Model for "`MoS2`"

General Condition

- Basis type: `lg`
- 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]`
- 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):
  $\boldsymbol{a}_1 = [\ 3.16610,\ 0.00000,\ 0.00000]$
  $\boldsymbol{a}_2 = [-1.58305,\ 2.74192,\ 0.00000]$
  $\boldsymbol{a}_3 = [\ 0.00000,\ 0.00000, 20.00000]$

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	$\{-6^-_{001}\|0\}$

continued …

Table 1

#	SO	#	SO	#	SO	#	SO	#	SO
6	$\{-6^+_{001}\|0\}$	7	$\{m_{110}\|0\}$	8	$\{m_{100}\|0\}$	9	$\{m_{010}\|0\}$	10	$\{2_{1-10}\|0\}$
11	$\{2_{120}\|0\}$	12	$\{2_{210}\|0\}$								

Harmonics

Table 2: Harmonics

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

continued …

2

Table 2

#	symbol	irrep.	rank	X	multiplicity	component	symmetry
11	$\mathbb{G}_1(A_2')$	A_2'	1	G, M	-	-	z
12	$\mathbb{G}_3(A_2')$	A_2'	3	G, M	-	-	$-\dfrac{z(3x^2+3y^2-2z^2)}{2}$
13	$\mathbb{Q}_3(A_2')$	A_2'	3	Q, T	-	-	$\dfrac{\sqrt{10}x(x^2-3y^2)}{4}$
14	$\mathbb{Q}_5(A_2')$	A_2'	5	Q, T	-	-	$-\dfrac{\sqrt{70}x(x^2-3y^2)(x^2+y^2-8z^2)}{16}$
15	$\mathbb{Q}_1(A_2'')$	A_2''	1	Q, T	-	-	z
16	$\mathbb{G}_3(A_2'')$	A_2''	3	G, M	-	-	$\dfrac{\sqrt{10}x(x^2-3y^2)}{4}$
17	$\mathbb{Q}_3(A_2'')$	A_2''	3	Q, T	-	-	$-\dfrac{z(3x^2+3y^2-2z^2)}{2}$
18	$\mathbb{Q}_4(A_2'')$	A_2''	4	Q, T	-	-	$\dfrac{\sqrt{70}yz(3x^2-y^2)}{4}$
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	$\dfrac{\sqrt{3}(x-y)(x+y)}{2}$
25	$\mathbb{G}_{3,1}(E')$	E'	3	G, M	-	1	$-\dfrac{\sqrt{15}z(x-y)(x+y)}{2}$
26	$\mathbb{G}_{3,2}(E')$					2	$\sqrt{15}xyz$
27	$\mathbb{Q}_{3,1}(E')$	E'	3	Q, T	-	1	$-\dfrac{\sqrt{6}x(x^2+y^2-4z^2)}{4}$
28	$\mathbb{Q}_{3,2}(E')$					2	$-\dfrac{\sqrt{6}y(x^2+y^2-4z^2)}{4}$
29	$\mathbb{Q}_{4,1}(E',1)$	E'	4	Q, T	1	1	$-\dfrac{\sqrt{35}xy(x-y)(x+y)}{2}$
30	$\mathbb{Q}_{4,2}(E',1)$					2	$\dfrac{\sqrt{35}(x^2-2xy-y^2)(x^2+2xy-y^2)}{8}$
31	$\mathbb{Q}_{4,1}(E',2)$	E'	4	Q, T	2	1	$-\dfrac{\sqrt{5}xy(x^2+y^2-6z^2)}{2}$

3

Table 2

#	symbol	irrep.	rank	X	multiplicity	component	symmetry
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	$\frac{\sqrt{10}xz(3x^2+3y^2-4z^2)}{4}$
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	$-\frac{3\sqrt{35}xyz(x-y)(x+y)}{2}$

continued …

4

Table 2

#	symbol	irrep.	rank	X	multiplicity	component	symmetry
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)
1	$\lvert d_u \rangle$ @Mo(1)	2	$\lvert d_{xz} \rangle$ @Mo(1)	3	$\lvert d_{yz} \rangle$ @Mo(1)	4	$\lvert d_{xy} \rangle$ @Mo(1)	5	$\lvert d_v \rangle$ @Mo(1)
6	$\lvert p_x \rangle$ @S(1)	7	$\lvert p_y \rangle$ @S(1)	8	$\lvert p_z \rangle$ @S(1)	9	$\lvert p_x \rangle$ @S(2)	10	$\lvert p_y \rangle$ @S(2)
11	$\lvert p_z \rangle$ @S(2)								

