

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):
 - $\mathbf{a}_1 = [3.16610, 0.00000, 0.00000]$
 - $\mathbf{a}_2 = [-1.58305, 2.74192, 0.00000]$
 - $\mathbf{a}_3 = [0.00000, 0.00000, 20.00000]$

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	$Q_0(A'_1)$	A'_1	0	Q, T	-	-	1
2	$Q_2(A'_1)$	A'_1	2	Q, T	-	-	$-\frac{x^2}{2} - \frac{y^2}{2} + z^2$
3	$Q_3(A'_1)$	A'_1	3	Q, T	-	-	$\frac{\sqrt{10}y(3x^2-y^2)}{4}$
4	$Q_4(A'_1)$	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	$Q_5(A'_1)$	A'_1	5	Q, T	-	-	$-\frac{\sqrt{70}y(3x^2-y^2)(x^2+y^2-8z^2)}{16}$
6	$G_0(A''_1)$	A''_1	0	G, M	-	-	1
7	$G_2(A''_1)$	A''_1	2	G, M	-	-	$-\frac{x^2}{2} - \frac{y^2}{2} + z^2$

continued ...

Table 2

#	symbol	irrep.	rank	X	multiplicity	component	symmetry
8	$\mathbb{G}_3(A_1'')$	A_1''	3	G, M	-	-	$\frac{\sqrt{10}y(3x^2-y^2)}{4}$
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	$-\frac{\sqrt{6}y(x^2+y^2-4z^2)}{4}$

continued ...

Table 2

#	symbol	irrep.	rank	X	multiplicity	component	symmetry
29	$\mathbb{Q}_{4,1}(E', 1)$	E'	4	Q, T	1	1	$-\frac{\sqrt{35}xy(x-y)(x+y)}{2}$
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	$-\frac{\sqrt{10}yz(3x^2+3y^2-4z^2)}{4}$

continued ...

Table 2

#	symbol	irrep.	rank	X	multiplicity	component	symmetry
50	$\mathbb{Q}_{4,2}(E'')$					2	$\frac{\sqrt{10}xz(3x^2+3y^2-4z^2)}{4}$
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 @\text{Mo}(1)$	1	$ d_{xy}\rangle @\text{Mo}(1)$	2	$ d_{xz}\rangle @\text{Mo}(1)$	3	$ d_{yz}\rangle @\text{Mo}(1)$	4	$ d_u\rangle @\text{Mo}(1)$
5	$ p_x\rangle @\text{S}(1)$	6	$ p_y\rangle @\text{S}(1)$	7	$ p_z\rangle @\text{S}(1)$	8	$ p_x\rangle @\text{S}(2)$	9	$ p_y\rangle @\text{S}(2)$
10	$ p_z\rangle @\text{S}(2)$								

Table 4: Atomic basis (orbital part only)

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

- 'Mo' site-cluster : Mo

- * 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**

$$\boxed{\text{z1}} \quad \mathbb{Q}_0^{(c)}(A'_1) = \mathbb{Q}_0^{(a)}(A'_1)\mathbb{Q}_0^{(s)}(A'_1)$$

$$\boxed{\text{z2}} \quad \mathbb{Q}_2^{(c)}(A'_1) = \mathbb{Q}_2^{(a)}(A'_1)\mathbb{Q}_0^{(s)}(A'_1)$$

$$\boxed{\text{z3}} \quad \mathbb{Q}_4^{(c)}(A'_1) = \mathbb{Q}_4^{(a)}(A'_1)\mathbb{Q}_0^{(s)}(A'_1)$$

$$\boxed{\text{z43}} \quad \mathbb{Q}_4^{(c)}(A''_1) = \mathbb{Q}_4^{(a)}(A''_1)\mathbb{Q}_0^{(s)}(A'_1)$$

$$\boxed{\text{z60}} \quad \mathbb{Q}_4^{(c)}(A_2'') = \mathbb{Q}_4^{(a)}(A_2'')\mathbb{Q}_0^{(s)}(A_1')$$

$$\boxed{\text{z83}} \quad \mathbb{Q}_{2,1}^{(c)}(E') = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E')\mathbb{Q}_0^{(s)}(A_1')}{2}$$

$$\boxed{\text{z84}} \quad \mathbb{Q}_{2,2}^{(c)}(E') = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E')\mathbb{Q}_0^{(s)}(A_1')}{2}$$

