2}^{(b)}(E')}{29} - \frac{\sqrt{58}\mathbb{Q}_{4,2}^{(a)}(E', 2)\mathbb{Q}_{1,2}^{(b)}(E')}{58}$$

$$\boxed{\text{z12}} \quad \mathbb{Q}_3^{(c)}(A'_1, c) = -\frac{\sqrt{2}\mathbb{M}_{3,1}^{(a)}(E')\mathbb{T}_{1,1}^{(b)}(E')}{2} - \frac{\sqrt{2}\mathbb{M}_{3,2}^{(a)}(E')\mathbb{T}_{1,2}^{(b)}(E')}{2}$$

$$\boxed{\text{z13}} \quad \mathbb{Q}_4^{(c)}(A'_1) = \mathbb{Q}_4^{(a)}(A'_1)\mathbb{Q}_0^{(b)}(A'_1)$$

$$\boxed{\text{z14}} \quad \mathbb{Q}_5^{(c)}(A'_1) = -\frac{\sqrt{58}\mathbb{Q}_{4,1}^{(a)}(E', 1)\mathbb{Q}_{1,1}^{(b)}(E')}{58} + \frac{\sqrt{406}\mathbb{Q}_{4,1}^{(a)}(E', 2)\mathbb{Q}_{1,1}^{(b)}(E')}{29} - \frac{\sqrt{58}\mathbb{Q}_{4,2}^{(a)}(E', 1)\mathbb{Q}_{1,2}^{(b)}(E')}{58} + \frac{\sqrt{406}\mathbb{Q}_{4,2}^{(a)}(E', 2)\mathbb{Q}_{1,2}^{(b)}(E')}{29}$$

$$\boxed{\text{z29}} \quad \mathbb{Q}_4^{(c)}(A''_1, a) = \mathbb{Q}_4^{(a)}(A''_1)\mathbb{Q}_0^{(b)}(A'_1)$$

$$\boxed{\text{z30}} \quad \mathbb{Q}_4^{(c)}(A''_1, b) = \mathbb{M}_3^{(a)}(A''_2)\mathbb{M}_1^{(b)}(A'_2)$$

$$\boxed{\text{z31}} \quad \mathbb{G}_0^{(c)}(A''_1) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(a)}(E'')\mathbb{T}_{1,1}^{(b)}(E')}{2} + \frac{\sqrt{2}\mathbb{M}_{1,2}^{(a)}(E'')\mathbb{T}_{1,2}^{(b)}(E')}{2}$$

$$\boxed{\text{z32}} \quad \mathbb{G}_2^{(c)}(A''_1, a) = -\frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{2} - \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{2}$$

$$\boxed{\text{z44}} \quad \mathbb{G}_2^{(c)}(A''_1, b) = \frac{\sqrt{2}\mathbb{M}_{3,1}^{(a)}(E'')\mathbb{T}_{1,1}^{(b)}(E')}{2} + \frac{\sqrt{2}\mathbb{M}_{3,2}^{(a)}(E'')\mathbb{T}_{1,2}^{(b)}(E')}{2}$$

$$\boxed{\text{z45}} \quad \mathbb{G}_4^{(c)}(A''_1) = -\frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{2} - \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{2}$$

$$\boxed{\text{z46}} \quad \mathbb{Q}_3^{(c)}(A'_2, a) = -\frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{2} + \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{2}$$

$$\boxed{\text{z47}} \quad \mathbb{Q}_3^{(c)}(A'_2, b) = -\frac{\sqrt{406}\mathbb{Q}_{4,1}^{(a)}(E', 1)\mathbb{Q}_{1,2}^{(b)}(E')}{29} + \frac{\sqrt{58}\mathbb{Q}_{4,1}^{(a)}(E', 2)\mathbb{Q}_{1,2}^{(b)}(E')}{58} + \frac{\sqrt{406}\mathbb{Q}_{4,2}^{(a)}(E', 1)\mathbb{Q}_{1,1}^{(b)}(E')}{29} - \frac{\sqrt{58}\mathbb{Q}_{4,2}^{(a)}(E', 2)\mathbb{Q}_{1,1}^{(b)}(E')}{58}$$

$$\boxed{\text{z48}} \quad \mathbb{Q}_3^{(c)}(A'_2, c) = \frac{\sqrt{2}\mathbb{M}_{3,1}^{(a)}(E')\mathbb{T}_{1,2}^{(b)}(E')}{2} - \frac{\sqrt{2}\mathbb{M}_{3,2}^{(a)}(E')\mathbb{T}_{1,1}^{(b)}(E')}{2}$$

$$\boxed{\text{z49}} \quad \mathbb{Q}_5^{(c)}(A'_2) = -\frac{\sqrt{58}\mathbb{Q}_{4,1}^{(a)}(E', 1)\mathbb{Q}_{1,2}^{(b)}(E')}{58} - \frac{\sqrt{406}\mathbb{Q}_{4,1}^{(a)}(E', 2)\mathbb{Q}_{1,2}^{(b)}(E')}{29} + \frac{\sqrt{58}\mathbb{Q}_{4,2}^{(a)}(E', 1)\mathbb{Q}_{1,1}^{(b)}(E')}{58} + \frac{\sqrt{406}\mathbb{Q}_{4,2}^{(a)}(E', 2)\mathbb{Q}_{1,1}^{(b)}(E')}{29}$$

$$\boxed{\text{z63}} \quad \mathbb{Q}_1^{(c)}(A''_2, a) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{2} - \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{2}$$

$$\boxed{\text{z64}} \quad \mathbb{Q}_1^{(c)}(A_2'', b) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(a)}(E'')\mathbb{T}_{1,2}^{(b)}(E')}{2} - \frac{\sqrt{2}\mathbb{M}_{1,2}^{(a)}(E'')\mathbb{T}_{1,1}^{(b)}(E')}{2}$$

$$\boxed{\text{z65}} \quad \mathbb{Q}_3^{(c)}(A_2'', a) = \frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{2} - \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{2}$$

$$\boxed{\text{z66}} \quad \mathbb{Q}_3^{(c)}(A_2'', b) = \frac{\sqrt{2}\mathbb{M}_{3,1}^{(a)}(E'')\mathbb{T}_{1,2}^{(b)}(E')}{2} - \frac{\sqrt{2}\mathbb{M}_{3,2}^{(a)}(E'')\mathbb{T}_{1,1}^{(b)}(E')}{2}$$

$$\boxed{\text{z67}} \quad \mathbb{Q}_4^{(c)}(A_2'', a) = \mathbb{Q}_4^{(a)}(A_2'')\mathbb{Q}_0^{(b)}(A_1')$$

$$\boxed{\text{z68}} \quad \mathbb{Q}_4^{(c)}(A_2'', b) = \mathbb{M}_3^{(a)}(A_1'')\mathbb{M}_1^{(b)}(A_2')$$

$$\boxed{\text{z93}} \quad \mathbb{Q}_{1,1}^{(c)}(E', a) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_1')\mathbb{Q}_{1,1}^{(b)}(E')}{2}$$

$$\boxed{\text{z94}} \quad \mathbb{Q}_{1,2}^{(c)}(E', a) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_1')\mathbb{Q}_{1,2}^{(b)}(E')}{2}$$

$$\boxed{\text{z95}} \quad \mathbb{Q}_{1,1}^{(c)}(E', b) = \frac{\sqrt{42}\mathbb{Q}_{2,1}^{(a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{14} + \frac{\sqrt{42}\mathbb{Q}_{2,2}^{(a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{14} - \frac{\sqrt{14}\mathbb{Q}_2^{(a)}(A_1')\mathbb{Q}_{1,1}^{(b)}(E')}{14}$$

$$\boxed{\text{z96}} \quad \mathbb{Q}_{1,2}^{(c)}(E', b) = \frac{\sqrt{42}\mathbb{Q}_{2,1}^{(a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{14} - \frac{\sqrt{42}\mathbb{Q}_{2,2}^{(a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{14} - \frac{\sqrt{14}\mathbb{Q}_2^{(a)}(A_1')\mathbb{Q}_{1,2}^{(b)}(E')}{14}$$

$$\boxed{\text{z97}} \quad \mathbb{Q}_{1,1}^{(c)}(E', c) = -\frac{\sqrt{2}\mathbb{M}_1^{(a)}(A_2')\mathbb{T}_{1,2}^{(b)}(E')}{2}$$

$$\boxed{\text{z98}} \quad \mathbb{Q}_{1,2}^{(c)}(E', c) = \frac{\sqrt{2}\mathbb{M}_1^{(a)}(A_2')\mathbb{T}_{1,1}^{(b)}(E')}{2}$$

$$\boxed{\text{z99}} \quad \mathbb{Q}_{2,1}^{(c)}(E', a) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E')\mathbb{Q}_0^{(b)}(A_1')}{2}$$

$$\boxed{\text{z100}} \quad \mathbb{Q}_{2,2}^{(c)}(E', a) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E')\mathbb{Q}_0^{(b)}(A_1')}{2}$$

$$\boxed{\text{z101}} \quad \mathbb{Q}_{2,1}^{(c)}(E', b) = \frac{\sqrt{2}\mathbb{M}_{3,2}^{(a)}(E')\mathbb{M}_1^{(b)}(A_2')}{2}$$

$$\boxed{\text{z102}} \quad \mathbb{Q}_{2,2}^{(c)}(E', b) = -\frac{\sqrt{2}\mathbb{M}_{3,1}^{(a)}(E')\mathbb{M}_1^{(b)}(A'_2)}{2}$$

$$\boxed{\text{z103}} \quad \mathbb{Q}_{3,1}^{(c)}(E', a) = \frac{\sqrt{7}\mathbb{Q}_{2,1}^{(a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{14} + \frac{\sqrt{7}\mathbb{Q}_{2,2}^{(a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{14} + \frac{\sqrt{21}\mathbb{Q}_2^{(a)}(A'_1)\mathbb{Q}_{1,1}^{(b)}(E')}{7}$$

$$\boxed{\text{z104}} \quad \mathbb{Q}_{3,2}^{(c)}(E', a) = \frac{\sqrt{7}\mathbb{Q}_{2,1}^{(a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{14} - \frac{\sqrt{7}\mathbb{Q}_{2,2}^{(a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{14} + \frac{\sqrt{21}\mathbb{Q}_2^{(a)}(A'_1)\mathbb{Q}_{1,2}^{(b)}(E')}{7}$$

$$\boxed{\text{z105}} \quad \mathbb{Q}_{3,1}^{(c)}(E', b) = \frac{\sqrt{35}\mathbb{Q}_{4,1}^{(a)}(E', 2)\mathbb{Q}_{1,2}^{(b)}(E')}{14} + \frac{\sqrt{35}\mathbb{Q}_{4,2}^{(a)}(E', 2)\mathbb{Q}_{1,1}^{(b)}(E')}{14} - \frac{\sqrt{7}\mathbb{Q}_4^{(a)}(A'_1)\mathbb{Q}_{1,1}^{(b)}(E')}{7}$$

$$\boxed{\text{z106}} \quad \mathbb{Q}_{3,2}^{(c)}(E', b) = \frac{\sqrt{35}\mathbb{Q}_{4,1}^{(a)}(E', 2)\mathbb{Q}_{1,1}^{(b)}(E')}{14} - \frac{\sqrt{35}\mathbb{Q}_{4,2}^{(a)}(E', 2)\mathbb{Q}_{1,2}^{(b)}(E')}{14} - \frac{\sqrt{7}\mathbb{Q}_4^{(a)}(A'_1)\mathbb{Q}_{1,2}^{(b)}(E')}{7}$$

$$\boxed{\text{z107}} \quad \mathbb{Q}_{3,1}^{(c)}(E', c) = -\frac{\sqrt{55}\mathbb{M}_{3,1}^{(a)}(E')\mathbb{T}_{1,2}^{(b)}(E')}{22} - \frac{\sqrt{55}\mathbb{M}_{3,2}^{(a)}(E')\mathbb{T}_{1,1}^{(b)}(E')}{22} - \frac{\sqrt{33}\mathbb{M}_3^{(a)}(A'_2)\mathbb{T}_{1,2}^{(b)}(E')}{11}$$

$$\boxed{\text{z108}} \quad \mathbb{Q}_{3,2}^{(c)}(E', c) = -\frac{\sqrt{55}\mathbb{M}_{3,1}^{(a)}(E')\mathbb{T}_{1,1}^{(b)}(E')}{22} + \frac{\sqrt{55}\mathbb{M}_{3,2}^{(a)}(E')\mathbb{T}_{1,2}^{(b)}(E')}{22} + \frac{\sqrt{33}\mathbb{M}_3^{(a)}(A'_2)\mathbb{T}_{1,1}^{(b)}(E')}{11}$$

$$\boxed{\text{z109}} \quad \mathbb{Q}_{4,1}^{(c)}(E', 1) = \frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E', 1)\mathbb{Q}_0^{(b)}(A'_1)}{2}$$

$$\boxed{\text{z110}} \quad \mathbb{Q}_{4,2}^{(c)}(E', 1) = \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E', 1)\mathbb{Q}_0^{(b)}(A'_1)}{2}$$

$$\boxed{\text{z111}} \quad \mathbb{Q}_{4,1}^{(c)}(E', 2) = \frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E', 2)\mathbb{Q}_0^{(b)}(A'_1)}{2}$$

$$\boxed{\text{z112}} \quad \mathbb{Q}_{4,2}^{(c)}(E', 2) = \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E', 2)\mathbb{Q}_0^{(b)}(A'_1)}{2}$$