Table 4: Atomic basis (orbital part only)

orbital	definition
$\lvert p_x \rangle$	x

continued …

5

Table 4

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

— **SAMB** ———————————————————————————————

164 (all 246) SAMBs

- 'Mo' site-cluster
  * bra: $\langle d_u \rvert$, $\langle d_{xz} \rvert$, $\langle d_{yz} \rvert$, $\langle d_{xy} \rvert$, $\langle d_v \rvert$
  * ket: $\lvert d_u \rangle$, $\lvert d_{xz} \rangle$, $\lvert d_{yz} \rangle$, $\lvert d_{xy} \rangle$, $\lvert d_v \rangle$
  * wyckoff: `1a`

$\boxed{\text{z1}}$ $\quad \mathbb{Q}_0^{(c)}(A_1') = \mathbb{Q}_0^{(a)}(A_1')\mathbb{Q}_0^{(s)}(A_1')$

$\boxed{\text{z2}}$ $\quad \mathbb{Q}_2^{(c)}(A_1') = \mathbb{Q}_2^{(a)}(A_1')\mathbb{Q}_0^{(s)}(A_1')$

$\boxed{\text{z3}}$ $\quad \mathbb{Q}_4^{(c)}(A_1') = \mathbb{Q}_4^{(a)}(A_1')\mathbb{Q}_0^{(s)}(A_1')$

$\boxed{\text{z43}}$ $\quad \mathbb{Q}_4^{(c)}(A_1'') = \mathbb{Q}_4^{(a)}(A_1'')\mathbb{Q}_0^{(s)}(A_1')$

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

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

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

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

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

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

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

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

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

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

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

- '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

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

$\boxed{\text{z5}}$ $\quad \mathbb{Q}_2^{(c)}(A_1') = \mathbb{Q}_2^{(a)}(A_1')\mathbb{Q}_0^{(s)}(A_1')$

$\boxed{\text{z61}}$ $\quad \mathbb{Q}_1^{(c)}(A_2'', a) = \mathbb{Q}_0^{(a)}(A_1')\mathbb{Q}_1^{(s)}(A_2'')$

$\boxed{\text{z62}}$ $\quad \mathbb{Q}_1^{(c)}(A_2'', b) = \mathbb{Q}_2^{(a)}(A_1')\mathbb{Q}_1^{(s)}(A_2'')$

$\boxed{\text{z89}}$ $\quad \mathbb{Q}_{1,1}^{(c)}(E') = -\dfrac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E'')\mathbb{Q}_1^{(s)}(A_2'')}{2}$

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

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

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

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

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

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

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

- 'Mo'-'Mo' bond-cluster
  * bra: $\langle d_u |$, $\langle d_{xz} |$, $\langle d_{yz} |$, $\langle d_{xy} |$, $\langle d_v |$
  * ket: $| d_u \rangle$, $| d_{xz} \rangle$, $| d_{yz} \rangle$, $| d_{xy} \rangle$, $| d_v \rangle$
  * wyckoff: `3b@3j`

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

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

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

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

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

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

$\boxed{\text{z12}}$ $\quad \mathbb{Q}_3^{(c)}(A_1', c) = -\dfrac{\sqrt{2}\mathbb{M}_{3,1}^{(a)}(E')\mathbb{T}_{1,1}^{(b)}(E')}{2} - \dfrac{\sqrt{2}\mathbb{M}_{3,2}^{(a)}(E')\mathbb{T}_{1,2}^{(b)}(E')}{2}$

$\boxed{\text{z13}}$ $\quad \mathbb{Q}_4^{(c)}(A_1') = \mathbb{Q}_4^{(a)}(A_1')\mathbb{Q}_0^{(b)}(A_1')$

$\boxed{\text{z14}}$ $\quad \mathbb{Q}_5^{(c)}(A_1') = -\dfrac{\sqrt{58}\mathbb{Q}_{4,1}^{(a)}(E',1)\mathbb{Q}_{1,1}^{(b)}(E')}{58} + \dfrac{\sqrt{406}\mathbb{Q}_{4,1}^{(a)}(E',2)\mathbb{Q}_{1,1}^{(b)}(E')}{29} - \dfrac{\sqrt{58}\mathbb{Q}_{4,2}^{(a)}(E',1)\mathbb{Q}_{1,2}^{(b)}(E')}{58} + \dfrac{\sqrt{406}\mathbb{Q}_{4,2}^{(a)}(E',2)\mathbb{Q}_{1,2}^{(b)}(E')}{29}$