$$\boxed{\text{z85}} \quad \mathbb{Q}_{4,1}^{(c)}(E', 1) = \frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E', 1)\mathbb{Q}_0^{(s)}(A_1')}{2}$$

$$\boxed{\text{z86}} \quad \mathbb{Q}_{4,2}^{(c)}(E', 1) = \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E', 1)\mathbb{Q}_0^{(s)}(A_1')}{2}$$

$$\boxed{\text{z87}} \quad \mathbb{Q}_{4,1}^{(c)}(E', 2) = \frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E', 2)\mathbb{Q}_0^{(s)}(A_1')}{2}$$

$$\boxed{\text{z88}} \quad \mathbb{Q}_{4,2}^{(c)}(E', 2) = \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E', 2)\mathbb{Q}_0^{(s)}(A_1')}{2}$$

$$\boxed{\text{z167}} \quad \mathbb{Q}_{2,1}^{(c)}(E'') = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E'')\mathbb{Q}_0^{(s)}(A_1')}{2}$$

$$\boxed{\text{z168}} \quad \mathbb{Q}_{2,2}^{(c)}(E'') = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E'')\mathbb{Q}_0^{(s)}(A_1')}{2}$$

$$\boxed{\text{z169}} \quad \mathbb{Q}_{4,1}^{(c)}(E'') = \frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E'')\mathbb{Q}_0^{(s)}(A_1')}{2}$$

$$\boxed{\text{z170}} \quad \mathbb{Q}_{4,2}^{(c)}(E'') = \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E'')\mathbb{Q}_0^{(s)}(A_1')}{2}$$

• 'S' site-cluster : S

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

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

* wyckoff: 2i

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

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

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

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

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

$$\boxed{\text{z90}} \quad \mathbb{Q}_{1,2}^{(c)}(E') = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E'')\mathbb{Q}_1^{(s)}(A'_2)}{2}$$

$$\boxed{\text{z91}} \quad \mathbb{Q}_{2,1}^{(c)}(E') = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E')\mathbb{Q}_0^{(s)}(A'_1)}{2}$$

$$\boxed{\text{z92}} \quad \mathbb{Q}_{2,2}^{(c)}(E') = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E')\mathbb{Q}_0^{(s)}(A'_1)}{2}$$

$$\boxed{\text{z171}} \quad \mathbb{Q}_{2,1}^{(c)}(E'') = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E'')\mathbb{Q}_0^{(s)}(A'_1)}{2}$$

$$\boxed{\text{z172}} \quad \mathbb{Q}_{2,2}^{(c)}(E'') = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E'')\mathbb{Q}_0^{(s)}(A'_1)}{2}$$

$$\boxed{\text{z173}} \quad \mathbb{Q}_{3,1}^{(c)}(E'') = -\frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E')\mathbb{Q}_1^{(s)}(A'_2)}{2}$$

$$\boxed{\text{z174}} \quad \mathbb{Q}_{3,2}^{(c)}(E'') = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E')\mathbb{Q}_1^{(s)}(A'_2)}{2}$$

- 'Mo'-'Mo' bond-cluster : Mo;Mo_001_1
 - * 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: 3b03j

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

$$\boxed{\text{z64}} \quad \mathbb{Q}_1^{(c)}(A'_2, b) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(a)}(E'')\mathbb{T}_{1,2}^{(b)}(E')}{2} - \frac{\sqrt{2}\mathbb{M}_{1,2}^{(a)}(E'')\mathbb{T}_{1,1}^{(b)}(E')}{2}$$

$$\boxed{\text{z65}} \quad \mathbb{Q}_3^{(c)}(A'_2, a) = \frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{2} - \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{2}$$

$$\boxed{\text{z66}} \quad \mathbb{Q}_3^{(c)}(A'_2, b) = \frac{\sqrt{2}\mathbb{M}_{3,1}^{(a)}(E'')\mathbb{T}_{1,2}^{(b)}(E')}{2} - \frac{\sqrt{2}\mathbb{M}_{3,2}^{(a)}(E'')\mathbb{T}_{1,1}^{(b)}(E')}{2}$$

$$\boxed{\text{z67}} \quad \mathbb{Q}_4^{(c)}(A'_2, a) = \mathbb{Q}_4^{(a)}(A'_2)\mathbb{Q}_0^{(b)}(A'_1)$$