$$\boxed{\text{z113}} \quad \mathbb{Q}_{5,1}^{(c)}(E', 1) = \frac{\mathbb{Q}_{4,1}^{(a)}(E', 1)\mathbb{Q}_{1,2}^{(b)}(E')}{2} + \frac{\mathbb{Q}_{4,2}^{(a)}(E', 1)\mathbb{Q}_{1,1}^{(b)}(E')}{2}$$

$$\boxed{\text{z114}} \quad \mathbb{Q}_{5,2}^{(c)}(E', 1) = \frac{\mathbb{Q}_{4,1}^{(a)}(E', 1)\mathbb{Q}_{1,1}^{(b)}(E')}{2} - \frac{\mathbb{Q}_{4,2}^{(a)}(E', 1)\mathbb{Q}_{1,2}^{(b)}(E')}{2}$$

$$\boxed{\text{z115}} \quad \mathbb{Q}_{5,1}^{(c)}(E', 2) = \frac{\sqrt{14}\mathbb{Q}_{4,1}^{(a)}(E', 2)\mathbb{Q}_{1,2}^{(b)}(E')}{14} + \frac{\sqrt{14}\mathbb{Q}_{4,2}^{(a)}(E', 2)\mathbb{Q}_{1,1}^{(b)}(E')}{14} + \frac{\sqrt{70}\mathbb{Q}_4^{(a)}(A'_1)\mathbb{Q}_{1,1}^{(b)}(E')}{14}$$

$$\boxed{\text{z116}} \quad \mathbb{Q}_{5,2}^{(c)}(E', 2) = \frac{\sqrt{14}\mathbb{Q}_{4,1}^{(a)}(E', 2)\mathbb{Q}_{1,1}^{(b)}(E')}{14} - \frac{\sqrt{14}\mathbb{Q}_{4,2}^{(a)}(E', 2)\mathbb{Q}_{1,2}^{(b)}(E')}{14} + \frac{\sqrt{70}\mathbb{Q}_4^{(a)}(A'_1)\mathbb{Q}_{1,2}^{(b)}(E')}{14}$$

$$\boxed{\text{z117}} \quad \mathbb{G}_{2,1}^{(c)}(E') = \frac{\sqrt{66}\mathbb{M}_{3,1}^{(a)}(E')\mathbb{T}_{1,2}^{(b)}(E')}{22} + \frac{\sqrt{66}\mathbb{M}_{3,2}^{(a)}(E')\mathbb{T}_{1,1}^{(b)}(E')}{22} - \frac{\sqrt{110}\mathbb{M}_3^{(a)}(A'_2)\mathbb{T}_{1,2}^{(b)}(E')}{22}$$

$$\boxed{\text{z118}} \quad \mathbb{G}_{2,2}^{(c)}(E') = \frac{\sqrt{66}\mathbb{M}_{3,1}^{(a)}(E')\mathbb{T}_{1,1}^{(b)}(E')}{22} - \frac{\sqrt{66}\mathbb{M}_{3,2}^{(a)}(E')\mathbb{T}_{1,2}^{(b)}(E')}{22} + \frac{\sqrt{110}\mathbb{M}_3^{(a)}(A'_2)\mathbb{T}_{1,1}^{(b)}(E')}{22}$$

$$\boxed{\text{z175}} \quad \mathbb{Q}_{2,1}^{(c)}(E'', a) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E'')\mathbb{Q}_0^{(b)}(A'_1)}{2}$$

$$\boxed{\text{z176}} \quad \mathbb{Q}_{2,2}^{(c)}(E'', a) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E'')\mathbb{Q}_0^{(b)}(A'_1)}{2}$$

$$\boxed{\text{z177}} \quad \mathbb{Q}_{2,1}^{(c)}(E'', b) = \frac{\sqrt{2}\mathbb{M}_{3,2}^{(a)}(E'')\mathbb{M}_1^{(b)}(A'_2)}{2}$$

$$\boxed{\text{z178}} \quad \mathbb{Q}_{2,2}^{(c)}(E'', b) = -\frac{\sqrt{2}\mathbb{M}_{3,1}^{(a)}(E'')\mathbb{M}_1^{(b)}(A'_2)}{2}$$

$$\boxed{\text{z179}} \quad \mathbb{Q}_{2,1}^{(c)}(E'', c) = \frac{\sqrt{2}\mathbb{M}_{1,2}^{(a)}(E'')\mathbb{M}_1^{(b)}(A'_2)}{2}$$

$$\boxed{\text{z180}} \quad \mathbb{Q}_{2,2}^{(c)}(E'', c) = -\frac{\sqrt{2}\mathbb{M}_{1,1}^{(a)}(E'')\mathbb{M}_1^{(b)}(A'_2)}{2}$$

$$\boxed{\text{z181}} \quad \mathbb{Q}_{3,1}^{(c)}(E'', a) = \frac{\mathbb{Q}_{2,1}^{(a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{2} + \frac{\mathbb{Q}_{2,2}^{(a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{2}$$

$$\boxed{\text{z182}} \quad \mathbb{Q}_{3,2}^{(c)}(E'', a) = \frac{\mathbb{Q}_{2,1}^{(a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{2} - \frac{\mathbb{Q}_{2,2}^{(a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{2}$$

$$\boxed{\text{z183}} \quad \mathbb{Q}_{3,1}^{(c)}(E'', b) = -\frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{8} - \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{8} - \frac{\sqrt{14}\mathbb{Q}_4^{(a)}(A''_1)\mathbb{Q}_{1,1}^{(b)}(E')}{8} - \frac{\sqrt{14}\mathbb{Q}_4^{(a)}(A''_2)\mathbb{Q}_{1,2}^{(b)}(E')}{8}$$

$$\boxed{\text{z184}} \quad \mathbb{Q}_{3,2}^{(c)}(E'', b) = -\frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{8} + \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{8} - \frac{\sqrt{14}\mathbb{Q}_4^{(a)}(A''_1)\mathbb{Q}_{1,2}^{(b)}(E')}{8} + \frac{\sqrt{14}\mathbb{Q}_4^{(a)}(A''_2)\mathbb{Q}_{1,1}^{(b)}(E')}{8}$$

$$\boxed{\text{z185}} \quad \mathbb{Q}_{3,1}^{(c)}(E'', c) = \frac{\sqrt{10}\mathbb{M}_{3,1}^{(a)}(E'')\mathbb{T}_{1,2}^{(b)}(E')}{8} + \frac{\sqrt{10}\mathbb{M}_{3,2}^{(a)}(E'')\mathbb{T}_{1,1}^{(b)}(E')}{8} + \frac{\sqrt{6}\mathbb{M}_3^{(a)}(A''_1)\mathbb{T}_{1,1}^{(b)}(E')}{8} - \frac{\sqrt{6}\mathbb{M}_3^{(a)}(A''_2)\mathbb{T}_{1,2}^{(b)}(E')}{8}$$

$$\boxed{\text{z186}} \quad \mathbb{Q}_{3,2}^{(c)}(E'', c) = \frac{\sqrt{10}\mathbb{M}_{3,1}^{(a)}(E'')\mathbb{T}_{1,1}^{(b)}(E')}{8} - \frac{\sqrt{10}\mathbb{M}_{3,2}^{(a)}(E'')\mathbb{T}_{1,2}^{(b)}(E')}{8} + \frac{\sqrt{6}\mathbb{M}_3^{(a)}(A_1'')\mathbb{T}_{1,2}^{(b)}(E')}{8} + \frac{\sqrt{6}\mathbb{M}_3^{(a)}(A_2'')\mathbb{T}_{1,1}^{(b)}(E')}{8}$$

$$\boxed{\text{z187}} \quad \mathbb{Q}_{4,1}^{(c)}(E'') = \frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E'')\mathbb{Q}_0^{(b)}(A'_1)}{2}$$

$$\boxed{\text{z188}} \quad \mathbb{Q}_{4,2}^{(c)}(E'') = \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E'')\mathbb{Q}_0^{(b)}(A'_1)}{2}$$

$$\boxed{\text{z189}} \quad \mathbb{Q}_{5,1}^{(c)}(E'', 1) = -\frac{\mathbb{Q}_4^{(a)}(A''_1)\mathbb{Q}_{1,1}^{(b)}(E')}{2} + \frac{\mathbb{Q}_4^{(a)}(A''_2)\mathbb{Q}_{1,2}^{(b)}(E')}{2}$$

$$\boxed{\text{z190}} \quad \mathbb{Q}_{5,2}^{(c)}(E'', 1) = -\frac{\mathbb{Q}_4^{(a)}(A''_1)\mathbb{Q}_{1,2}^{(b)}(E')}{2} - \frac{\mathbb{Q}_4^{(a)}(A''_2)\mathbb{Q}_{1,1}^{(b)}(E')}{2}$$

$$\boxed{\text{z191}} \quad \mathbb{Q}_{5,1}^{(c)}(E'', 2) = \frac{\sqrt{14}\mathbb{Q}_{4,1}^{(a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{8} + \frac{\sqrt{14}\mathbb{Q}_{4,2}^{(a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{8} - \frac{\sqrt{2}\mathbb{Q}_4^{(a)}(A''_1)\mathbb{Q}_{1,1}^{(b)}(E')}{8} - \frac{\sqrt{2}\mathbb{Q}_4^{(a)}(A''_2)\mathbb{Q}_{1,2}^{(b)}(E')}{8}$$

$$\boxed{\text{z192}} \quad \mathbb{Q}_{5,2}^{(c)}(E'', 2) = \frac{\sqrt{14}\mathbb{Q}_{4,1}^{(a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{8} - \frac{\sqrt{14}\mathbb{Q}_{4,2}^{(a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{8} - \frac{\sqrt{2}\mathbb{Q}_4^{(a)}(A''_1)\mathbb{Q}_{1,2}^{(b)}(E')}{8} + \frac{\sqrt{2}\mathbb{Q}_4^{(a)}(A''_2)\mathbb{Q}_{1,1}^{(b)}(E')}{8}$$

$$\boxed{\text{z193}} \quad \mathbb{G}_{2,1}^{(c)}(E'', a) = -\frac{\sqrt{6}\mathbb{M}_{3,1}^{(a)}(E'')\mathbb{T}_{1,2}^{(b)}(E')}{8} - \frac{\sqrt{6}\mathbb{M}_{3,2}^{(a)}(E'')\mathbb{T}_{1,1}^{(b)}(E')}{8} + \frac{\sqrt{10}\mathbb{M}_3^{(a)}(A''_1)\mathbb{T}_{1,1}^{(b)}(E')}{8} - \frac{\sqrt{10}\mathbb{M}_3^{(a)}(A''_2)\mathbb{T}_{1,2}^{(b)}(E')}{8}$$

$$\boxed{\text{z194}} \quad \mathbb{G}_{2,2}^{(c)}(E'', a) = -\frac{\sqrt{6}\mathbb{M}_{3,1}^{(a)}(E'')\mathbb{T}_{1,1}^{(b)}(E')}{8} + \frac{\sqrt{6}\mathbb{M}_{3,2}^{(a)}(E'')\mathbb{T}_{1,2}^{(b)}(E')}{8} + \frac{\sqrt{10}\mathbb{M}_3^{(a)}(A''_1)\mathbb{T}_{1,2}^{(b)}(E')}{8} + \frac{\sqrt{10}\mathbb{M}_3^{(a)}(A''_2)\mathbb{T}_{1,1}^{(b)}(E')}{8}$$

$$\boxed{\text{z195}} \quad \mathbb{G}_{2,1}^{(c)}(E'', b) = \frac{\mathbb{M}_{1,1}^{(a)}(E'')\mathbb{T}_{1,2}^{(b)}(E')}{2} + \frac{\mathbb{M}_{1,2}^{(a)}(E'')\mathbb{T}_{1,1}^{(b)}(E')}{2}$$

$$\boxed{\text{z196}} \quad \mathbb{G}_{2,2}^{(c)}(E'', b) = \frac{\mathbb{M}_{1,1}^{(a)}(E'')\mathbb{T}_{1,1}^{(b)}(E')}{2} - \frac{\mathbb{M}_{1,2}^{(a)}(E'')\mathbb{T}_{1,2}^{(b)}(E')}{2}$$

$$\boxed{\text{z197}} \quad \mathbb{G}_{4,1}^{(c)}(E'', 1) = -\frac{\mathbb{M}_3^{(a)}(A''_1)\mathbb{T}_{1,1}^{(b)}(E')}{2} - \frac{\mathbb{M}_3^{(a)}(A''_2)\mathbb{T}_{1,2}^{(b)}(E')}{2}$$

$$\boxed{\text{z198}} \quad \mathbb{G}_{4,2}^{(c)}(E'', 1) = -\frac{\mathbb{M}_3^{(a)}(A''_1)\mathbb{T}_{1,2}^{(b)}(E')}{2} + \frac{\mathbb{M}_3^{(a)}(A''_2)\mathbb{T}_{1,1}^{(b)}(E')}{2}$$

- S;Mo_001_1 : 'Mo'-'S' bond-cluster

* bra: $\langle d_v |, \langle d_{xy} |, \langle d_{xz} |, \langle d_{yz} |, \langle d_u |$