$\boxed{\text{z29}}$ $\quad \mathbb{Q}_4^{(c)}(A_1'', a) = \mathbb{Q}_4^{(a)}(A_1'')\mathbb{Q}_0^{(b)}(A_1')$

$\boxed{\text{z30}}$ $\quad \mathbb{Q}_4^{(c)}(A_1'', b) = \mathbb{M}_3^{(a)}(A_2'')\mathbb{M}_1^{(b)}(A_2')$

$\boxed{\text{z31}}$ $\quad \mathbb{Q}_3^{(c)}(A_2', a) = -\dfrac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{2} + \dfrac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{2}$

$\boxed{\text{z32}}$ $\quad \mathbb{Q}_3^{(c)}(A_2', b) = -\dfrac{\sqrt{406}\mathbb{Q}_{4,1}^{(a)}(E',1)\mathbb{Q}_{1,2}^{(b)}(E')}{29} + \dfrac{\sqrt{58}\mathbb{Q}_{4,1}^{(a)}(E',2)\mathbb{Q}_{1,2}^{(b)}(E')}{58} + \dfrac{\sqrt{406}\mathbb{Q}_{4,2}^{(a)}(E',1)\mathbb{Q}_{1,1}^{(b)}(E')}{29} - \dfrac{\sqrt{58}\mathbb{Q}_{4,2}^{(a)}(E',2)\mathbb{Q}_{1,1}^{(b)}(E')}{58}$

$\boxed{\text{z44}}$ $\quad \mathbb{Q}_3^{(c)}(A_2', c) = \dfrac{\sqrt{2}\mathbb{M}_{3,1}^{(a)}(E')\mathbb{T}_{1,2}^{(b)}(E')}{2} - \dfrac{\sqrt{2}\mathbb{M}_{3,2}^{(a)}(E')\mathbb{T}_{1,1}^{(b)}(E')}{2}$

$\boxed{\text{z45}}$ $\quad \mathbb{Q}_5^{(c)}(A_2') = -\dfrac{\sqrt{58}\mathbb{Q}_{4,1}^{(a)}(E',1)\mathbb{Q}_{1,2}^{(b)}(E')}{58} - \dfrac{\sqrt{406}\mathbb{Q}_{4,1}^{(a)}(E',2)\mathbb{Q}_{1,2}^{(b)}(E')}{29} + \dfrac{\sqrt{58}\mathbb{Q}_{4,2}^{(a)}(E',1)\mathbb{Q}_{1,1}^{(b)}(E')}{58} + \dfrac{\sqrt{406}\mathbb{Q}_{4,2}^{(a)}(E',2)\mathbb{Q}_{1,1}^{(b)}(E')}{29}$

$\boxed{\text{z46}}$ $\quad \mathbb{Q}_1^{(c)}(A_2'', a) = \dfrac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{2} - \dfrac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{2}$

$\boxed{\text{z47}}$ $\quad \mathbb{Q}_1^{(c)}(A_2'', b) = \dfrac{\sqrt{2}\mathbb{M}_{1,1}^{(a)}(E'')\mathbb{T}_{1,2}^{(b)}(E')}{2} - \dfrac{\sqrt{2}\mathbb{M}_{1,2}^{(a)}(E'')\mathbb{T}_{1,1}^{(b)}(E')}{2}$

$\boxed{\text{z48}}$ $\quad \mathbb{Q}_3^{(c)}(A_2'', a) = \dfrac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{2} - \dfrac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{2}$

$$\boxed{\text{z49}} \quad \mathbb{Q}_3^{(c)}(A_2'',b) = \frac{\sqrt{2}\mathbb{M}_{3,1}^{(a)}(E'')\mathbb{T}_{1,2}^{(b)}(E')}{2} - \frac{\sqrt{2}\mathbb{M}_{3,2}^{(a)}(E'')\mathbb{T}_{1,1}^{(b)}(E')}{2}$$

$$\boxed{\text{z63}} \quad \mathbb{Q}_4^{(c)}(A_2'',a) = \mathbb{Q}_4^{(a)}(A_2'')\mathbb{Q}_0^{(b)}(A_1')$$