$$\boxed{\text{z68}} \quad \mathbb{Q}_4^{(c)}(A'_2, b) = \mathbb{M}_3^{(a)}(A'_1)\mathbb{M}_1^{(b)}(A'_2)$$

$$\boxed{\text{z93}} \quad \mathbb{Q}_{1,1}^{(c)}(E', a) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A'_1)\mathbb{Q}_{1,1}^{(b)}(E')}{2}$$

$$\boxed{\text{z94}} \quad \mathbb{Q}_{1,2}^{(c)}(E', a) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A'_1)\mathbb{Q}_{1,2}^{(b)}(E')}{2}$$

$$\boxed{\text{z95}} \quad \mathbb{Q}_{1,1}^{(c)}(E', b) = \frac{\sqrt{42}\mathbb{Q}_{2,1}^{(a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{14} + \frac{\sqrt{42}\mathbb{Q}_{2,2}^{(a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{14} - \frac{\sqrt{14}\mathbb{Q}_2^{(a)}(A'_1)\mathbb{Q}_{1,1}^{(b)}(E')}{14}$$

$$\boxed{\text{z96}} \quad \mathbb{Q}_{1,2}^{(c)}(E', b) = \frac{\sqrt{42}\mathbb{Q}_{2,1}^{(a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{14} - \frac{\sqrt{42}\mathbb{Q}_{2,2}^{(a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{14} - \frac{\sqrt{14}\mathbb{Q}_2^{(a)}(A'_1)\mathbb{Q}_{1,2}^{(b)}(E')}{14}$$

$$\boxed{\text{z97}} \quad \mathbb{Q}_{1,1}^{(c)}(E', c) = -\frac{\sqrt{2}\mathbb{M}_1^{(a)}(A'_2)\mathbb{T}_{1,2}^{(b)}(E')}{2}$$

$$\boxed{\text{z98}} \quad \mathbb{Q}_{1,2}^{(c)}(E', c) = \frac{\sqrt{2}\mathbb{M}_1^{(a)}(A'_2)\mathbb{T}_{1,1}^{(b)}(E')}{2}$$

$$\begin{aligned}
\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}
\end{aligned}$$

$$\begin{aligned}
\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} \\
\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} \\
\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} \\
\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} \\
\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} \\
\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} \\
\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} \\
\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} \\
\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} \\
\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} \\
\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} \\
\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} \\
\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} \\
\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}
\end{aligned}$$

$$\begin{aligned}
\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} \\
\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} \\
\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} \\
\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} \\
\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} \\
\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} \\
\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} \\
\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} \\
\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} \\
\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} \\
\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} \\
\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} \\
\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} \\
\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}
\end{aligned}$$

$$\boxed{\text{z197}} \quad \mathbb{G}_{4,1}^{(c)}(E'', 1) = -\frac{\mathbb{M}_3^{(a)}(A_1'')\mathbb{T}_{1,1}^{(b)}(E')}{2} - \frac{\mathbb{M}_3^{(a)}(A_2'')\mathbb{T}_{1,2}^{(b)}(E')}{2}$$

$$\boxed{\text{z198}} \quad \mathbb{G}_{4,2}^{(c)}(E'', 1) = -\frac{\mathbb{M}_3^{(a)}(A_1'')\mathbb{T}_{1,2}^{(b)}(E')}{2} + \frac{\mathbb{M}_3^{(a)}(A_2'')\mathbb{T}_{1,1}^{(b)}(E')}{2}$$

• 'Mo'-'S' bond-cluster : S;Mo_001_1

* 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

$$\boxed{\text{z15}} \quad \mathbb{Q}_0^{(c)}(A_1') = \frac{\sqrt{3}\mathbb{Q}_{1,1}^{(a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{3} + \frac{\sqrt{3}\mathbb{Q}_{1,2}^{(a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{3} + \frac{\sqrt{3}\mathbb{Q}_1^{(a)}(A_2'')\mathbb{Q}_1^{(b)}(A_2'')}{3}$$

$$\boxed{\text{z16}} \quad \mathbb{Q}_2^{(c)}(A_1', a) = \frac{\sqrt{14}\mathbb{Q}_{3,1}^{(a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{7} + \frac{\sqrt{14}\mathbb{Q}_{3,2}^{(a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{7} + \frac{\sqrt{21}\mathbb{Q}_3^{(a)}(A_2'')\mathbb{Q}_1^{(b)}(A_2'')}{7}$$