* ket: $|p_x\rangle, |p_y\rangle, |p_z\rangle$

* wyckoff: **6a@6n**

$$\boxed{\text{z15}} \quad \mathbb{Q}_0^{(c)}(A'_1) = \frac{\sqrt{3}\mathbb{Q}_{1,1}^{(a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{3} + \frac{\sqrt{3}\mathbb{Q}_{1,2}^{(a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{3} + \frac{\sqrt{3}\mathbb{Q}_1^{(a)}(A''_2)\mathbb{Q}_1^{(b)}(A''_2)}{3}$$

$$\boxed{\text{z16}} \quad \mathbb{Q}_2^{(c)}(A'_1, a) = \frac{\sqrt{14}\mathbb{Q}_{3,1}^{(a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{7} + \frac{\sqrt{14}\mathbb{Q}_{3,2}^{(a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{7} + \frac{\sqrt{21}\mathbb{Q}_3^{(a)}(A''_2)\mathbb{Q}_1^{(b)}(A''_2)}{7}$$

$$\boxed{\text{z17}} \quad \mathbb{Q}_2^{(c)}(A'_1, b) = -\frac{\sqrt{6}\mathbb{Q}_{1,1}^{(a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{6} - \frac{\sqrt{6}\mathbb{Q}_{1,2}^{(a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{6} + \frac{\sqrt{6}\mathbb{Q}_1^{(a)}(A''_2)\mathbb{Q}_1^{(b)}(A''_2)}{3}$$

$$\boxed{\text{z18}} \quad \mathbb{Q}_2^{(c)}(A'_1, c) = -\frac{\sqrt{2}\mathbb{G}_{2,1}^{(a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{2} - \frac{\sqrt{2}\mathbb{G}_{2,2}^{(a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{2}$$

$$\boxed{\text{z19}} \quad \mathbb{Q}_3^{(c)}(A'_1, a) = \mathbb{Q}_3^{(a)}(A'_1)\mathbb{Q}_0^{(b)}(A'_1)$$

$$\boxed{\text{z20}} \quad \mathbb{Q}_3^{(c)}(A'_1, b) = -\frac{\sqrt{2}\mathbb{Q}_{3,1}^{(a)}(E'')\mathbb{Q}_{2,1}^{(b)}(E'')}{2} - \frac{\sqrt{2}\mathbb{Q}_{3,2}^{(a)}(E'')\mathbb{Q}_{2,2}^{(b)}(E'')}{2}$$

$$\boxed{\text{z21}} \quad \mathbb{Q}_3^{(c)}(A'_1, c) = \frac{\sqrt{2}\mathbb{G}_{2,1}^{(a)}(E'')\mathbb{Q}_{2,1}^{(b)}(E'')}{2} + \frac{\sqrt{2}\mathbb{G}_{2,2}^{(a)}(E'')\mathbb{Q}_{2,2}^{(b)}(E'')}{2}$$

$$\boxed{\text{z22}} \quad \mathbb{Q}_4^{(c)}(A'_1) = -\frac{\sqrt{42}\mathbb{Q}_{3,1}^{(a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{14} - \frac{\sqrt{42}\mathbb{Q}_{3,2}^{(a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{14} + \frac{2\sqrt{7}\mathbb{Q}_3^{(a)}(A''_2)\mathbb{Q}_1^{(b)}(A''_2)}{7}$$

$$\boxed{\text{z33}} \quad \mathbb{Q}_4^{(c)}(A''_1) = -\frac{\sqrt{6}\mathbb{Q}_{3,1}^{(a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{4} - \frac{\sqrt{6}\mathbb{Q}_{3,2}^{(a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{4} + \frac{\mathbb{Q}_3^{(a)}(A''_2)\mathbb{Q}_1^{(b)}(A''_2)}{2}$$

$$\boxed{\text{z34}} \quad \mathbb{G}_0^{(c)}(A''_1) = \frac{\sqrt{2}\mathbb{G}_{2,1}^{(a)}(E')\mathbb{Q}_{2,1}^{(b)}(E'')}{2} + \frac{\sqrt{2}\mathbb{G}_{2,2}^{(a)}(E')\mathbb{Q}_{2,2}^{(b)}(E'')}{2}$$

$$\boxed{\text{z35}} \quad \mathbb{G}_2^{(c)}(A''_1, a) = \frac{\sqrt{2}\mathbb{Q}_{3,1}^{(a)}(E')\mathbb{Q}_{2,1}^{(b)}(E'')}{2} + \frac{\sqrt{2}\mathbb{Q}_{3,2}^{(a)}(E')\mathbb{Q}_{2,2}^{(b)}(E'')}{2}$$

$$\boxed{\text{z36}} \quad \mathbb{G}_2^{(c)}(A''_1, b) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E')\mathbb{Q}_{2,1}^{(b)}(E'')}{2} + \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E')\mathbb{Q}_{2,2}^{(b)}(E'')}{2}$$

$$\boxed{\text{z37}} \quad \mathbb{G}_2^{(c)}(A''_1, c) = \mathbb{G}_2^{(a)}(A''_1)\mathbb{Q}_0^{(b)}(A'_1)$$

$$\boxed{\text{z38}} \quad \mathbb{G}_3^{(c)}(A_1'', a) = -\frac{\sqrt{2}\mathbb{Q}_{3,1}^{(a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{4} - \frac{\sqrt{2}\mathbb{Q}_{3,2}^{(a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{4} - \frac{\sqrt{3}\mathbb{Q}_3^{(a)}(A_2')\mathbb{Q}_1^{(b)}(A_2'')}{2}$$

$$\boxed{\text{z39}} \quad \mathbb{G}_3^{(c)}(A_1'', b) = \frac{\sqrt{2}\mathbb{G}_{2,1}^{(a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{2} + \frac{\sqrt{2}\mathbb{G}_{2,2}^{(a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{2}$$

$$\boxed{\text{z50}} \quad \mathbb{Q}_3^{(c)}(A_2', a) = \mathbb{Q}_3^{(a)}(A_2')\mathbb{Q}_0^{(b)}(A_1')$$

$$\boxed{\text{z51}} \quad \mathbb{Q}_3^{(c)}(A_2', b) = \frac{\sqrt{2}\mathbb{Q}_{3,1}^{(a)}(E'')\mathbb{Q}_{2,2}^{(b)}(E'')}{2} - \frac{\sqrt{2}\mathbb{Q}_{3,2}^{(a)}(E'')\mathbb{Q}_{2,1}^{(b)}(E'')}{2}$$

$$\boxed{\text{z52}} \quad \mathbb{Q}_3^{(c)}(A_2', c) = -\frac{\sqrt{2}\mathbb{G}_{2,1}^{(a)}(E'')\mathbb{Q}_{2,2}^{(b)}(E'')}{2} + \frac{\sqrt{2}\mathbb{G}_{2,2}^{(a)}(E'')\mathbb{Q}_{2,1}^{(b)}(E'')}{2}$$

$$\boxed{\text{z53}} \quad \mathbb{G}_1^{(c)}(A_2', a) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{2} - \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{2}$$

$$\boxed{\text{z54}} \quad \mathbb{G}_1^{(c)}(A_2', b) = \frac{\sqrt{30}\mathbb{G}_{2,1}^{(a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{10} - \frac{\sqrt{30}\mathbb{G}_{2,2}^{(a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{10} + \frac{\sqrt{10}\mathbb{G}_2^{(a)}(A_1'')\mathbb{Q}_1^{(b)}(A_2'')}{5}$$

$$\boxed{\text{z55}} \quad \mathbb{G}_3^{(c)}(A_2', a) = \frac{\sqrt{2}\mathbb{Q}_{3,1}^{(a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{2} - \frac{\sqrt{2}\mathbb{Q}_{3,2}^{(a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{2}$$

$$\boxed{\text{z56}} \quad \mathbb{G}_3^{(c)}(A_2', b) = -\frac{\sqrt{5}\mathbb{G}_{2,1}^{(a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{5} + \frac{\sqrt{5}\mathbb{G}_{2,2}^{(a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{5} + \frac{\sqrt{15}\mathbb{G}_2^{(a)}(A_1'')\mathbb{Q}_1^{(b)}(A_2'')}{5}$$

$$\boxed{\text{z69}} \quad \mathbb{Q}_1^{(c)}(A_2'', a) = -\frac{\sqrt{2}\mathbb{Q}_{3,1}^{(a)}(E')\mathbb{Q}_{2,2}^{(b)}(E'')}{2} + \frac{\sqrt{2}\mathbb{Q}_{3,2}^{(a)}(E')\mathbb{Q}_{2,1}^{(b)}(E'')}{2}$$

$$\boxed{\text{z70}} \quad \mathbb{Q}_1^{(c)}(A_2'', b) = \mathbb{Q}_1^{(a)}(A_2'')\mathbb{Q}_0^{(b)}(A_1')$$

$$\boxed{\text{z71}} \quad \mathbb{Q}_1^{(c)}(A_2'', c) = -\frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E')\mathbb{Q}_{2,2}^{(b)}(E'')}{2} + \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E')\mathbb{Q}_{2,1}^{(b)}(E'')}{2}$$

$$\boxed{\text{z72}} \quad \mathbb{Q}_1^{(c)}(A_2'', d) = \frac{\sqrt{2}\mathbb{G}_{2,1}^{(a)}(E')\mathbb{Q}_{2,2}^{(b)}(E'')}{2} - \frac{\sqrt{2}\mathbb{G}_{2,2}^{(a)}(E')\mathbb{Q}_{2,1}^{(b)}(E'')}{2}$$

$$\boxed{\text{z73}} \quad \mathbb{Q}_3^{(c)}(A_2'') = \mathbb{Q}_3^{(a)}(A_2'')\mathbb{Q}_0^{(b)}(A_1')$$

$$\boxed{z74} \quad \mathbb{Q}_4^{(c)}(A_2'') = -\frac{\sqrt{6}\mathbb{Q}_{3,1}^{(a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{4} + \frac{\sqrt{6}\mathbb{Q}_{3,2}^{(a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{4} + \frac{\mathbb{Q}_3^{(a)}(A'_1)\mathbb{Q}_1^{(b)}(A_2'')}{2}$$

$$\boxed{z75} \quad \mathbb{G}_3^{(c)}(A_2'', a) = \frac{\sqrt{2}\mathbb{Q}_{3,1}^{(a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{4} - \frac{\sqrt{2}\mathbb{Q}_{3,2}^{(a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{4} + \frac{\sqrt{3}\mathbb{Q}_3^{(a)}(A'_1)\mathbb{Q}_1^{(b)}(A_2'')}{2}$$

$$\boxed{z76} \quad \mathbb{G}_3^{(c)}(A_2'', b) = -\frac{\sqrt{2}\mathbb{G}_{2,1}^{(a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{2} + \frac{\sqrt{2}\mathbb{G}_{2,2}^{(a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{2}$$

$$\boxed{z119} \quad \mathbb{Q}_{1,1}^{(c)}(E', a) = \frac{\sqrt{130}\mathbb{Q}_{3,1}^{(a)}(E'')\mathbb{Q}_{2,2}^{(b)}(E'')}{26} + \frac{\sqrt{130}\mathbb{Q}_{3,2}^{(a)}(E'')\mathbb{Q}_{2,1}^{(b)}(E'')}{26} + \frac{\sqrt{78}\mathbb{Q}_3^{(a)}(A_2'')\mathbb{Q}_{2,2}^{(b)}(E'')}{26}$$

$$\boxed{z120} \quad \mathbb{Q}_{1,2}^{(c)}(E', a) = \frac{\sqrt{130}\mathbb{Q}_{3,1}^{(a)}(E'')\mathbb{Q}_{2,1}^{(b)}(E'')}{26} - \frac{\sqrt{130}\mathbb{Q}_{3,2}^{(a)}(E'')\mathbb{Q}_{2,2}^{(b)}(E'')}{26} - \frac{\sqrt{78}\mathbb{Q}_3^{(a)}(A_2'')\mathbb{Q}_{2,1}^{(b)}(E'')}{26}$$

$$\boxed{z121} \quad \mathbb{Q}_{1,1}^{(c)}(E', b) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E')\mathbb{Q}_0^{(b)}(A'_1)}{2}$$

$$\boxed{z122} \quad \mathbb{Q}_{1,2}^{(c)}(E', b) = \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E')\mathbb{Q}_0^{(b)}(A'_1)}{2}$$

$$\boxed{z123} \quad \mathbb{Q}_{1,1}^{(c)}(E', c) = -\frac{\sqrt{2}\mathbb{Q}_1^{(a)}(A_2'')\mathbb{Q}_{2,2}^{(b)}(E'')}{2}$$

$$\boxed{z124} \quad \mathbb{Q}_{1,2}^{(c)}(E', c) = \frac{\sqrt{2}\mathbb{Q}_1^{(a)}(A_2'')\mathbb{Q}_{2,1}^{(b)}(E'')}{2}$$

$$\boxed{z125} \quad \mathbb{Q}_{1,1}^{(c)}(E', d) = -\frac{\sqrt{10}\mathbb{G}_{2,1}^{(a)}(E'')\mathbb{Q}_{2,2}^{(b)}(E'')}{10} - \frac{\sqrt{10}\mathbb{G}_{2,2}^{(a)}(E'')\mathbb{Q}_{2,1}^{(b)}(E'')}{10} - \frac{\sqrt{30}\mathbb{G}_2^{(a)}(A_1'')\mathbb{Q}_{2,1}^{(b)}(E'')}{10}$$

$$\boxed{z126} \quad \mathbb{Q}_{1,2}^{(c)}(E', d) = -\frac{\sqrt{10}\mathbb{G}_{2,1}^{(a)}(E'')\mathbb{Q}_{2,1}^{(b)}(E'')}{10} + \frac{\sqrt{10}\mathbb{G}_{2,2}^{(a)}(E'')\mathbb{Q}_{2,2}^{(b)}(E'')}{10} - \frac{\sqrt{30}\mathbb{G}_2^{(a)}(A_1'')\mathbb{Q}_{2,2}^{(b)}(E'')}{10}$$

$$\boxed{z127} \quad \mathbb{Q}_{2,1}^{(c)}(E', a) = -\frac{\sqrt{21}\mathbb{Q}_{3,1}^{(a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{42} + \frac{\sqrt{210}\mathbb{Q}_{3,2}^{(a)}(E'')\mathbb{Q}_1^{(b)}(A_2'')}{42} - \frac{\sqrt{21}\mathbb{Q}_{3,2}^{(a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{42} + \frac{\sqrt{35}\mathbb{Q}_3^{(a)}(A'_1)\mathbb{Q}_{1,1}^{(b)}(E')}{14} - \frac{\sqrt{35}\mathbb{Q}_3^{(a)}(A'_2)\mathbb{Q}_{1,2}^{(b)}(E')}{14}$$

$$\boxed{z128} \quad \mathbb{Q}_{2,2}^{(c)}(E', a) = -\frac{\sqrt{210}\mathbb{Q}_{3,1}^{(a)}(E'')\mathbb{Q}_1^{(b)}(A_2'')}{42} - \frac{\sqrt{21}\mathbb{Q}_{3,1}^{(a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{42} + \frac{\sqrt{21}\mathbb{Q}_{3,2}^{(a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{42} + \frac{\sqrt{35}\mathbb{Q}_3^{(a)}(A'_1)\mathbb{Q}_{1,2}^{(b)}(E')}{14} + \frac{\sqrt{35}\mathbb{Q}_3^{(a)}(A'_2)\mathbb{Q}_{1,1}^{(b)}(E')}{14}$$

$$\boxed{z129} \quad \mathbb{Q}_{2,1}^{(c)}(E', b) = \frac{\mathbb{Q}_{1,1}^{(a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{2} + \frac{\mathbb{Q}_{1,2}^{(a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{2}$$

