

# 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**

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

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**Symmetry Operation**


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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	$\{2_{210} 0\}$						

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**Harmonics**


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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	$-\frac{\sqrt{105}xyz(x^2+y^2-2z^2)}{2}$

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**Basis in full matrix**


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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$	$y$

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

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**SAMB: 246 (all 246)**


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- 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**

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

• **S** : '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

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

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

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

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

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

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

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

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

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

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

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

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

- Mo;Mo\_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: **3b03j**

$$\boxed{\text{z6}} \quad \mathbb{Q}_0^{(c)}(A_1', a) = \mathbb{Q}_0^{(a)}(A_1')\mathbb{Q}_0^{(b)}(A_1')$$

$$\boxed{\text{z7}} \quad \mathbb{Q}_0^{(c)}(A_1', b) = \mathbb{M}_1^{(a)}(A_2')\mathbb{M}_1^{(b)}(A_2')$$

$$\boxed{\text{z8}} \quad \mathbb{Q}_2^{(c)}(A_1', a) = \mathbb{Q}_2^{(a)}(A_1')\mathbb{Q}_0^{(b)}(A_1')$$

$$\boxed{\text{z9}} \quad \mathbb{Q}_2^{(c)}(A_1', b) = \mathbb{M}_3^{(a)}(A_2')\mathbb{M}_1^{(b)}(A_2')$$

$$\boxed{\text{z10}} \quad \mathbb{Q}_3^{(c)}(A_1', a) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{2} + \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{2}$$

$$\boxed{\text{z11}} \quad \mathbb{Q}_3^{(c)}(A_1', b) = -\frac{\sqrt{406}\mathbb{Q}_{4,1}^{(a)}(E', 1)\mathbb{Q}_{1,1}^{(b)}(E')}{29} - \frac{\sqrt{58}\mathbb{Q}_{4,1}^{(a)}(E', 2)\mathbb{Q}_{1,1}^{(b)}(E')}{58} - \frac{\sqrt{406}\mathbb{Q}_{4,2}^{(a)}(E', 1)\mathbb{Q}_{1,2}^{(b)}(E')}{29} - \frac{\sqrt{58}\mathbb{Q}_{4,2}^{(a)}(E', 2)\mathbb{Q}_{1,2}^{(b)}(E')}{58}$$



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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

• 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: 6a06n

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

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

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

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

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

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

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

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

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

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

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

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

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

$$\begin{aligned}
\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')
\end{aligned}$$

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



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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