$$\boxed{\text{z17}} \quad \mathbb{Q}_2^{(c)}(A_1', b) = -\frac{\sqrt{6}\mathbb{Q}_{1,1}^{(a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{6} - \frac{\sqrt{6}\mathbb{Q}_{1,2}^{(a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{6} + \frac{\sqrt{6}\mathbb{Q}_1^{(a)}(A_2'')\mathbb{Q}_1^{(b)}(A_2'')}{3}$$

$$\boxed{\text{z18}} \quad \mathbb{Q}_2^{(c)}(A_1', c) = -\frac{\sqrt{2}\mathbb{G}_{2,1}^{(a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{2} - \frac{\sqrt{2}\mathbb{G}_{2,2}^{(a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{2}$$

$$\boxed{\text{z19}} \quad \mathbb{Q}_3^{(c)}(A_1', a) = \mathbb{Q}_3^{(a)}(A_1')\mathbb{Q}_0^{(b)}(A_1')$$

$$\boxed{\text{z20}} \quad \mathbb{Q}_3^{(c)}(A_1', b) = -\frac{\sqrt{2}\mathbb{Q}_{3,1}^{(a)}(E'')\mathbb{Q}_{2,1}^{(b)}(E'')}{2} - \frac{\sqrt{2}\mathbb{Q}_{3,2}^{(a)}(E'')\mathbb{Q}_{2,2}^{(b)}(E'')}{2}$$

$$\boxed{\text{z21}} \quad \mathbb{Q}_3^{(c)}(A_1', c) = \frac{\sqrt{2}\mathbb{G}_{2,1}^{(a)}(E'')\mathbb{Q}_{2,1}^{(b)}(E'')}{2} + \frac{\sqrt{2}\mathbb{G}_{2,2}^{(a)}(E'')\mathbb{Q}_{2,2}^{(b)}(E'')}{2}$$

$$\boxed{\text{z22}} \quad \mathbb{Q}_4^{(c)}(A_1') = -\frac{\sqrt{42}\mathbb{Q}_{3,1}^{(a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{14} - \frac{\sqrt{42}\mathbb{Q}_{3,2}^{(a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{14} + \frac{2\sqrt{7}\mathbb{Q}_3^{(a)}(A_2'')\mathbb{Q}_1^{(b)}(A_2'')}{7}$$

$$\boxed{\text{z33}} \quad \mathbb{Q}_4^{(c)}(A_1'') = -\frac{\sqrt{6}\mathbb{Q}_{3,1}^{(a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{4} - \frac{\sqrt{6}\mathbb{Q}_{3,2}^{(a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{4} + \frac{\mathbb{Q}_3^{(a)}(A_2'')\mathbb{Q}_1^{(b)}(A_2'')}{2}$$

$$\boxed{\text{z34}} \quad \mathbb{G}_0^{(c)}(A_1'') = \frac{\sqrt{2}\mathbb{G}_{2,1}^{(a)}(E')\mathbb{Q}_{2,1}^{(b)}(E'')}{2} + \frac{\sqrt{2}\mathbb{G}_{2,2}^{(a)}(E')\mathbb{Q}_{2,2}^{(b)}(E'')}{2}$$

$$\boxed{\text{z35}} \quad \mathbb{G}_2^{(c)}(A_1'', a) = \frac{\sqrt{2}\mathbb{Q}_{3,1}^{(a)}(E')\mathbb{Q}_{2,1}^{(b)}(E'')}{2} + \frac{\sqrt{2}\mathbb{Q}_{3,2}^{(a)}(E')\mathbb{Q}_{2,2}^{(b)}(E'')}{2}$$

$$\boxed{\text{z36}} \quad \mathbb{G}_2^{(c)}(A_1'', b) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E')\mathbb{Q}_{2,1}^{(b)}(E'')}{2} + \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E')\mathbb{Q}_{2,2}^{(b)}(E'')}{2}$$

$$\boxed{\text{z37}} \quad \mathbb{G}_2^{(c)}(A_1'', c) = \mathbb{G}_2^{(a)}(A_1'')\mathbb{Q}_0^{(b)}(A_1')$$