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

$$\boxed{\text{z131}} \quad \mathbb{Q}_{2,1}^{(c)}(E', c) = -\frac{\sqrt{3}\mathbb{G}_{2,1}^{(a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{6} - \frac{\sqrt{3}\mathbb{G}_{2,2}^{(a)}(E'')\mathbb{Q}_1^{(b)}(A_2'')}{3} - \frac{\sqrt{3}\mathbb{G}_{2,2}^{(a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{6}$$

$$\boxed{\text{z132}} \quad \mathbb{Q}_{2,2}^{(c)}(E', c) = \frac{\sqrt{3}\mathbb{G}_{2,1}^{(a)}(E'')\mathbb{Q}_1^{(b)}(A_2'')}{3} - \frac{\sqrt{3}\mathbb{G}_{2,1}^{(a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{6} + \frac{\sqrt{3}\mathbb{G}_{2,2}^{(a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{6}$$

$$\boxed{\text{z133}} \quad \mathbb{Q}_{3,1}^{(c)}(E', a) = \frac{\sqrt{2}\mathbb{Q}_{3,1}^{(a)}(E')\mathbb{Q}_0^{(b)}(A'_1)}{2}$$

$$\boxed{\text{z134}} \quad \mathbb{Q}_{3,2}^{(c)}(E', a) = \frac{\sqrt{2}\mathbb{Q}_{3,2}^{(a)}(E')\mathbb{Q}_0^{(b)}(A'_1)}{2}$$

$$\boxed{\text{z135}} \quad \mathbb{Q}_{3,1}^{(c)}(E', b) = \frac{\sqrt{39}\mathbb{Q}_{3,1}^{(a)}(E'')\mathbb{Q}_{2,2}^{(b)}(E'')}{26} + \frac{\sqrt{39}\mathbb{Q}_{3,2}^{(a)}(E'')\mathbb{Q}_{2,1}^{(b)}(E'')}{26} - \frac{\sqrt{65}\mathbb{Q}_3^{(a)}(A_2'')\mathbb{Q}_{2,2}^{(b)}(E'')}{13}$$

$$\boxed{\text{z136}} \quad \mathbb{Q}_{3,2}^{(c)}(E', b) = \frac{\sqrt{39}\mathbb{Q}_{3,1}^{(a)}(E'')\mathbb{Q}_{2,1}^{(b)}(E'')}{26} - \frac{\sqrt{39}\mathbb{Q}_{3,2}^{(a)}(E'')\mathbb{Q}_{2,2}^{(b)}(E'')}{26} + \frac{\sqrt{65}\mathbb{Q}_3^{(a)}(A_2'')\mathbb{Q}_{2,1}^{(b)}(E'')}{13}$$

$$\boxed{\text{z137}} \quad \mathbb{Q}_{3,1}^{(c)}(E', c) = \frac{\sqrt{15}\mathbb{G}_{2,1}^{(a)}(E'')\mathbb{Q}_{2,2}^{(b)}(E'')}{10} + \frac{\sqrt{15}\mathbb{G}_{2,2}^{(a)}(E'')\mathbb{Q}_{2,1}^{(b)}(E'')}{10} - \frac{\sqrt{5}\mathbb{G}_2^{(a)}(A_1'')\mathbb{Q}_{2,1}^{(b)}(E'')}{5}$$

$$\boxed{\text{z138}} \quad \mathbb{Q}_{3,2}^{(c)}(E', c) = \frac{\sqrt{15}\mathbb{G}_{2,1}^{(a)}(E'')\mathbb{Q}_{2,1}^{(b)}(E'')}{10} - \frac{\sqrt{15}\mathbb{G}_{2,2}^{(a)}(E'')\mathbb{Q}_{2,2}^{(b)}(E'')}{10} - \frac{\sqrt{5}\mathbb{G}_2^{(a)}(A_1'')\mathbb{Q}_{2,2}^{(b)}(E'')}{5}$$

$$\boxed{\text{z139}} \quad \mathbb{Q}_{4,1}^{(c)}(E', 1) = -\frac{\mathbb{Q}_3^{(a)}(A'_1)\mathbb{Q}_{1,1}^{(b)}(E')}{2} - \frac{\mathbb{Q}_3^{(a)}(A'_2)\mathbb{Q}_{1,2}^{(b)}(E')}{2}$$

$$\boxed{\text{z140}} \quad \mathbb{Q}_{4,2}^{(c)}(E', 1) = -\frac{\mathbb{Q}_3^{(a)}(A'_1)\mathbb{Q}_{1,2}^{(b)}(E')}{2} + \frac{\mathbb{Q}_3^{(a)}(A'_2)\mathbb{Q}_{1,1}^{(b)}(E')}{2}$$

$$\boxed{\text{z141}} \quad \mathbb{Q}_{4,1}^{(c)}(E', 2) = \frac{\sqrt{105}\mathbb{Q}_{3,1}^{(a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{28} + \frac{\sqrt{42}\mathbb{Q}_{3,2}^{(a)}(E'')\mathbb{Q}_1^{(b)}(A_2'')}{14} + \frac{\sqrt{105}\mathbb{Q}_{3,2}^{(a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{28} - \frac{\sqrt{7}\mathbb{Q}_3^{(a)}(A'_1)\mathbb{Q}_{1,1}^{(b)}(E')}{28} + \frac{\sqrt{7}\mathbb{Q}_3^{(a)}(A'_2)\mathbb{Q}_{1,2}^{(b)}(E')}{28}$$

$$\boxed{\text{z142}} \quad \mathbb{Q}_{4,2}^{(c)}(E', 2) = -\frac{\sqrt{42}\mathbb{Q}_{3,1}^{(a)}(E'')\mathbb{Q}_1^{(b)}(A_2'')}{14} + \frac{\sqrt{105}\mathbb{Q}_{3,1}^{(a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{28} - \frac{\sqrt{105}\mathbb{Q}_{3,2}^{(a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{28} - \frac{\sqrt{7}\mathbb{Q}_3^{(a)}(A'_1)\mathbb{Q}_{1,2}^{(b)}(E')}{28} - \frac{\sqrt{7}\mathbb{Q}_3^{(a)}(A'_2)\mathbb{Q}_{1,1}^{(b)}(E')}{28}$$

$$\boxed{\text{z143}} \quad \mathbb{G}_{2,1}^{(c)}(E') = \frac{\sqrt{2}\mathbb{G}_{2,1}^{(a)}(E')\mathbb{Q}_0^{(b)}(A'_1)}{2}$$

$$\boxed{\text{z144}} \quad \mathbb{G}_{2,2}^{(c)}(E') = \frac{\sqrt{2}\mathbb{G}_{2,2}^{(a)}(E')\mathbb{Q}_0^{(b)}(A'_1)}{2}$$

$$\boxed{\text{z145}} \quad \mathbb{G}_{3,1}^{(c)}(E', a) = \frac{\sqrt{15}\mathbb{Q}_{3,1}^{(a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{12} - \frac{\sqrt{6}\mathbb{Q}_{3,2}^{(a)}(E'')\mathbb{Q}_1^{(b)}(A''_2)}{6} + \frac{\sqrt{15}\mathbb{Q}_{3,2}^{(a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{12} + \frac{\mathbb{Q}_3^{(a)}(A'_1)\mathbb{Q}_{1,1}^{(b)}(E')}{4} - \frac{\mathbb{Q}_3^{(a)}(A'_2)\mathbb{Q}_{1,2}^{(b)}(E')}{4}$$

$$\boxed{\text{z146}} \quad \mathbb{G}_{3,2}^{(c)}(E', a) = \frac{\sqrt{6}\mathbb{Q}_{3,1}^{(a)}(E'')\mathbb{Q}_1^{(b)}(A''_2)}{6} + \frac{\sqrt{15}\mathbb{Q}_{3,1}^{(a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{12} - \frac{\sqrt{15}\mathbb{Q}_{3,2}^{(a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{12} + \frac{\mathbb{Q}_3^{(a)}(A'_1)\mathbb{Q}_{1,2}^{(b)}(E')}{4} + \frac{\mathbb{Q}_3^{(a)}(A'_2)\mathbb{Q}_{1,1}^{(b)}(E')}{4}$$

$$\boxed{\text{z147}} \quad \mathbb{G}_{3,1}^{(c)}(E', b) = \frac{\sqrt{6}\mathbb{G}_{2,1}^{(a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{6} - \frac{\sqrt{6}\mathbb{G}_{2,2}^{(a)}(E'')\mathbb{Q}_1^{(b)}(A''_2)}{6} + \frac{\sqrt{6}\mathbb{G}_{2,2}^{(a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{6}$$

$$\boxed{\text{z148}} \quad \mathbb{G}_{3,2}^{(c)}(E', b) = \frac{\sqrt{6}\mathbb{G}_{2,1}^{(a)}(E'')\mathbb{Q}_1^{(b)}(A''_2)}{6} + \frac{\sqrt{6}\mathbb{G}_{2,1}^{(a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{6} - \frac{\sqrt{6}\mathbb{G}_{2,2}^{(a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{6}$$

$$\boxed{\text{z199}} \quad \mathbb{Q}_{2,1}^{(c)}(E'', a) = \frac{\sqrt{210}\mathbb{Q}_{3,1}^{(a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{42} + \frac{\sqrt{210}\mathbb{Q}_{3,2}^{(a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{42} + \frac{2\sqrt{21}\mathbb{Q}_{3,2}^{(a)}(E')\mathbb{Q}_1^{(b)}(A''_2)}{21} - \frac{\sqrt{14}\mathbb{Q}_3^{(a)}(A''_2)\mathbb{Q}_{1,2}^{(b)}(E')}{14}$$

$$\boxed{\text{z200}} \quad \mathbb{Q}_{2,2}^{(c)}(E'', a) = \frac{\sqrt{210}\mathbb{Q}_{3,1}^{(a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{42} - \frac{2\sqrt{21}\mathbb{Q}_{3,1}^{(a)}(E')\mathbb{Q}_1^{(b)}(A''_2)}{21} - \frac{\sqrt{210}\mathbb{Q}_{3,2}^{(a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{42} + \frac{\sqrt{14}\mathbb{Q}_3^{(a)}(A''_2)\mathbb{Q}_{1,1}^{(b)}(E')}{14}$$

$$\boxed{\text{z201}} \quad \mathbb{Q}_{2,1}^{(c)}(E'', b) = \frac{\mathbb{Q}_{1,2}^{(a)}(E')\mathbb{Q}_1^{(b)}(A''_2)}{2} + \frac{\mathbb{Q}_1^{(a)}(A''_2)\mathbb{Q}_{1,2}^{(b)}(E')}{2}$$

$$\boxed{\text{z202}} \quad \mathbb{Q}_{2,2}^{(c)}(E'', b) = -\frac{\mathbb{Q}_{1,1}^{(a)}(E')\mathbb{Q}_1^{(b)}(A''_2)}{2} - \frac{\mathbb{Q}_1^{(a)}(A''_2)\mathbb{Q}_{1,1}^{(b)}(E')}{2}$$

$$\boxed{\text{z203}} \quad \mathbb{Q}_{2,1}^{(c)}(E'', c) = \frac{\sqrt{3}\mathbb{G}_{2,1}^{(a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{6} + \frac{\sqrt{3}\mathbb{G}_{2,2}^{(a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{6} + \frac{\sqrt{3}\mathbb{G}_{2,2}^{(a)}(E')\mathbb{Q}_1^{(b)}(A''_2)}{6} + \frac{\mathbb{G}_2^{(a)}(A''_1)\mathbb{Q}_{1,1}^{(b)}(E')}{2}$$

$$\boxed{\text{z204}} \quad \mathbb{Q}_{2,2}^{(c)}(E'', c) = \frac{\sqrt{3}\mathbb{G}_{2,1}^{(a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{6} - \frac{\sqrt{3}\mathbb{G}_{2,1}^{(a)}(E')\mathbb{Q}_1^{(b)}(A''_2)}{6} - \frac{\sqrt{3}\mathbb{G}_{2,2}^{(a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{6} + \frac{\mathbb{G}_2^{(a)}(A''_1)\mathbb{Q}_{1,2}^{(b)}(E')}{2}$$