• **S;S\_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**

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

$$\begin{aligned}
\boxed{\text{z240}} \quad \mathbb{Q}_{4,2}^{(c)}(E'') &= \frac{\sqrt{7}\mathbb{Q}_{2,1}^{(a)}(E')\mathbb{Q}_{2,1}^{(b)}(E'')}{14} - \frac{\sqrt{7}\mathbb{Q}_{2,2}^{(a)}(E')\mathbb{Q}_{2,2}^{(b)}(E'')}{14} + \frac{\sqrt{21}\mathbb{Q}_2^{(a)}(A'_1)\mathbb{Q}_{2,2}^{(b)}(E'')}{7} \\
\boxed{\text{z241}} \quad \mathbb{G}_{1,1}^{(c)}(E'') &= \frac{\mathbb{M}_{1,2}^{(a)}(E'')\mathbb{M}_1^{(b)}(A'_2)}{2} - \frac{\mathbb{M}_1^{(a)}(A'_2)\mathbb{M}_{1,2}^{(b)}(E'')}{2} \\
\boxed{\text{z242}} \quad \mathbb{G}_{1,2}^{(c)}(E'') &= -\frac{\mathbb{M}_{1,1}^{(a)}(E'')\mathbb{M}_1^{(b)}(A'_2)}{2} + \frac{\mathbb{M}_1^{(a)}(A'_2)\mathbb{M}_{1,1}^{(b)}(E'')}{2} \\
\boxed{\text{z243}} \quad \mathbb{G}_{2,1}^{(c)}(E'', a) &= -\frac{\sqrt{3}\mathbb{Q}_{2,1}^{(a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{6} - \frac{\sqrt{3}\mathbb{Q}_{2,2}^{(a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{6} - \frac{\sqrt{3}\mathbb{Q}_{2,2}^{(a)}(E')\mathbb{Q}_1^{(b)}(A'_2)}{3} \\
\boxed{\text{z244}} \quad \mathbb{G}_{2,2}^{(c)}(E'', a) &= -\frac{\sqrt{3}\mathbb{Q}_{2,1}^{(a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{6} + \frac{\sqrt{3}\mathbb{Q}_{2,1}^{(a)}(E')\mathbb{Q}_1^{(b)}(A'_2)}{3} + \frac{\sqrt{3}\mathbb{Q}_{2,2}^{(a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{6} \\
\boxed{\text{z245}} \quad \mathbb{G}_{2,1}^{(c)}(E'', b) &= \frac{\mathbb{M}_{1,1}^{(a)}(E'')\mathbb{T}_{1,2}^{(b)}(E')}{2} + \frac{\mathbb{M}_{1,2}^{(a)}(E'')\mathbb{T}_{1,1}^{(b)}(E')}{2} \\
\boxed{\text{z246}} \quad \mathbb{G}_{2,2}^{(c)}(E'', b) &= \frac{\mathbb{M}_{1,1}^{(a)}(E'')\mathbb{T}_{1,1}^{(b)}(E')}{2} - \frac{\mathbb{M}_{1,2}^{(a)}(E'')\mathbb{T}_{1,2}^{(b)}(E')}{2}
\end{aligned}$$

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## Atomic SAMB

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

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

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

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

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

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

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

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

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

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

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## Cluster SAMB

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- 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: 6a@6n

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

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

$$\boxed{\text{y12}} \quad \mathbb{Q}_1^{(s)}(A_2'') = \left[ \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, -\frac{\sqrt{6}}{6}, -\frac{\sqrt{6}}{6}, -\frac{\sqrt{6}}{6} \right]$$

$$\boxed{\text{y13}} \quad \mathbb{T}_1^{(s)}(A_2'') = \left[ \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, -\frac{\sqrt{6}i}{6}, -\frac{\sqrt{6}i}{6}, -\frac{\sqrt{6}i}{6} \right]$$

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

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

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

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

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

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

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

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

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

$$\boxed{\text{y22}} \quad \mathbb{Q}_0^{(s)}(A_1') = \left[ \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6} \right]$$

$$\boxed{\text{y23}} \quad \mathbb{M}_2^{(s)}(A_1'') = \left[ \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, -\frac{\sqrt{6}i}{6}, -\frac{\sqrt{6}i}{6}, -\frac{\sqrt{6}i}{6} \right]$$

$$\boxed{\text{y24}} \quad \mathbb{M}_1^{(s)}(A_2') = \left[ \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6} \right]$$



$$\boxed{\text{y25}} \quad \mathbb{Q}_1^{(s)}(A_2'') = \left[ \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, -\frac{\sqrt{6}}{6}, -\frac{\sqrt{6}}{6}, -\frac{\sqrt{6}}{6} \right]$$

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

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

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

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

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

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

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

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

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— Site and Bond

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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 ( <i>s</i> )	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 (3b03j), ND,  $|\mathbf{v}|=3.1661$  (cartesian)

SL	vector ( <i>v</i> )	center ( <i>c</i> )	mapping	head	tail	<i>R</i> (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 (6a06n), D,  $|\mathbf{v}|=3.0849$  (cartesian)

SL	vector ( <i>v</i> )	center ( <i>c</i> )	mapping	head	tail	<i>R</i> (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 ( $\boldsymbol{v}$ )	center ( $\boldsymbol{c}$ )	mapping	head	tail	$\boldsymbol{R}$ (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,  $|\boldsymbol{v}|=3.1661$  (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]