$$\boxed{\text{z64}} \quad \mathbb{Q}_4^{(c)}(A_2'',b) = \mathbb{M}_3^{(a)}(A_1'')\mathbb{M}_1^{(b)}(A_2')$$

$$\boxed{\text{z65}} \quad \mathbb{Q}_{1,1}^{(c)}(E',a) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_1')\mathbb{Q}_{1,1}^{(b)}(E')}{2}$$

$$\boxed{\text{z66}} \quad \mathbb{Q}_{1,2}^{(c)}(E',a) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_1')\mathbb{Q}_{1,2}^{(b)}(E')}{2}$$

$$\boxed{\text{z67}} \quad \mathbb{Q}_{1,1}^{(c)}(E',b) = \frac{\sqrt{42}\mathbb{Q}_{2,1}^{(a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{14} + \frac{\sqrt{42}\mathbb{Q}_{2,2}^{(a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{14} - \frac{\sqrt{14}\mathbb{Q}_2^{(a)}(A_1')\mathbb{Q}_{1,1}^{(b)}(E')}{14}$$

$$\boxed{\text{z68}} \quad \mathbb{Q}_{1,2}^{(c)}(E',b) = \frac{\sqrt{42}\mathbb{Q}_{2,1}^{(a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{14} - \frac{\sqrt{42}\mathbb{Q}_{2,2}^{(a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{14} - \frac{\sqrt{14}\mathbb{Q}_2^{(a)}(A_1')\mathbb{Q}_{1,2}^{(b)}(E')}{14}$$

$$\boxed{\text{z93}} \quad \mathbb{Q}_{1,1}^{(c)}(E',c) = -\frac{\sqrt{2}\mathbb{M}_1^{(a)}(A_2')\mathbb{T}_{1,2}^{(b)}(E')}{2}$$

$$\boxed{\text{z94}} \quad \mathbb{Q}_{1,2}^{(c)}(E',c) = \frac{\sqrt{2}\mathbb{M}_1^{(a)}(A_2')\mathbb{T}_{1,1}^{(b)}(E')}{2}$$

$$\boxed{\text{z95}} \quad \mathbb{Q}_{2,1}^{(c)}(E',a) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E')\mathbb{Q}_0^{(b)}(A_1')}{2}$$

$$\boxed{\text{z96}} \quad \mathbb{Q}_{2,2}^{(c)}(E',a) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E')\mathbb{Q}_0^{(b)}(A_1')}{2}$$

$$\boxed{\text{z97}} \quad \mathbb{Q}_{2,1}^{(c)}(E',b) = \frac{\sqrt{2}\mathbb{M}_{3,2}^{(a)}(E')\mathbb{M}_1^{(b)}(A_2')}{2}$$

$$\boxed{\text{z98}} \quad \mathbb{Q}_{2,2}^{(c)}(E',b) = -\frac{\sqrt{2}\mathbb{M}_{3,1}^{(a)}(E')\mathbb{M}_1^{(b)}(A_2')}{2}$$

$$\boxed{\text{z99}} \quad \mathbb{Q}_{3,1}^{(c)}(E',a) = \frac{\sqrt{7}\mathbb{Q}_{2,1}^{(a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{14} + \frac{\sqrt{7}\mathbb{Q}_{2,2}^{(a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{14} + \frac{\sqrt{21}\mathbb{Q}_2^{(a)}(A_1')\mathbb{Q}_{1,1}^{(b)}(E')}{7}$$

$\boxed{\text{z100}}$ $\quad \mathbb{Q}_{3,2}^{(c)}(E',a) = \dfrac{\sqrt{7}\mathbb{Q}_{2,1}^{(a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{14} - \dfrac{\sqrt{7}\mathbb{Q}_{2,2}^{(a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{14} + \dfrac{\sqrt{21}\mathbb{Q}_{2}^{(a)}(A_1')\mathbb{Q}_{1,2}^{(b)}(E')}{7}$

$\boxed{\text{z101}}$ $\quad \mathbb{Q}_{3,1}^{(c)}(E',b) = \dfrac{\sqrt{35}\mathbb{Q}_{4,1}^{(a)}(E',2)\mathbb{Q}_{1,2}^{(b)}(E')}{14} + \dfrac{\sqrt{35}\mathbb{Q}_{4,2}^{(a)}(E',2)\mathbb{Q}_{1,1}^{(b)}(E')}{14} - \dfrac{\sqrt{7}\mathbb{Q}_{4}^{(a)}(A_1')\mathbb{Q}_{1,1}^{(b)}(E')}{7}$