$$\boxed{\text{z205}} \quad \mathbb{Q}_{3,1}^{(c)}(E'', a) = \frac{\sqrt{2}\mathbb{Q}_{3,1}^{(a)}(E'')\mathbb{Q}_0^{(b)}(A'_1)}{2}$$

$$\boxed{\text{z206}} \quad \mathbb{Q}_{3,2}^{(c)}(E'', a) = \frac{\sqrt{2}\mathbb{Q}_{3,2}^{(a)}(E'')\mathbb{Q}_0^{(b)}(A'_1)}{2}$$

$$\boxed{\text{z207}} \quad \mathbb{Q}_{3,1}^{(c)}(E'', b) = \frac{\sqrt{6}\mathbb{Q}_{3,1}^{(a)}(E')\mathbb{Q}_{2,2}^{(b)}(E'')}{8} + \frac{\sqrt{6}\mathbb{Q}_{3,2}^{(a)}(E')\mathbb{Q}_{2,1}^{(b)}(E'')}{8} - \frac{\sqrt{10}\mathbb{Q}_3^{(a)}(A'_1)\mathbb{Q}_{2,1}^{(b)}(E'')}{8} + \frac{\sqrt{10}\mathbb{Q}_3^{(a)}(A'_2)\mathbb{Q}_{2,2}^{(b)}(E'')}{8}$$

$$\boxed{\text{z208}} \quad \mathbb{Q}_{3,2}^{(c)}(E'', b) = \frac{\sqrt{6}\mathbb{Q}_{3,1}^{(a)}(E')\mathbb{Q}_{2,1}^{(b)}(E'')}{8} - \frac{\sqrt{6}\mathbb{Q}_{3,2}^{(a)}(E')\mathbb{Q}_{2,2}^{(b)}(E'')}{8} - \frac{\sqrt{10}\mathbb{Q}_3^{(a)}(A'_1)\mathbb{Q}_{2,2}^{(b)}(E'')}{8} - \frac{\sqrt{10}\mathbb{Q}_3^{(a)}(A'_2)\mathbb{Q}_{2,1}^{(b)}(E'')}{8}$$

$$\boxed{\text{z209}} \quad \mathbb{Q}_{3,1}^{(c)}(E'', c) = \frac{\mathbb{Q}_{1,1}^{(a)}(E')\mathbb{Q}_{2,2}^{(b)}(E'')}{2} + \frac{\mathbb{Q}_{1,2}^{(a)}(E')\mathbb{Q}_{2,1}^{(b)}(E'')}{2}$$

$$\boxed{\text{z210}} \quad \mathbb{Q}_{3,2}^{(c)}(E'', c) = \frac{\mathbb{Q}_{1,1}^{(a)}(E')\mathbb{Q}_{2,1}^{(b)}(E'')}{2} - \frac{\mathbb{Q}_{1,2}^{(a)}(E')\mathbb{Q}_{2,2}^{(b)}(E'')}{2}$$

$$\boxed{\text{z211}} \quad \mathbb{Q}_{4,1}^{(c)}(E'') = -\frac{\sqrt{21}\mathbb{Q}_{3,1}^{(a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{28} - \frac{\sqrt{21}\mathbb{Q}_{3,2}^{(a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{28} + \frac{\sqrt{210}\mathbb{Q}_{3,2}^{(a)}(E')\mathbb{Q}_1^{(b)}(A''_2)}{28} + \frac{\sqrt{35}\mathbb{Q}_3^{(a)}(A''_2)\mathbb{Q}_{1,2}^{(b)}(E')}{14}$$

$$\boxed{\text{z212}} \quad \mathbb{Q}_{4,2}^{(c)}(E'') = -\frac{\sqrt{21}\mathbb{Q}_{3,1}^{(a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{28} - \frac{\sqrt{210}\mathbb{Q}_{3,1}^{(a)}(E')\mathbb{Q}_1^{(b)}(A''_2)}{28} + \frac{\sqrt{21}\mathbb{Q}_{3,2}^{(a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{28} - \frac{\sqrt{35}\mathbb{Q}_3^{(a)}(A''_2)\mathbb{Q}_{1,1}^{(b)}(E')}{14}$$

$$\boxed{\text{z213}} \quad \mathbb{Q}_{5,1}^{(c)}(E'', 1) = \frac{\mathbb{Q}_3^{(a)}(A'_1)\mathbb{Q}_{2,1}^{(b)}(E'')}{2} + \frac{\mathbb{Q}_3^{(a)}(A'_2)\mathbb{Q}_{2,2}^{(b)}(E'')}{2}$$

$$\boxed{\text{z214}} \quad \mathbb{Q}_{5,2}^{(c)}(E'', 1) = \frac{\mathbb{Q}_3^{(a)}(A'_1)\mathbb{Q}_{2,2}^{(b)}(E'')}{2} - \frac{\mathbb{Q}_3^{(a)}(A'_2)\mathbb{Q}_{2,1}^{(b)}(E'')}{2}$$

$$\boxed{\text{z215}} \quad \mathbb{Q}_{5,1}^{(c)}(E'', 2) = \frac{\sqrt{10}\mathbb{Q}_{3,1}^{(a)}(E')\mathbb{Q}_{2,2}^{(b)}(E'')}{8} + \frac{\sqrt{10}\mathbb{Q}_{3,2}^{(a)}(E')\mathbb{Q}_{2,1}^{(b)}(E'')}{8} + \frac{\sqrt{6}\mathbb{Q}_3^{(a)}(A'_1)\mathbb{Q}_{2,1}^{(b)}(E'')}{8} - \frac{\sqrt{6}\mathbb{Q}_3^{(a)}(A'_2)\mathbb{Q}_{2,2}^{(b)}(E'')}{8}$$

$$\boxed{\text{z216}} \quad \mathbb{Q}_{5,2}^{(c)}(E'', 2) = \frac{\sqrt{10}\mathbb{Q}_{3,1}^{(a)}(E')\mathbb{Q}_{2,1}^{(b)}(E'')}{8} - \frac{\sqrt{10}\mathbb{Q}_{3,2}^{(a)}(E')\mathbb{Q}_{2,2}^{(b)}(E'')}{8} + \frac{\sqrt{6}\mathbb{Q}_3^{(a)}(A'_1)\mathbb{Q}_{2,2}^{(b)}(E'')}{8} + \frac{\sqrt{6}\mathbb{Q}_3^{(a)}(A'_2)\mathbb{Q}_{2,1}^{(b)}(E'')}{8}$$

$$\boxed{\text{z217}} \quad \mathbb{G}_{1,1}^{(c)}(E'', a) = \frac{\mathbb{Q}_{1,2}^{(a)}(E')\mathbb{Q}_1^{(b)}(A''_2)}{2} - \frac{\mathbb{Q}_1^{(a)}(A''_2)\mathbb{Q}_{1,2}^{(b)}(E')}{2}$$

$$\boxed{\text{z218}} \quad \mathbb{G}_{1,2}^{(c)}(E'', a) = -\frac{\mathbb{Q}_{1,1}^{(a)}(E')\mathbb{Q}_1^{(b)}(A''_2)}{2} + \frac{\mathbb{Q}_1^{(a)}(A''_2)\mathbb{Q}_{1,1}^{(b)}(E')}{2}$$

$$\boxed{\text{z219}} \quad \mathbb{G}_{1,1}^{(c)}(E'', b) = \frac{\sqrt{15}\mathbb{G}_{2,1}^{(a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{10} + \frac{\sqrt{15}\mathbb{G}_{2,2}^{(a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{10} - \frac{\sqrt{15}\mathbb{G}_{2,2}^{(a)}(E')\mathbb{Q}_1^{(b)}(A''_2)}{10} - \frac{\sqrt{5}\mathbb{G}_2^{(a)}(A''_1)\mathbb{Q}_{1,1}^{(b)}(E')}{10}$$

$$\boxed{\text{z220}} \quad \mathbb{G}_{1,2}^{(c)}(E'', b) = \frac{\sqrt{15}\mathbb{G}_{2,1}^{(a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{10} + \frac{\sqrt{15}\mathbb{G}_{2,1}^{(a)}(E')\mathbb{Q}_1^{(b)}(A''_2)}{10} - \frac{\sqrt{15}\mathbb{G}_{2,2}^{(a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{10} - \frac{\sqrt{5}\mathbb{G}_2^{(a)}(A''_1)\mathbb{Q}_{1,2}^{(b)}(E')}{10}$$

$$\boxed{\text{z221}} \quad \mathbb{G}_{2,1}^{(c)}(E'', a) = \frac{\sqrt{2}\mathbb{G}_{2,1}^{(a)}(E'')\mathbb{Q}_0^{(b)}(A'_1)}{2}$$

$$\boxed{z222} \quad \mathbb{G}_{2,2}^{(c)}(E'', a) = \frac{\sqrt{2}\mathbb{G}_{2,2}^{(a)}(E'')\mathbb{Q}_0^{(b)}(A'_1)}{2}$$

$$\boxed{z223} \quad \mathbb{G}_{2,1}^{(c)}(E'', b) = -\frac{\mathbb{G}_{2,1}^{(a)}(E')\mathbb{Q}_{2,2}^{(b)}(E'')}{2} - \frac{\mathbb{G}_{2,2}^{(a)}(E')\mathbb{Q}_{2,1}^{(b)}(E'')}{2}$$

$$\boxed{z224} \quad \mathbb{G}_{2,2}^{(c)}(E'', b) = -\frac{\mathbb{G}_{2,1}^{(a)}(E')\mathbb{Q}_{2,1}^{(b)}(E'')}{2} + \frac{\mathbb{G}_{2,2}^{(a)}(E')\mathbb{Q}_{2,2}^{(b)}(E'')}{2}$$

$$\boxed{z225} \quad \mathbb{G}_{3,1}^{(c)}(E'', a) = -\frac{\sqrt{15}\mathbb{Q}_{3,1}^{(a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{12} - \frac{\sqrt{15}\mathbb{Q}_{3,2}^{(a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{12} + \frac{\sqrt{6}\mathbb{Q}_{3,2}^{(a)}(E')\mathbb{Q}_1^{(b)}(A''_2)}{12} - \frac{\mathbb{Q}_3^{(a)}(A''_2)\mathbb{Q}_{1,2}^{(b)}(E')}{2}$$

$$\boxed{z226} \quad \mathbb{G}_{3,2}^{(c)}(E'', a) = -\frac{\sqrt{15}\mathbb{Q}_{3,1}^{(a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{12} - \frac{\sqrt{6}\mathbb{Q}_{3,1}^{(a)}(E')\mathbb{Q}_1^{(b)}(A''_2)}{12} + \frac{\sqrt{15}\mathbb{Q}_{3,2}^{(a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{12} + \frac{\mathbb{Q}_3^{(a)}(A''_2)\mathbb{Q}_{1,1}^{(b)}(E')}{2}$$

$$\boxed{z227} \quad \mathbb{G}_{3,1}^{(c)}(E'', b) = -\frac{\sqrt{15}\mathbb{G}_{2,1}^{(a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{30} - \frac{\sqrt{15}\mathbb{G}_{2,2}^{(a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{30} - \frac{2\sqrt{15}\mathbb{G}_{2,2}^{(a)}(E')\mathbb{Q}_1^{(b)}(A''_2)}{15} + \frac{\sqrt{5}\mathbb{G}_2^{(a)}(A''_1)\mathbb{Q}_{1,1}^{(b)}(E')}{5}$$

$$\boxed{z228} \quad \mathbb{G}_{3,2}^{(c)}(E'', b) = -\frac{\sqrt{15}\mathbb{G}_{2,1}^{(a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{30} + \frac{2\sqrt{15}\mathbb{G}_{2,1}^{(a)}(E')\mathbb{Q}_1^{(b)}(A''_2)}{15} + \frac{\sqrt{15}\mathbb{G}_{2,2}^{(a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{30} + \frac{\sqrt{5}\mathbb{G}_2^{(a)}(A''_1)\mathbb{Q}_{1,2}^{(b)}(E')}{5}$$