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

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

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

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

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

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

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

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

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

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

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

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

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

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

$$\boxed{\text{z74}} \quad \mathbb{Q}_4^{(c)}(A_2'') = -\frac{\sqrt{6}\mathbb{Q}_{3,1}^{(a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{4} + \frac{\sqrt{6}\mathbb{Q}_{3,2}^{(a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{4} + \frac{\mathbb{Q}_3^{(a)}(A_1')\mathbb{Q}_1^{(b)}(A_2'')}{2}$$

$$\boxed{\text{z75}} \quad \mathbb{G}_3^{(c)}(A_2'', a) = \frac{\sqrt{2}\mathbb{Q}_{3,1}^{(a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{4} - \frac{\sqrt{2}\mathbb{Q}_{3,2}^{(a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{4} + \frac{\sqrt{3}\mathbb{Q}_3^{(a)}(A_1')\mathbb{Q}_1^{(b)}(A_2'')}{2}$$

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

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

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

$$\boxed{\text{z121}} \quad \mathbb{Q}_{1,1}^{(c)}(E', b) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E')\mathbb{Q}_0^{(b)}(A_1')}{2}$$

$$\boxed{\text{z122}} \quad \mathbb{Q}_{1,2}^{(c)}(E', b) = \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E')\mathbb{Q}_0^{(b)}(A_1')}{2}$$

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

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

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

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

$$\begin{aligned}
\boxed{\text{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{\text{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{\text{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}
\end{aligned}$$

$$\begin{aligned}
\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} \\
\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} \\
\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} \\
\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} \\
\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} \\
\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} \\
\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} \\
\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} \\
\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} \\
\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} \\
\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} \\
\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} \\
\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} \\
\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}
\end{aligned}$$

$$\begin{aligned}
\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} \\
\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} \\
\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} \\
\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} \\
\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} \\
\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} \\
\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} \\
\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} \\
\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} \\
\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} \\
\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} \\
\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} \\
\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} \\
\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}
\end{aligned}$$

$$\boxed{\text{z219}} \quad \mathbb{G}_{1,1}^{(c)}(E'', b) = \frac{\sqrt{15}\mathbb{G}_{2,1}^{(a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{10} + \frac{\sqrt{15}\mathbb{G}_{2,2}^{(a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{10} - \frac{\sqrt{15}\mathbb{G}_{2,2}^{(a)}(E')\mathbb{Q}_1^{(b)}(A_2'')}{10} - \frac{\sqrt{5}\mathbb{G}_2^{(a)}(A_1'')\mathbb{Q}_{1,1}^{(b)}(E')}{10}$$

$$\boxed{\text{z220}} \quad \mathbb{G}_{1,2}^{(c)}(E'', b) = \frac{\sqrt{15}\mathbb{G}_{2,1}^{(a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{10} + \frac{\sqrt{15}\mathbb{G}_{2,1}^{(a)}(E')\mathbb{Q}_1^{(b)}(A_2'')}{10} - \frac{\sqrt{15}\mathbb{G}_{2,2}^{(a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{10} - \frac{\sqrt{5}\mathbb{G}_2^{(a)}(A_1'')\mathbb{Q}_{1,2}^{(b)}(E')}{10}$$

$$\boxed{\text{z221}} \quad \mathbb{G}_{2,1}^{(c)}(E'', a) = \frac{\sqrt{2}\mathbb{G}_{2,1}^{(a)}(E'')\mathbb{Q}_0^{(b)}(A_1')}{2}$$

$$\boxed{\text{z222}} \quad \mathbb{G}_{2,2}^{(c)}(E'', a) = \frac{\sqrt{2}\mathbb{G}_{2,2}^{(a)}(E'')\mathbb{Q}_0^{(b)}(A_1')}{2}$$

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

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

$$\boxed{\text{z225}} \quad \mathbb{G}_{3,1}^{(c)}(E'', a) = -\frac{\sqrt{15}\mathbb{Q}_{3,1}^{(a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{12} - \frac{\sqrt{15}\mathbb{Q}_{3,2}^{(a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{12} + \frac{\sqrt{6}\mathbb{Q}_{3,2}^{(a)}(E')\mathbb{Q}_1^{(b)}(A_2'')}{12} - \frac{\mathbb{Q}_3^{(a)}(A_2'')\mathbb{Q}_{1,2}^{(b)}(E')}{2}$$

$$\boxed{\text{z226}} \quad \mathbb{G}_{3,2}^{(c)}(E'', a) = -\frac{\sqrt{15}\mathbb{Q}_{3,1}^{(a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{12} - \frac{\sqrt{6}\mathbb{Q}_{3,1}^{(a)}(E')\mathbb{Q}_1^{(b)}(A_2'')}{12} + \frac{\sqrt{15}\mathbb{Q}_{3,2}^{(a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{12} + \frac{\mathbb{Q}_3^{(a)}(A_2'')\mathbb{Q}_{1,1}^{(b)}(E')}{2}$$