$\boxed{\text{z102}}$ $\quad \mathbb{Q}_{3,2}^{(c)}(E',b) = \dfrac{\sqrt{35}\mathbb{Q}_{4,1}^{(a)}(E',2)\mathbb{Q}_{1,1}^{(b)}(E')}{14} - \dfrac{\sqrt{35}\mathbb{Q}_{4,2}^{(a)}(E',2)\mathbb{Q}_{1,2}^{(b)}(E')}{14} - \dfrac{\sqrt{7}\mathbb{Q}_{4}^{(a)}(A_1')\mathbb{Q}_{1,2}^{(b)}(E')}{7}$

$\boxed{\text{z103}}$ $\quad \mathbb{Q}_{3,1}^{(c)}(E',c) = -\dfrac{\sqrt{55}\mathbb{M}_{3,1}^{(a)}(E')\mathbb{T}_{1,2}^{(b)}(E')}{22} - \dfrac{\sqrt{55}\mathbb{M}_{3,2}^{(a)}(E')\mathbb{T}_{1,1}^{(b)}(E')}{22} - \dfrac{\sqrt{33}\mathbb{M}_{3}^{(a)}(A_2')\mathbb{T}_{1,2}^{(b)}(E')}{11}$

$\boxed{\text{z104}}$ $\quad \mathbb{Q}_{3,2}^{(c)}(E',c) = -\dfrac{\sqrt{55}\mathbb{M}_{3,1}^{(a)}(E')\mathbb{T}_{1,1}^{(b)}(E')}{22} + \dfrac{\sqrt{55}\mathbb{M}_{3,2}^{(a)}(E')\mathbb{T}_{1,2}^{(b)}(E')}{22} + \dfrac{\sqrt{33}\mathbb{M}_{3}^{(a)}(A_2')\mathbb{T}_{1,1}^{(b)}(E')}{11}$

$\boxed{\text{z105}}$ $\quad \mathbb{Q}_{4,1}^{(c)}(E',1) = \dfrac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E',1)\mathbb{Q}_{0}^{(b)}(A_1')}{2}$

$\boxed{\text{z106}}$ $\quad \mathbb{Q}_{4,2}^{(c)}(E',1) = \dfrac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E',1)\mathbb{Q}_{0}^{(b)}(A_1')}{2}$

$\boxed{\text{z107}}$ $\quad \mathbb{Q}_{4,1}^{(c)}(E',2) = \dfrac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E',2)\mathbb{Q}_{0}^{(b)}(A_1')}{2}$

$\boxed{\text{z108}}$ $\quad \mathbb{Q}_{4,2}^{(c)}(E',2) = \dfrac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E',2)\mathbb{Q}_{0}^{(b)}(A_1')}{2}$

$\boxed{\text{z109}}$ $\quad \mathbb{Q}_{5,1}^{(c)}(E',1) = \dfrac{\mathbb{Q}_{4,1}^{(a)}(E',1)\mathbb{Q}_{1,2}^{(b)}(E')}{2} + \dfrac{\mathbb{Q}_{4,2}^{(a)}(E',1)\mathbb{Q}_{1,1}^{(b)}(E')}{2}$

$\boxed{\text{z110}}$ $\quad \mathbb{Q}_{5,2}^{(c)}(E',1) = \dfrac{\mathbb{Q}_{4,1}^{(a)}(E',1)\mathbb{Q}_{1,1}^{(b)}(E')}{2} - \dfrac{\mathbb{Q}_{4,2}^{(a)}(E',1)\mathbb{Q}_{1,2}^{(b)}(E')}{2}$

$\boxed{\text{z111}}$ $\quad \mathbb{Q}_{5,1}^{(c)}(E',2) = \dfrac{\sqrt{14}\mathbb{Q}_{4,1}^{(a)}(E',2)\mathbb{Q}_{1,2}^{(b)}(E')}{14} + \dfrac{\sqrt{14}\mathbb{Q}_{4,2}^{(a)}(E',2)\mathbb{Q}_{1,1}^{(b)}(E')}{14} + \dfrac{\sqrt{70}\mathbb{Q}_{4}^{(a)}(A_1')\mathbb{Q}_{1,1}^{(b)}(E')}{14}$