- S;S_001_1 : 'S'-'S' bond-cluster

* bra: $\langle p_x |, \langle p_y |, \langle p_z |$

* ket: $|p_x\rangle, |p_y\rangle, |p_z\rangle$

* wyckoff: 6b06n

$$\boxed{z23} \quad \mathbb{Q}_0^{(c)}(A'_1, a) = \mathbb{Q}_0^{(a)}(A'_1)\mathbb{Q}_0^{(b)}(A'_1)$$

$$\boxed{z24} \quad \mathbb{Q}_0^{(c)}(A'_1, b) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E'')\mathbb{Q}_{2,1}^{(b)}(E'')}{2} + \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E'')\mathbb{Q}_{2,2}^{(b)}(E'')}{2}$$

$$\boxed{z25} \quad \mathbb{Q}_0^{(c)}(A'_1, c) = \frac{\sqrt{3}\mathbb{M}_{1,1}^{(a)}(E'')\mathbb{M}_{1,1}^{(b)}(E'')}{3} + \frac{\sqrt{3}\mathbb{M}_{1,2}^{(a)}(E'')\mathbb{M}_{1,2}^{(b)}(E'')}{3} + \frac{\sqrt{3}\mathbb{M}_1^{(a)}(A'_2)\mathbb{M}_1^{(b)}(A'_2)}{3}$$

$$\boxed{z26} \quad \mathbb{Q}_2^{(c)}(A'_1, a) = \mathbb{Q}_2^{(a)}(A'_1)\mathbb{Q}_0^{(b)}(A'_1)$$

$$\boxed{z27} \quad \mathbb{Q}_2^{(c)}(A'_1, b) = -\frac{\sqrt{6}\mathbb{M}_{1,1}^{(a)}(E'')\mathbb{M}_{1,1}^{(b)}(E'')}{6} - \frac{\sqrt{6}\mathbb{M}_{1,2}^{(a)}(E'')\mathbb{M}_{1,2}^{(b)}(E'')}{6} + \frac{\sqrt{6}\mathbb{M}_1^{(a)}(A'_2)\mathbb{M}_1^{(b)}(A'_2)}{3}$$

$$\boxed{z28} \quad \mathbb{Q}_3^{(c)}(A'_1) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{2} + \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{2}$$

$$\boxed{z40} \quad \mathbb{Q}_4^{(c)}(A''_1) = -\frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E')\mathbb{Q}_{2,1}^{(b)}(E'')}{2} - \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E')\mathbb{Q}_{2,2}^{(b)}(E'')}{2}$$

$$\boxed{z41} \quad \mathbb{G}_0^{(c)}(A''_1) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(a)}(E'')\mathbb{T}_{1,1}^{(b)}(E')}{2} + \frac{\sqrt{2}\mathbb{M}_{1,2}^{(a)}(E'')\mathbb{T}_{1,2}^{(b)}(E')}{2}$$

$$\boxed{z42} \quad \mathbb{G}_2^{(c)}(A''_1) = -\frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{2} - \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{2}$$

$$\boxed{z57} \quad \mathbb{Q}_3^{(c)}(A'_2) = -\frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{2} + \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{2}$$

$$\boxed{z58} \quad \mathbb{G}_1^{(c)}(A'_2, a) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E'')\mathbb{Q}_{2,2}^{(b)}(E'')}{2} - \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E'')\mathbb{Q}_{2,1}^{(b)}(E'')}{2}$$

$$\boxed{z59} \quad \mathbb{G}_1^{(c)}(A'_2, b) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(a)}(E'')\mathbb{M}_{1,2}^{(b)}(E'')}{2} - \frac{\sqrt{2}\mathbb{M}_{1,2}^{(a)}(E'')\mathbb{M}_{1,1}^{(b)}(E'')}{2}$$

$$\boxed{z77} \quad \mathbb{Q}_1^{(c)}(A''_2, a) = \mathbb{Q}_0^{(a)}(A'_1)\mathbb{Q}_1^{(b)}(A''_2)$$

$$\boxed{z78} \quad \mathbb{Q}_1^{(c)}(A''_2, b) = \frac{\sqrt{30}\mathbb{Q}_{2,1}^{(a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{10} - \frac{\sqrt{30}\mathbb{Q}_{2,2}^{(a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{10} + \frac{\sqrt{10}\mathbb{Q}_2^{(a)}(A'_1)\mathbb{Q}_1^{(b)}(A''_2)}{5}$$

$$\boxed{z79} \quad \mathbb{Q}_1^{(c)}(A''_2, c) = \mathbb{M}_1^{(a)}(A'_2)\mathbb{M}_2^{(b)}(A''_1)$$

$$\boxed{z80} \quad \mathbb{Q}_1^{(c)}(A''_2, d) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(a)}(E'')\mathbb{T}_{1,2}^{(b)}(E')}{2} - \frac{\sqrt{2}\mathbb{M}_{1,2}^{(a)}(E'')\mathbb{T}_{1,1}^{(b)}(E')}{2}$$

$$\boxed{z81} \quad \mathbb{Q}_3^{(c)}(A''_2) = -\frac{\sqrt{5}\mathbb{Q}_{2,1}^{(a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{5} + \frac{\sqrt{5}\mathbb{Q}_{2,2}^{(a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{5} + \frac{\sqrt{15}\mathbb{Q}_2^{(a)}(A'_1)\mathbb{Q}_1^{(b)}(A''_2)}{5}$$

$$\boxed{z82} \quad \mathbb{Q}_4^{(c)}(A''_2) = -\frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E')\mathbb{Q}_{2,2}^{(b)}(E'')}{2} + \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E')\mathbb{Q}_{2,1}^{(b)}(E'')}{2}$$

$$\boxed{z149} \quad \mathbb{Q}_{1,1}^{(c)}(E', a) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A'_1)\mathbb{Q}_{1,1}^{(b)}(E')}{2}$$

$$\boxed{\text{z150}} \quad \mathbb{Q}_{1,2}^{(c)}(E', a) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A'_1)\mathbb{Q}_{1,2}^{(b)}(E')}{2}$$

$$\boxed{\text{z151}} \quad \mathbb{Q}_{1,1}^{(c)}(E', b) = \frac{\sqrt{15}\mathbb{Q}_{2,1}^{(a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{10} - \frac{\sqrt{15}\mathbb{Q}_{2,2}^{(a)}(E'')\mathbb{Q}_1^{(b)}(A''_2)}{10} + \frac{\sqrt{15}\mathbb{Q}_{2,2}^{(a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{10} - \frac{\sqrt{5}\mathbb{Q}_2^{(a)}(A'_1)\mathbb{Q}_{1,1}^{(b)}(E')}{10}$$

$$\boxed{\text{z152}} \quad \mathbb{Q}_{1,2}^{(c)}(E', b) = \frac{\sqrt{15}\mathbb{Q}_{2,1}^{(a)}(E'')\mathbb{Q}_1^{(b)}(A''_2)}{10} + \frac{\sqrt{15}\mathbb{Q}_{2,1}^{(a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{10} - \frac{\sqrt{15}\mathbb{Q}_{2,2}^{(a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{10} - \frac{\sqrt{5}\mathbb{Q}_2^{(a)}(A'_1)\mathbb{Q}_{1,2}^{(b)}(E')}{10}$$

$$\boxed{\text{z153}} \quad \mathbb{Q}_{1,1}^{(c)}(E', c) = -\frac{\sqrt{2}\mathbb{M}_{1,1}^{(a)}(E'')\mathbb{M}_2^{(b)}(A''_1)}{2}$$

$$\boxed{\text{z154}} \quad \mathbb{Q}_{1,2}^{(c)}(E', c) = -\frac{\sqrt{2}\mathbb{M}_{1,2}^{(a)}(E'')\mathbb{M}_2^{(b)}(A''_1)}{2}$$

$$\boxed{\text{z155}} \quad \mathbb{Q}_{1,1}^{(c)}(E', d) = -\frac{\sqrt{2}\mathbb{M}_1^{(a)}(A'_2)\mathbb{T}_{1,2}^{(b)}(E')}{2}$$

$$\boxed{\text{z156}} \quad \mathbb{Q}_{1,2}^{(c)}(E', d) = \frac{\sqrt{2}\mathbb{M}_1^{(a)}(A'_2)\mathbb{T}_{1,1}^{(b)}(E')}{2}$$

$$\boxed{\text{z157}} \quad \mathbb{Q}_{2,1}^{(c)}(E', a) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E')\mathbb{Q}_0^{(b)}(A'_1)}{2}$$

$$\boxed{\text{z158}} \quad \mathbb{Q}_{2,2}^{(c)}(E', a) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E')\mathbb{Q}_0^{(b)}(A'_1)}{2}$$

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

$$\boxed{\text{z160}} \quad \mathbb{Q}_{2,2}^{(c)}(E', b) = -\frac{\mathbb{Q}_{2,1}^{(a)}(E'')\mathbb{Q}_{2,1}^{(b)}(E'')}{2} + \frac{\mathbb{Q}_{2,2}^{(a)}(E'')\mathbb{Q}_{2,2}^{(b)}(E'')}{2}$$

$$\boxed{\text{z161}} \quad \mathbb{Q}_{2,1}^{(c)}(E', c) = \frac{\mathbb{M}_{1,1}^{(a)}(E'')\mathbb{M}_{1,2}^{(b)}(E'')}{2} + \frac{\mathbb{M}_{1,2}^{(a)}(E'')\mathbb{M}_{1,1}^{(b)}(E'')}{2}$$

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

$$\boxed{\text{z163}} \quad \mathbb{Q}_{3,1}^{(c)}(E') = -\frac{\sqrt{15}\mathbb{Q}_{2,1}^{(a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{30} - \frac{2\sqrt{15}\mathbb{Q}_{2,2}^{(a)}(E'')\mathbb{Q}_1^{(b)}(A''_2)}{15} - \frac{\sqrt{15}\mathbb{Q}_{2,2}^{(a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{30} + \frac{\sqrt{5}\mathbb{Q}_2^{(a)}(A'_1)\mathbb{Q}_{1,1}^{(b)}(E')}{5}$$

$$\boxed{\text{z164}} \quad \mathbb{Q}_{3,2}^{(c)}(E') = \frac{2\sqrt{15}\mathbb{Q}_{2,1}^{(a)}(E'')\mathbb{Q}_1^{(b)}(A_2'')}{15} - \frac{\sqrt{15}\mathbb{Q}_{2,1}^{(a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{30} + \frac{\sqrt{15}\mathbb{Q}_{2,2}^{(a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{30} + \frac{\sqrt{5}\mathbb{Q}_2^{(a)}(A_1')\mathbb{Q}_{1,2}^{(b)}(E')}{5}$$

$$\boxed{\text{z165}} \quad \mathbb{G}_{2,1}^{(c)}(E') = \frac{\sqrt{3}\mathbb{Q}_{2,1}^{(a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{6} + \frac{\sqrt{3}\mathbb{Q}_{2,2}^{(a)}(E'')\mathbb{Q}_1^{(b)}(A_2'')}{6} + \frac{\sqrt{3}\mathbb{Q}_{2,2}^{(a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{6} + \frac{\mathbb{Q}_2^{(a)}(A_1')\mathbb{Q}_{1,1}^{(b)}(E')}{2}$$

$$\boxed{\text{z166}} \quad \mathbb{G}_{2,2}^{(c)}(E') = -\frac{\sqrt{3}\mathbb{Q}_{2,1}^{(a)}(E'')\mathbb{Q}_1^{(b)}(A_2'')}{6} + \frac{\sqrt{3}\mathbb{Q}_{2,1}^{(a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{6} - \frac{\sqrt{3}\mathbb{Q}_{2,2}^{(a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{6} + \frac{\mathbb{Q}_2^{(a)}(A_1')\mathbb{Q}_{1,2}^{(b)}(E')}{2}$$

$$\boxed{\text{z229}} \quad \mathbb{Q}_{2,1}^{(c)}(E'', a) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_1')\mathbb{Q}_{2,1}^{(b)}(E'')}{2}$$

$$\boxed{\text{z230}} \quad \mathbb{Q}_{2,2}^{(c)}(E'', a) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_1')\mathbb{Q}_{2,2}^{(b)}(E'')}{2}$$

$$\boxed{\text{z231}} \quad \mathbb{Q}_{2,1}^{(c)}(E'', b) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E'')\mathbb{Q}_0^{(b)}(A_1')}{2}$$

$$\boxed{\text{z232}} \quad \mathbb{Q}_{2,2}^{(c)}(E'', b) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E'')\mathbb{Q}_0^{(b)}(A_1')}{2}$$

$$\boxed{\text{z233}} \quad \mathbb{Q}_{2,1}^{(c)}(E'', c) = -\frac{\sqrt{42}\mathbb{Q}_{2,1}^{(a)}(E')\mathbb{Q}_{2,2}^{(b)}(E'')}{14} - \frac{\sqrt{42}\mathbb{Q}_{2,2}^{(a)}(E')\mathbb{Q}_{2,1}^{(b)}(E'')}{14} + \frac{\sqrt{14}\mathbb{Q}_2^{(a)}(A_1')\mathbb{Q}_{2,1}^{(b)}(E'')}{14}$$

$$\boxed{\text{z234}} \quad \mathbb{Q}_{2,2}^{(c)}(E'', c) = -\frac{\sqrt{42}\mathbb{Q}_{2,1}^{(a)}(E')\mathbb{Q}_{2,1}^{(b)}(E'')}{14} + \frac{\sqrt{42}\mathbb{Q}_{2,2}^{(a)}(E')\mathbb{Q}_{2,2}^{(b)}(E'')}{14} + \frac{\sqrt{14}\mathbb{Q}_2^{(a)}(A_1')\mathbb{Q}_{2,2}^{(b)}(E'')}{14}$$

$$\boxed{\text{z235}} \quad \mathbb{Q}_{2,1}^{(c)}(E'', d) = \frac{\mathbb{M}_{1,2}^{(a)}(E'')\mathbb{M}_1^{(b)}(A_2')}{2} + \frac{\mathbb{M}_1^{(a)}(A_2')\mathbb{M}_{1,2}^{(b)}(E'')}{2}$$

$$\boxed{\text{z236}} \quad \mathbb{Q}_{2,2}^{(c)}(E'', d) = -\frac{\mathbb{M}_{1,1}^{(a)}(E'')\mathbb{M}_1^{(b)}(A_2')}{2} - \frac{\mathbb{M}_1^{(a)}(A_2')\mathbb{M}_{1,1}^{(b)}(E'')}{2}$$

$$\boxed{\text{z237}} \quad \mathbb{Q}_{3,1}^{(c)}(E'') = \frac{\sqrt{6}\mathbb{Q}_{2,1}^{(a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{6} + \frac{\sqrt{6}\mathbb{Q}_{2,2}^{(a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{6} - \frac{\sqrt{6}\mathbb{Q}_{2,2}^{(a)}(E')\mathbb{Q}_1^{(b)}(A_2'')}{6}$$