$$\boxed{\text{z227}} \quad \mathbb{G}_{3,1}^{(c)}(E'', b) = -\frac{\sqrt{15}\mathbb{G}_{2,1}^{(a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{30} - \frac{\sqrt{15}\mathbb{G}_{2,2}^{(a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{30} - \frac{2\sqrt{15}\mathbb{G}_{2,2}^{(a)}(E')\mathbb{Q}_1^{(b)}(A_2'')}{15} + \frac{\sqrt{5}\mathbb{G}_2^{(a)}(A_1'')\mathbb{Q}_{1,1}^{(b)}(E')}{5}$$

$$\boxed{\text{z228}} \quad \mathbb{G}_{3,2}^{(c)}(E'', b) = -\frac{\sqrt{15}\mathbb{G}_{2,1}^{(a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{30} + \frac{2\sqrt{15}\mathbb{G}_{2,1}^{(a)}(E')\mathbb{Q}_1^{(b)}(A_2'')}{15} + \frac{\sqrt{15}\mathbb{G}_{2,2}^{(a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{30} + \frac{\sqrt{5}\mathbb{G}_2^{(a)}(A_1'')\mathbb{Q}_{1,2}^{(b)}(E')}{5}$$

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

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

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

* wyckoff: **6b@6n**

$$\boxed{\text{z23}} \quad \mathbb{Q}_0^{(c)}(A_1', a) = \mathbb{Q}_0^{(a)}(A_1')\mathbb{Q}_0^{(b)}(A_1')$$

$$\boxed{\text{z24}} \quad \mathbb{Q}_0^{(c)}(A_1', b) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E'')\mathbb{Q}_{2,1}^{(b)}(E'')}{2} + \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E'')\mathbb{Q}_{2,2}^{(b)}(E'')}{2}$$

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

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

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

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

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

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

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

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

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

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

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

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

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

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

$$\begin{aligned}
\boxed{\text{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{\text{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{\text{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}
\end{aligned}$$

$$\begin{aligned}
\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} \\
\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} \\
\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} \\
\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} \\
\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} \\
\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} \\
\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} \\
\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} \\
\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} \\
\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} \\
\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} \\
\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} \\
\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} \\
\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}
\end{aligned}$$

$$\begin{aligned}
\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}
\end{aligned}$$

Atomic SAMB

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

$$\boxed{\text{x16}} \quad \mathbb{M}_3^{(a)}(A_1'') = \begin{bmatrix} 0 & 0 & \frac{i}{2} & 0 & 0 \\ 0 & 0 & 0 & -\frac{i}{2} & 0 \\ -\frac{i}{2} & 0 & 0 & 0 & 0 \\ 0 & \frac{i}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x17}} \quad \mathbb{M}_1^{(a)}(A_2') = \begin{bmatrix} 0 & -\frac{\sqrt{10}i}{5} & 0 & 0 & 0 \\ \frac{\sqrt{10}i}{5} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{10}i}{10} & 0 \\ 0 & 0 & \frac{\sqrt{10}i}{10} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x18}} \quad \mathbb{M}_3^{(a)}(A_2') = \begin{bmatrix} 0 & \frac{\sqrt{10}i}{10} & 0 & 0 & 0 \\ -\frac{\sqrt{10}i}{10} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{10}i}{5} & 0 \\ 0 & 0 & \frac{\sqrt{10}i}{5} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x19}} \quad \mathbb{M}_3^{(a)}(A_2'') = \begin{bmatrix} 0 & 0 & 0 & -\frac{i}{2} & 0 \\ 0 & 0 & -\frac{i}{2} & 0 & 0 \\ 0 & \frac{i}{2} & 0 & 0 & 0 \\ \frac{i}{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Cluster SAMB

- Site cluster

** Wyckoff: 1a

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

** Wyckoff: 2i

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

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

- Bond cluster

** Wyckoff: **3b@3j**

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

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

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

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

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

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

** Wyckoff: **6b@6n**

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

$$\boxed{\text{y11}} \quad \mathbb{M}_2^{(s)}(A''_1) = \left[\frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, -\frac{\sqrt{6}i}{6}, -\frac{\sqrt{6}i}{6}, -\frac{\sqrt{6}i}{6} \right]$$