$\boxed{\text{z112}}$ $\quad \mathbb{Q}_{5,2}^{(c)}(E',2) = \dfrac{\sqrt{14}\mathbb{Q}_{4,1}^{(a)}(E',2)\mathbb{Q}_{1,1}^{(b)}(E')}{14} - \dfrac{\sqrt{14}\mathbb{Q}_{4,2}^{(a)}(E',2)\mathbb{Q}_{1,2}^{(b)}(E')}{14} + \dfrac{\sqrt{70}\mathbb{Q}_{4}^{(a)}(A_1')\mathbb{Q}_{1,2}^{(b)}(E')}{14}$

$\boxed{\text{z113}}$ $\quad \mathbb{Q}_{2,1}^{(c)}(E'',a) = \dfrac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E'')\mathbb{Q}_{0}^{(b)}(A_1')}{2}$

$\boxed{\text{z114}}$ $\quad \mathbb{Q}_{2,2}^{(c)}(E'',a) = \dfrac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E'')\mathbb{Q}_0^{(b)}(A_1')}{2}$

$\boxed{\text{z115}}$ $\quad \mathbb{Q}_{2,1}^{(c)}(E'',b) = \dfrac{\sqrt{2}\mathbb{M}_{3,2}^{(a)}(E'')\mathbb{M}_1^{(b)}(A_2')}{2}$

$\boxed{\text{z116}}$ $\quad \mathbb{Q}_{2,2}^{(c)}(E'',b) = -\dfrac{\sqrt{2}\mathbb{M}_{3,1}^{(a)}(E'')\mathbb{M}_1^{(b)}(A_2')}{2}$

$\boxed{\text{z117}}$ $\quad \mathbb{Q}_{2,1}^{(c)}(E'',c) = \dfrac{\sqrt{2}\mathbb{M}_{1,2}^{(a)}(E'')\mathbb{M}_1^{(b)}(A_2')}{2}$

$\boxed{\text{z118}}$ $\quad \mathbb{Q}_{2,2}^{(c)}(E'',c) = -\dfrac{\sqrt{2}\mathbb{M}_{1,1}^{(a)}(E'')\mathbb{M}_1^{(b)}(A_2')}{2}$

$\boxed{\text{z175}}$ $\quad \mathbb{Q}_{3,1}^{(c)}(E'',a) = \dfrac{\mathbb{Q}_{2,1}^{(a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{2} + \dfrac{\mathbb{Q}_{2,2}^{(a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{2}$

$\boxed{\text{z176}}$ $\quad \mathbb{Q}_{3,2}^{(c)}(E'',a) = \dfrac{\mathbb{Q}_{2,1}^{(a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{2} - \dfrac{\mathbb{Q}_{2,2}^{(a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{2}$

$\boxed{\text{z177}}$ $\quad \mathbb{Q}_{3,1}^{(c)}(E'',b) = -\dfrac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{8} - \dfrac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{8} - \dfrac{\sqrt{14}\mathbb{Q}_4^{(a)}(A_1'')\mathbb{Q}_{1,1}^{(b)}(E')}{8} - \dfrac{\sqrt{14}\mathbb{Q}_4^{(a)}(A_2'')\mathbb{Q}_{1,2}^{(b)}(E')}{8}$

$\boxed{\text{z178}}$ $\quad \mathbb{Q}_{3,2}^{(c)}(E'',b) = -\dfrac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{8} + \dfrac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{8} - \dfrac{\sqrt{14}\mathbb{Q}_4^{(a)}(A_1'')\mathbb{Q}_{1,2}^{(b)}(E')}{8} + \dfrac{\sqrt{14}\mathbb{Q}_4^{(a)}(A_2'')\mathbb{Q}_{1,1}^{(b)}(E')}{8}$

$\boxed{\text{z179}}$ $\quad \mathbb{Q}_{3,1}^{(c)}(E'',c) = \dfrac{\sqrt{10}\mathbb{M}_{3,1}^{(a)}(E'')\mathbb{T}_{1,2}^{(b)}(E')}{8} + \dfrac{\sqrt{10}\mathbb{M}_{3,2}^{(a)}(E'')\mathbb{T}_{1,1}^{(b)}(E')}{8} + \dfrac{\sqrt{6}\mathbb{M}_3^{(a)}(A_1'')\mathbb{T}_{1,1}^{(b)}(E')}{8} - \dfrac{\sqrt{6}\mathbb{M}_3^{(a)}(A_2'')\mathbb{T}_{1,2}^{(b)}(E')}{8}$