$$\boxed{\text{z238}} \quad \mathbb{Q}_{3,2}^{(c)}(E'') = \frac{\sqrt{6}\mathbb{Q}_{2,1}^{(a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{6} + \frac{\sqrt{6}\mathbb{Q}_{2,1}^{(a)}(E')\mathbb{Q}_1^{(b)}(A_2'')}{6} - \frac{\sqrt{6}\mathbb{Q}_{2,2}^{(a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{6}$$

$$\boxed{\text{z239}} \quad \mathbb{Q}_{4,1}^{(c)}(E'') = \frac{\sqrt{7}\mathbb{Q}_{2,1}^{(a)}(E')\mathbb{Q}_{2,2}^{(b)}(E'')}{14} + \frac{\sqrt{7}\mathbb{Q}_{2,2}^{(a)}(E')\mathbb{Q}_{2,1}^{(b)}(E'')}{14} + \frac{\sqrt{21}\mathbb{Q}_2^{(a)}(A_1')\mathbb{Q}_{2,1}^{(b)}(E'')}{7}$$

$$\boxed{\text{z240}} \quad \mathbb{Q}_{4,2}^{(c)}(E'') = \frac{\sqrt{7}\mathbb{Q}_{2,1}^{(a)}(E')\mathbb{Q}_{2,1}^{(b)}(E'')}{14} - \frac{\sqrt{7}\mathbb{Q}_{2,2}^{(a)}(E')\mathbb{Q}_{2,2}^{(b)}(E'')}{14} + \frac{\sqrt{21}\mathbb{Q}_2^{(a)}(A'_1)\mathbb{Q}_{2,2}^{(b)}(E'')}{7}$$

$$\boxed{\text{z241}} \quad \mathbb{G}_{1,1}^{(c)}(E'') = \frac{\mathbb{M}_{1,2}^{(a)}(E'')\mathbb{M}_1^{(b)}(A'_2)}{2} - \frac{\mathbb{M}_1^{(a)}(A'_2)\mathbb{M}_{1,2}^{(b)}(E'')}{2}$$

$$\boxed{\text{z242}} \quad \mathbb{G}_{1,2}^{(c)}(E'') = -\frac{\mathbb{M}_{1,1}^{(a)}(E'')\mathbb{M}_1^{(b)}(A'_2)}{2} + \frac{\mathbb{M}_1^{(a)}(A'_2)\mathbb{M}_{1,1}^{(b)}(E'')}{2}$$

$$\boxed{\text{z243}} \quad \mathbb{G}_{2,1}^{(c)}(E'', a) = -\frac{\sqrt{3}\mathbb{Q}_{2,1}^{(a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{6} - \frac{\sqrt{3}\mathbb{Q}_{2,2}^{(a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{6} - \frac{\sqrt{3}\mathbb{Q}_{2,2}^{(a)}(E')\mathbb{Q}_1^{(b)}(A''_2)}{3}$$

$$\boxed{\text{z244}} \quad \mathbb{G}_{2,2}^{(c)}(E'', a) = -\frac{\sqrt{3}\mathbb{Q}_{2,1}^{(a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{6} + \frac{\sqrt{3}\mathbb{Q}_{2,1}^{(a)}(E')\mathbb{Q}_1^{(b)}(A''_2)}{3} + \frac{\sqrt{3}\mathbb{Q}_{2,2}^{(a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{6}$$

$$\boxed{\text{z245}} \quad \mathbb{G}_{2,1}^{(c)}(E'', b) = \frac{\mathbb{M}_{1,1}^{(a)}(E'')\mathbb{T}_{1,2}^{(b)}(E')}{2} + \frac{\mathbb{M}_{1,2}^{(a)}(E'')\mathbb{T}_{1,1}^{(b)}(E')}{2}$$

$$\boxed{\text{z246}} \quad \mathbb{G}_{2,2}^{(c)}(E'', b) = \frac{\mathbb{M}_{1,1}^{(a)}(E'')\mathbb{T}_{1,1}^{(b)}(E')}{2} - \frac{\mathbb{M}_{1,2}^{(a)}(E'')\mathbb{T}_{1,2}^{(b)}(E')}{2}$$

— Atomic SAMB —

- bra: $\langle d_v |$, $\langle d_{xy} |$, $\langle d_{xz} |$, $\langle d_{yz} |$, $\langle d_u |$
- ket: $|d_v\rangle$, $|d_{xy}\rangle$, $|d_{xz}\rangle$, $|d_{yz}\rangle$, $|d_u\rangle$

$$\boxed{\text{x1}} \quad \mathbb{Q}_0^{(a)}(A'_1) = \begin{bmatrix} \frac{\sqrt{5}}{5} & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{5}}{5} & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{5}}{5} & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{5}}{5} & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{5}}{5} \end{bmatrix}$$

$$\boxed{\text{x2}} \quad \mathbb{Q}_2^{(a)}(A'_1) = \begin{bmatrix} -\frac{\sqrt{14}}{7} & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{14}}{7} & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{14}}{14} & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{14}}{14} & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{14}}{7} \end{bmatrix}$$

$$\boxed{x3} \quad \mathbb{Q}_4^{(a)}(A'_1) = \begin{bmatrix} \frac{\sqrt{70}}{70} & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{70}}{70} & 0 & 0 & 0 \\ 0 & 0 & -\frac{2\sqrt{70}}{35} & 0 & 0 \\ 0 & 0 & 0 & -\frac{2\sqrt{70}}{35} & 0 \\ 0 & 0 & 0 & 0 & \frac{3\sqrt{70}}{35} \end{bmatrix}$$

$$\boxed{x4} \quad \mathbb{Q}_4^{(a)}(A''_1) = \begin{bmatrix} 0 & 0 & \frac{1}{2} & 0 & 0 \\ 0 & 0 & 0 & -\frac{1}{2} & 0 \\ \frac{1}{2} & 0 & 0 & 0 & 0 \\ 0 & -\frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{x5} \quad \mathbb{Q}_4^{(a)}(A''_2) = \begin{bmatrix} 0 & 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & \frac{1}{2} & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 & 0 \\ \frac{1}{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{x6} \quad \mathbb{Q}_{2,1}^{(a)}(E') = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{14}}{7} \\ 0 & 0 & 0 & \frac{\sqrt{42}}{14} & 0 \\ 0 & 0 & \frac{\sqrt{42}}{14} & 0 & 0 \\ 0 & -\frac{\sqrt{14}}{7} & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{x7} \quad \mathbb{Q}_{2,2}^{(a)}(E') = \begin{bmatrix} 0 & 0 & 0 & 0 & -\frac{\sqrt{14}}{7} \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{42}}{14} & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{42}}{14} & 0 \\ -\frac{\sqrt{14}}{7} & 0 & 0 & 0 & 0 \end{bmatrix}$$

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

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

$$\boxed{x10} \quad \mathbb{Q}_{4,1}^{(a)}(E', 2) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{42}}{14} \\ 0 & 0 & 0 & \frac{\sqrt{14}}{7} & 0 \\ 0 & 0 & \frac{\sqrt{14}}{7} & 0 & 0 \\ 0 & \frac{\sqrt{42}}{14} & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{x11} \quad \mathbb{Q}_{4,2}^{(a)}(E', 2) = \begin{bmatrix} 0 & 0 & 0 & 0 & \frac{\sqrt{42}}{14} \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{14}}{7} & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{14}}{7} & 0 \\ \frac{\sqrt{42}}{14} & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{x12} \quad \mathbb{Q}_{2,1}^{(a)}(E'') = \begin{bmatrix} 0 & 0 & 0 & -\frac{\sqrt{42}}{14} & 0 \\ 0 & 0 & \frac{\sqrt{42}}{14} & 0 & 0 \\ 0 & \frac{\sqrt{42}}{14} & 0 & 0 & 0 \\ -\frac{\sqrt{42}}{14} & 0 & 0 & 0 & \frac{\sqrt{14}}{14} \\ 0 & 0 & 0 & \frac{\sqrt{14}}{14} & 0 \end{bmatrix}$$

$$\boxed{x13} \quad \mathbb{Q}_{2,2}^{(a)}(E'') = \begin{bmatrix} 0 & 0 & -\frac{\sqrt{42}}{14} & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{42}}{14} & 0 \\ -\frac{\sqrt{42}}{14} & 0 & 0 & 0 & -\frac{\sqrt{14}}{14} \\ 0 & -\frac{\sqrt{42}}{14} & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{14}}{14} & 0 & 0 \end{bmatrix}$$

$$\boxed{x14} \quad \mathbb{Q}_{4,1}^{(a)}(E'') = \begin{bmatrix} 0 & 0 & 0 & \frac{\sqrt{7}}{14} & 0 \\ 0 & 0 & -\frac{\sqrt{7}}{14} & 0 & 0 \\ 0 & -\frac{\sqrt{7}}{14} & 0 & 0 & 0 \\ \frac{\sqrt{7}}{14} & 0 & 0 & 0 & \frac{\sqrt{21}}{7} \\ 0 & 0 & 0 & \frac{\sqrt{21}}{7} & 0 \end{bmatrix}$$

$$\boxed{x15} \quad \mathbb{Q}_{4,2}^{(a)}(E'') = \begin{bmatrix} 0 & 0 & \frac{\sqrt{7}}{14} & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{7}}{14} & 0 \\ \frac{\sqrt{7}}{14} & 0 & 0 & 0 & -\frac{\sqrt{21}}{7} \\ 0 & \frac{\sqrt{7}}{14} & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{21}}{7} & 0 & 0 \end{bmatrix}$$

$$\boxed{x16} \quad \mathbb{M}_3^{(a)}(A''_1) = \begin{bmatrix} 0 & 0 & \frac{i}{2} & 0 & 0 \\ 0 & 0 & 0 & -\frac{i}{2} & 0 \\ -\frac{i}{2} & 0 & 0 & 0 & 0 \\ 0 & \frac{i}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{x17} \quad \mathbb{M}_1^{(a)}(A'_2) = \begin{bmatrix} 0 & -\frac{\sqrt{10}i}{5} & 0 & 0 & 0 \\ \frac{\sqrt{10}i}{5} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{10}i}{10} & 0 \\ 0 & 0 & \frac{\sqrt{10}i}{10} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{x18} \quad \mathbb{M}_3^{(a)}(A'_2) = \begin{bmatrix} 0 & \frac{\sqrt{10}i}{10} & 0 & 0 & 0 \\ -\frac{\sqrt{10}i}{10} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{10}i}{5} & 0 \\ 0 & 0 & \frac{\sqrt{10}i}{5} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{x19} \quad \mathbb{M}_3^{(a)}(A''_2) = \begin{bmatrix} 0 & 0 & 0 & -\frac{i}{2} & 0 \\ 0 & 0 & -\frac{i}{2} & 0 & 0 \\ 0 & \frac{i}{2} & 0 & 0 & 0 \\ \frac{i}{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{x20} \quad \mathbb{M}_{3,1}^{(a)}(E') = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{2}i}{2} \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{2}i}{2} & 0 & 0 & 0 \end{bmatrix}$$

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

$$\boxed{x22} \quad \mathbb{M}_{1,1}^{(a)}(E'') = \begin{bmatrix} 0 & 0 & 0 & \frac{\sqrt{10}i}{10} & 0 \\ 0 & 0 & -\frac{\sqrt{10}i}{10} & 0 & 0 \\ 0 & \frac{\sqrt{10}i}{10} & 0 & 0 & 0 \\ -\frac{\sqrt{10}i}{10} & 0 & 0 & 0 & -\frac{\sqrt{30}i}{10} \\ 0 & 0 & 0 & \frac{\sqrt{30}i}{10} & 0 \end{bmatrix}$$

$$\boxed{x23} \quad \mathbb{M}_{1,2}^{(a)}(E'') = \begin{bmatrix} 0 & 0 & \frac{\sqrt{10}i}{10} & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{10}i}{10} & 0 \\ -\frac{\sqrt{10}i}{10} & 0 & 0 & 0 & \frac{\sqrt{30}i}{10} \\ 0 & -\frac{\sqrt{10}i}{10} & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{30}i}{10} & 0 & 0 \end{bmatrix}$$

$$\boxed{x24} \quad \mathbb{M}_{3,1}^{(a)}(E'') = \begin{bmatrix} 0 & 0 & 0 & -\frac{\sqrt{15}i}{10} & 0 \\ 0 & 0 & \frac{\sqrt{15}i}{10} & 0 & 0 \\ 0 & -\frac{\sqrt{15}i}{10} & 0 & 0 & 0 \\ \frac{\sqrt{15}i}{10} & 0 & 0 & 0 & -\frac{\sqrt{5}i}{5} \\ 0 & 0 & 0 & \frac{\sqrt{5}i}{5} & 0 \end{bmatrix}$$

$$\boxed{x25} \quad \mathbb{M}_{3,2}^{(a)}(E'') = \begin{bmatrix} 0 & 0 & -\frac{\sqrt{15}i}{10} & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{15}i}{10} & 0 \\ \frac{\sqrt{15}i}{10} & 0 & 0 & 0 & \frac{\sqrt{5}i}{5} \\ 0 & \frac{\sqrt{15}i}{10} & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{5}i}{5} & 0 & 0 \end{bmatrix}$$