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

$$\boxed{\text{y13}} \quad \mathbb{Q}_1^{(s)}(A''_2) = \left[\frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, -\frac{\sqrt{6}}{6}, -\frac{\sqrt{6}}{6}, -\frac{\sqrt{6}}{6} \right]$$

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

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

$$\boxed{\text{y16}} \quad \mathbb{T}_{1,1}^{(s)}(E') = \left[\frac{\sqrt{3}i}{6}, -\frac{\sqrt{3}i}{3}, \frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{6}, -\frac{\sqrt{3}i}{3}, \frac{\sqrt{3}i}{6} \right]$$

$$\boxed{\text{y17}} \quad \mathbb{T}_{1,2}^{(s)}(E') = \left[\frac{i}{2}, 0, -\frac{i}{2}, \frac{i}{2}, 0, -\frac{i}{2} \right]$$

$$\boxed{\text{y18}} \quad \mathbb{M}_{1,1}^{(s)}(E'') = \left[\frac{i}{2}, 0, -\frac{i}{2}, -\frac{i}{2}, 0, \frac{i}{2} \right]$$

$$\boxed{\text{y19}} \quad \mathbb{M}_{1,2}^{(s)}(E'') = \left[-\frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{3}, -\frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{6}, -\frac{\sqrt{3}i}{3}, \frac{\sqrt{3}i}{6} \right]$$

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

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

** Wyckoff: **6a@6n**

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

$$\boxed{\text{y23}} \quad \mathbb{T}_0^{(s)}(A'_1) = \left[\frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6} \right]$$

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

$$\boxed{\text{y25}} \quad \mathbb{T}_1^{(s)}(A'_2) = \left[\frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, -\frac{\sqrt{6}i}{6}, -\frac{\sqrt{6}i}{6}, -\frac{\sqrt{6}i}{6} \right]$$

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

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

$$\boxed{\text{y28}} \quad \mathbb{T}_{1,1}^{(s)}(E') = \left[\frac{i}{2}, 0, -\frac{i}{2}, \frac{i}{2}, 0, -\frac{i}{2} \right]$$

$$\boxed{\text{y29}} \quad \mathbb{T}_{1,2}^{(s)}(E') = \left[-\frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{3}, -\frac{\sqrt{3}i}{6}, -\frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{3}, -\frac{\sqrt{3}i}{6} \right]$$

$$\boxed{\text{y30}} \quad \mathbb{M}_{1,1}^{(s)}(E'') = \left[-\frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{3}, -\frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{6}, -\frac{\sqrt{3}i}{3}, \frac{\sqrt{3}i}{6} \right]$$

$$\boxed{\text{y31}} \quad \mathbb{M}_{1,2}^{(s)}(E'') = \left[-\frac{i}{2}, 0, \frac{i}{2}, \frac{i}{2}, 0, -\frac{i}{2} \right]$$

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

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

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$
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 (\mathbf{s})	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 (\mathbf{s})	mapping
1	[0.66667, 0.33333, 0.12425]	[1,2,3,7,8,9]

continued ...

Table 8

SL	position (\mathbf{s})	mapping
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, $|\mathbf{v}| = 3.1661$ (cartesian)

SL	vector (\mathbf{v})	center (\mathbf{c})	mapping	head	tail	\mathbf{R} (primitive)
1	[-1.00000, -1.00000, 0.00000]	[0.50000, 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, $|\mathbf{v}| = 3.0849$ (cartesian)

SL	vector (\mathbf{v})	center (\mathbf{c})	mapping	head	tail	\mathbf{R} (primitive)
1	[0.33333, -0.33333, -0.12425]	[0.83333, 0.16667, 0.06212]	[1,7]	(1,1)	(1,1)	[-1,0,0]

continued ...

Table 10

SL	vector (\boldsymbol{v})	center (\boldsymbol{c})	mapping	head	tail	\boldsymbol{R} (primitive)
2	[0.33333, 0.66667, -0.12425]	[0.83333, 0.66667, 0.06212]	[2,9]	(1,1)	(1,1)	[-1,-1,0]
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 (6b06n), ND, $|\boldsymbol{v}|= 3.1661$ (cartesian)

SL	vector (\boldsymbol{v})	center (\boldsymbol{c})	mapping	head	tail	\boldsymbol{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]