$\boxed{\text{z180}}$ $\quad \mathbb{Q}_{3,2}^{(c)}(E'',c) = \dfrac{\sqrt{10}\mathbb{M}_{3,1}^{(a)}(E'')\mathbb{T}_{1,1}^{(b)}(E')}{8} - \dfrac{\sqrt{10}\mathbb{M}_{3,2}^{(a)}(E'')\mathbb{T}_{1,2}^{(b)}(E')}{8} + \dfrac{\sqrt{6}\mathbb{M}_3^{(a)}(A_1'')\mathbb{T}_{1,2}^{(b)}(E')}{8} + \dfrac{\sqrt{6}\mathbb{M}_3^{(a)}(A_2'')\mathbb{T}_{1,1}^{(b)}(E')}{8}$

$\boxed{\text{z181}}$ $\quad \mathbb{Q}_{4,1}^{(c)}(E'') = \dfrac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E'')\mathbb{Q}_0^{(b)}(A_1')}{2}$

$\boxed{\text{z182}}$ $\quad \mathbb{Q}_{4,2}^{(c)}(E'') = \dfrac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E'')\mathbb{Q}_0^{(b)}(A_1')}{2}$

$\boxed{\text{z183}}$ $\quad \mathbb{Q}_{5,1}^{(c)}(E'',1) = -\dfrac{\mathbb{Q}_4^{(a)}(A_1'')\mathbb{Q}_{1,1}^{(b)}(E')}{2} + \dfrac{\mathbb{Q}_4^{(a)}(A_2'')\mathbb{Q}_{1,2}^{(b)}(E')}{2}$

12

$\boxed{\text{z184}}$ $\quad \mathbb{Q}_{5,2}^{(c)}(E'',1) = -\dfrac{\mathbb{Q}_4^{(a)}(A_1'')\mathbb{Q}_{1,2}^{(b)}(E')}{2} - \dfrac{\mathbb{Q}_4^{(a)}(A_2'')\mathbb{Q}_{1,1}^{(b)}(E')}{2}$

$\boxed{\text{z185}}$ $\quad \mathbb{Q}_{5,1}^{(c)}(E'',2) = \dfrac{\sqrt{14}\mathbb{Q}_{4,1}^{(a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{8} + \dfrac{\sqrt{14}\mathbb{Q}_{4,2}^{(a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{8} - \dfrac{\sqrt{2}\mathbb{Q}_4^{(a)}(A_1'')\mathbb{Q}_{1,1}^{(b)}(E')}{8} - \dfrac{\sqrt{2}\mathbb{Q}_4^{(a)}(A_2'')\mathbb{Q}_{1,2}^{(b)}(E')}{8}$

$\boxed{\text{z186}}$ $\quad \mathbb{Q}_{5,2}^{(c)}(E'',2) = \dfrac{\sqrt{14}\mathbb{Q}_{4,1}^{(a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{8} - \dfrac{\sqrt{14}\mathbb{Q}_{4,2}^{(a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{8} - \dfrac{\sqrt{2}\mathbb{Q}_4^{(a)}(A_1'')\mathbb{Q}_{1,2}^{(b)}(E')}{8} + \dfrac{\sqrt{2}\mathbb{Q}_4^{(a)}(A_2'')\mathbb{Q}_{1,1}^{(b)}(E')}{8}$

$\boxed{\text{z187}}$ $\quad \mathbb{G}_0^{(c)}(A_1'') = \dfrac{\sqrt{2}\mathbb{M}_{1,1}^{(a)}(E'')\mathbb{T}_{1,1}^{(b)}(E')}{2} + \dfrac{\sqrt{2}\mathbb{M}_{1,2}^{(a)}(E'')\mathbb{T}_{1,2}^{(b)}(E')}{2}$

$\boxed{\text{z188}}$ $\quad \mathbb{G}_2^{(c)}(A_1'',a) = -\dfrac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{2} - \dfrac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{2}$