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

$$\boxed{x26} \quad \mathbb{Q}_0^{(a)}(A'_1) = \begin{bmatrix} \frac{\sqrt{3}}{3} & 0 & 0 \\ 0 & \frac{\sqrt{3}}{3} & 0 \\ 0 & 0 & \frac{\sqrt{3}}{3} \end{bmatrix}$$

$$\boxed{x27} \quad \mathbb{Q}_2^{(a)}(A'_1) = \begin{bmatrix} -\frac{\sqrt{6}}{6} & 0 & 0 \\ 0 & -\frac{\sqrt{6}}{6} & 0 \\ 0 & 0 & \frac{\sqrt{6}}{3} \end{bmatrix}$$

$$\boxed{x28} \quad \mathbb{Q}_{2,1}^{(a)}(E') = \begin{bmatrix} 0 & \frac{\sqrt{2}}{2} & 0 \\ \frac{\sqrt{2}}{2} & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{x29} \quad \mathbb{Q}_{2,2}^{(a)}(E') = \begin{bmatrix} \frac{\sqrt{2}}{2} & 0 & 0 \\ 0 & -\frac{\sqrt{2}}{2} & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

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

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

$$\boxed{x32} \quad \mathbb{M}_1^{(a)}(A'_2) = \begin{bmatrix} 0 & -\frac{\sqrt{2}i}{2} & 0 \\ \frac{\sqrt{2}i}{2} & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

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

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

— Cluster SAMB —

- Site cluster

** Wyckoff: **1a**

$$\boxed{y1} \quad \mathbb{Q}_0^{(s)}(A'_1) = [1]$$

** Wyckoff: 2i

$$\boxed{y2} \quad \mathbb{Q}_0^{(s)}(A'_1) = \left[\frac{\sqrt{2}}{2}, \frac{\sqrt{2}}{2} \right]$$

$$\boxed{y3} \quad \mathbb{Q}_1^{(s)}(A''_2) = \left[\frac{\sqrt{2}}{2}, -\frac{\sqrt{2}}{2} \right]$$

- Bond cluster

** Wyckoff: 3b@3j

$$\boxed{y4} \quad \mathbb{Q}_0^{(s)}(A'_1) = \left[\frac{\sqrt{3}}{3}, \frac{\sqrt{3}}{3}, \frac{\sqrt{3}}{3} \right]$$

$$\boxed{y5} \quad \mathbb{M}_1^{(s)}(A'_2) = \left[\frac{\sqrt{3}i}{3}, \frac{\sqrt{3}i}{3}, \frac{\sqrt{3}i}{3} \right]$$

$$\boxed{y6} \quad \mathbb{Q}_{1,1}^{(s)}(E') = \left[\frac{\sqrt{2}}{2}, 0, -\frac{\sqrt{2}}{2} \right]$$

$$\boxed{y7} \quad \mathbb{Q}_{1,2}^{(s)}(E') = \left[-\frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{3}, -\frac{\sqrt{6}}{6} \right]$$

$$\boxed{y8} \quad \mathbb{T}_{1,1}^{(s)}(E') = \left[\frac{\sqrt{6}i}{6}, -\frac{\sqrt{6}i}{3}, \frac{\sqrt{6}i}{6} \right]$$

$$\boxed{y9} \quad \mathbb{T}_{1,2}^{(s)}(E') = \left[\frac{\sqrt{2}i}{2}, 0, -\frac{\sqrt{2}i}{2} \right]$$

** Wyckoff: 6a@6n

$$\boxed{y10} \quad \mathbb{Q}_0^{(s)}(A'_1) = \left[\frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6} \right]$$

$$\boxed{y11} \quad \mathbb{T}_0^{(s)}(A'_1) = \left[\frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6} \right]$$

$$\boxed{\text{y12}} \quad \mathbb{Q}_1^{(s)}(A''_2) = \left[\frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, -\frac{\sqrt{6}}{6}, -\frac{\sqrt{6}}{6}, -\frac{\sqrt{6}}{6} \right]$$

$$\boxed{\text{y13}} \quad \mathbb{T}_1^{(s)}(A''_2) = \left[\frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, -\frac{\sqrt{6}i}{6}, -\frac{\sqrt{6}i}{6}, -\frac{\sqrt{6}i}{6} \right]$$

$$\boxed{\text{y14}} \quad \mathbb{Q}_{1,1}^{(s)}(E') = \left[\frac{1}{2}, 0, -\frac{1}{2}, \frac{1}{2}, 0, -\frac{1}{2} \right]$$

$$\boxed{\text{y15}} \quad \mathbb{Q}_{1,2}^{(s)}(E') = \left[-\frac{\sqrt{3}}{6}, \frac{\sqrt{3}}{3}, -\frac{\sqrt{3}}{6}, -\frac{\sqrt{3}}{6}, \frac{\sqrt{3}}{3}, -\frac{\sqrt{3}}{6} \right]$$

$$\boxed{\text{y16}} \quad \mathbb{T}_{1,1}^{(s)}(E') = \left[\frac{i}{2}, 0, -\frac{i}{2}, \frac{i}{2}, 0, -\frac{i}{2} \right]$$

$$\boxed{\text{y17}} \quad \mathbb{T}_{1,2}^{(s)}(E') = \left[-\frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{3}, -\frac{\sqrt{3}i}{6}, -\frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{3}, -\frac{\sqrt{3}i}{6} \right]$$

$$\boxed{\text{y18}} \quad \mathbb{M}_{1,1}^{(s)}(E'') = \left[-\frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{3}, -\frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{6}, -\frac{\sqrt{3}i}{3}, \frac{\sqrt{3}i}{6} \right]$$

$$\boxed{\text{y19}} \quad \mathbb{M}_{1,2}^{(s)}(E'') = \left[-\frac{i}{2}, 0, \frac{i}{2}, \frac{i}{2}, 0, -\frac{i}{2} \right]$$

$$\boxed{\text{y20}} \quad \mathbb{Q}_{2,1}^{(s)}(E'') = \left[-\frac{\sqrt{3}}{6}, \frac{\sqrt{3}}{3}, -\frac{\sqrt{3}}{6}, \frac{\sqrt{3}}{6}, -\frac{\sqrt{3}}{3}, \frac{\sqrt{3}}{6} \right]$$

$$\boxed{\text{y21}} \quad \mathbb{Q}_{2,2}^{(s)}(E'') = \left[-\frac{1}{2}, 0, \frac{1}{2}, \frac{1}{2}, 0, -\frac{1}{2} \right]$$

** Wyckoff: 6b@6n

$$\boxed{\text{y22}} \quad \mathbb{Q}_0^{(s)}(A'_1) = \left[\frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6} \right]$$

$$\boxed{\text{y23}} \quad \mathbb{M}_2^{(s)}(A''_1) = \left[\frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, -\frac{\sqrt{6}i}{6}, -\frac{\sqrt{6}i}{6}, -\frac{\sqrt{6}i}{6} \right]$$

$$\boxed{\text{y24}} \quad \mathbb{M}_1^{(s)}(A'_2) = \left[\frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6} \right]$$

$$\boxed{y25} \quad \mathbb{Q}_1^{(s)}(A''_2) = \left[\frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, -\frac{\sqrt{6}}{6}, -\frac{\sqrt{6}}{6}, -\frac{\sqrt{6}}{6} \right]$$

$$\boxed{y26} \quad \mathbb{Q}_{1,1}^{(s)}(E') = \left[\frac{1}{2}, 0, -\frac{1}{2}, \frac{1}{2}, 0, -\frac{1}{2} \right]$$

$$\boxed{y27} \quad \mathbb{Q}_{1,2}^{(s)}(E') = \left[-\frac{\sqrt{3}}{6}, \frac{\sqrt{3}}{3}, -\frac{\sqrt{3}}{6}, -\frac{\sqrt{3}}{6}, \frac{\sqrt{3}}{3}, -\frac{\sqrt{3}}{6} \right]$$

$$\boxed{y28} \quad \mathbb{T}_{1,1}^{(s)}(E') = \left[\frac{\sqrt{3}i}{6}, -\frac{\sqrt{3}i}{3}, \frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{6}, -\frac{\sqrt{3}i}{3}, \frac{\sqrt{3}i}{6} \right]$$

$$\boxed{y29} \quad \mathbb{T}_{1,2}^{(s)}(E') = \left[\frac{i}{2}, 0, -\frac{i}{2}, \frac{i}{2}, 0, -\frac{i}{2} \right]$$

$$\boxed{y30} \quad \mathbb{M}_{1,1}^{(s)}(E'') = \left[\frac{i}{2}, 0, -\frac{i}{2}, -\frac{i}{2}, 0, \frac{i}{2} \right]$$

$$\boxed{y31} \quad \mathbb{M}_{1,2}^{(s)}(E'') = \left[-\frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{3}, -\frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{6}, -\frac{\sqrt{3}i}{3}, \frac{\sqrt{3}i}{6} \right]$$

$$\boxed{y32} \quad \mathbb{Q}_{2,1}^{(s)}(E'') = \left[-\frac{\sqrt{3}}{6}, \frac{\sqrt{3}}{3}, -\frac{\sqrt{3}}{6}, \frac{\sqrt{3}}{6}, -\frac{\sqrt{3}}{3}, \frac{\sqrt{3}}{6} \right]$$

$$\boxed{y33} \quad \mathbb{Q}_{2,2}^{(s)}(E'') = \left[-\frac{1}{2}, 0, \frac{1}{2}, \frac{1}{2}, 0, -\frac{1}{2} \right]$$

— Site and Bond —

Table 5: Orbital of each site

#	site	orbital
1	Mo	$ d_v\rangle, d_{xy}\rangle, d_{xz}\rangle, d_{yz}\rangle, d_u\rangle$

continued ...

Table 5

#	site	orbital
2	s	$ p_x\rangle, p_y\rangle, p_z\rangle$

Table 6: Neighbor and bra-ket of each bond

#	head	tail	neighbor	head (bra)	tail (ket)
1	Mo	Mo	[1]	[d]	[d]
2	Mo	s	[1]	[d]	[p]
3	s	s	[1]	[p]	[p]

— Site in Unit Cell —

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

Table 7: 'Mo' (#1) site cluster (1a), -6m2

SL	position (<i>s</i>)	mapping
1	[0.00000, 0.00000, 0.00000]	[1,2,3,4,5,6,7,8,9,10,11,12]

Table 8: 'S' (#2) site cluster (2i), 3m.

SL	position (s)	mapping
1	[0.66667, 0.33333, 0.12425]	[1,2,3,7,8,9]
2	[0.66667, 0.33333, 0.87575]	[4,5,6,10,11,12]

Bond in Unit Cell

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

Table 9: 1-th 'Mo'-'Mo' [1] (#1) bond cluster (3b@3j), ND, $|v|=3.1661$ (cartesian)

SL	vector (v)	center (c)	mapping	head	tail	R (primitive)
1	[-1.00000, -1.00000, 0.00000]	[0.50000, 0.50000, 0.00000]	[1,4,-7,-10]	(1,1)	(1,1)	[1,1,0]
2	[1.00000, 0.00000, 0.00000]	[0.50000, 0.00000, 0.00000]	[2,5,-9,-12]	(1,1)	(1,1)	[-1,0,0]
3	[0.00000, 1.00000, 0.00000]	[0.00000, 0.50000, 0.00000]	[3,6,-8,-11]	(1,1)	(1,1)	[0,-1,0]

Table 10: 1-th 'Mo'-'S' [1] (#2) bond cluster (6a@6n), D, $|v|=3.0849$ (cartesian)

SL	vector (v)	center (c)	mapping	head	tail	R (primitive)
1	[0.33333, -0.33333, -0.12425]	[0.83333, 0.16667, 0.06212]	[1,7]	(1,1)	(1,1)	[-1,0,0]
2	[0.33333, 0.66667, -0.12425]	[0.83333, 0.66667, 0.06212]	[2,9]	(1,1)	(1,1)	[-1,-1,0]

continued ...

Table 10

SL	vector (\mathbf{v})	center (\mathbf{c})	mapping	head	tail	\mathbf{R} (primitive)
3	[-0.66667, -0.33333, -0.12425]	[0.33333, 0.16667, 0.06212]	[3,8]	(1,1)	(1,1)	[0,0,0]
4	[0.33333, -0.33333, 0.12425]	[0.83333, 0.16667, 0.93788]	[4,10]	(1,1)	(2,1)	[-1,0,-1]
5	[0.33333, 0.66667, 0.12425]	[0.83333, 0.66667, 0.93788]	[5,12]	(1,1)	(2,1)	[-1,-1,-1]
6	[-0.66667, -0.33333, 0.12425]	[0.33333, 0.16667, 0.93788]	[6,11]	(1,1)	(2,1)	[0,0,-1]

Table 11: 1-th 'S'-'S' [1] (#3) bond cluster (6b@6n), ND, $|\mathbf{v}|=3.1661$ (cartesian)

SL	vector (\mathbf{v})	center (\mathbf{c})	mapping	head	tail	\mathbf{R} (primitive)
1	[-1.00000, -1.00000, 0.00000]	[0.16667, 0.83333, 0.12425]	[1,-7]	(1,1)	(1,1)	[1,1,0]
2	[1.00000, 0.00000, 0.00000]	[0.16667, 0.33333, 0.12425]	[2,-9]	(1,1)	(1,1)	[-1,0,0]
3	[0.00000, 1.00000, 0.00000]	[0.66667, 0.83333, 0.12425]	[3,-8]	(1,1)	(1,1)	[0,-1,0]
4	[-1.00000, -1.00000, 0.00000]	[0.16667, 0.83333, 0.87575]	[4,-10]	(2,1)	(2,1)	[1,1,0]
5	[1.00000, 0.00000, 0.00000]	[0.16667, 0.33333, 0.87575]	[5,-12]	(2,1)	(2,1)	[-1,0,0]
6	[0.00000, 1.00000, 0.00000]	[0.66667, 0.83333, 0.87575]	[6,-11]	(2,1)	(2,1)	[0,-1,0]