$\boxed{\text{z189}}$ $\quad \mathbb{G}_2^{(c)}(A_1'',b) = \dfrac{\sqrt{2}\mathbb{M}_{3,1}^{(a)}(E'')\mathbb{T}_{1,1}^{(b)}(E')}{2} + \dfrac{\sqrt{2}\mathbb{M}_{3,2}^{(a)}(E'')\mathbb{T}_{1,2}^{(b)}(E')}{2}$

$\boxed{\text{z190}}$ $\quad \mathbb{G}_4^{(c)}(A_1'') = -\dfrac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{2} - \dfrac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{2}$

$\boxed{\text{z191}}$ $\quad \mathbb{G}_{2,1}^{(c)}(E') = \dfrac{\sqrt{66}\mathbb{M}_{3,1}^{(a)}(E')\mathbb{T}_{1,2}^{(b)}(E')}{22} + \dfrac{\sqrt{66}\mathbb{M}_{3,2}^{(a)}(E')\mathbb{T}_{1,1}^{(b)}(E')}{22} - \dfrac{\sqrt{110}\mathbb{M}_3^{(a)}(A_2')\mathbb{T}_{1,2}^{(b)}(E')}{22}$

$\boxed{\text{z192}}$ $\quad \mathbb{G}_{2,2}^{(c)}(E') = \dfrac{\sqrt{66}\mathbb{M}_{3,1}^{(a)}(E')\mathbb{T}_{1,1}^{(b)}(E')}{22} - \dfrac{\sqrt{66}\mathbb{M}_{3,2}^{(a)}(E')\mathbb{T}_{1,2}^{(b)}(E')}{22} + \dfrac{\sqrt{110}\mathbb{M}_3^{(a)}(A_2')\mathbb{T}_{1,1}^{(b)}(E')}{22}$

$\boxed{\text{z193}}$ $\quad \mathbb{G}_{2,1}^{(c)}(E'',a) = -\dfrac{\sqrt{6}\mathbb{M}_{3,1}^{(a)}(E'')\mathbb{T}_{1,2}^{(b)}(E')}{8} - \dfrac{\sqrt{6}\mathbb{M}_{3,2}^{(a)}(E'')\mathbb{T}_{1,1}^{(b)}(E')}{8} + \dfrac{\sqrt{10}\mathbb{M}_3^{(a)}(A_1'')\mathbb{T}_{1,1}^{(b)}(E')}{8} - \dfrac{\sqrt{10}\mathbb{M}_3^{(a)}(A_2'')\mathbb{T}_{1,2}^{(b)}(E')}{8}$

$\boxed{\text{z194}}$ $\quad \mathbb{G}_{2,2}^{(c)}(E'',a) = -\dfrac{\sqrt{6}\mathbb{M}_{3,1}^{(a)}(E'')\mathbb{T}_{1,1}^{(b)}(E')}{8} + \dfrac{\sqrt{6}\mathbb{M}_{3,2}^{(a)}(E'')\mathbb{T}_{1,2}^{(b)}(E')}{8} + \dfrac{\sqrt{10}\mathbb{M}_3^{(a)}(A_1'')\mathbb{T}_{1,2}^{(b)}(E')}{8} + \dfrac{\sqrt{10}\mathbb{M}_3^{(a)}(A_2'')\mathbb{T}_{1,1}^{(b)}(E')}{8}$

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

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

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

13

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

- 'Mo'-'S' bond-cluster
  * bra: $\langle d_u|$, $\langle d_{xz}|$, $\langle d_{yz}|$, $\langle d_{xy}|$, $\langle d_v|$
  * ket: $|p_x\rangle$, $|p_y\rangle$, $|p_z\rangle$
  * wyckoff: `6a@6n`

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

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

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

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

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

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

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

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

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

$\boxed{\text{z34}}$ $\mathbb{Q}_3^{(c)}(A_2',a) = \mathbb{Q}_3^{(a)}(A_2')\mathbb{Q}_0^{(b)}(A_1')$

$\boxed{\text{z35}}$ $\mathbb{Q}_3^{(c)}(A_2',b) = \dfrac{\sqrt{2}\mathbb{Q}_{3,1}^{(a)}(E'')\mathbb{Q}_{2,2}^{(b)}(E'')}{2} - \dfrac{\sqrt{2}\mathbb{Q}_{3,2}^{(a)}(E'')\mathbb{Q}_{2,1}^{(b)}(E'')}{2}$

$$\boxed{\text{z36}} \quad \mathbb{Q}_3^{(c)}(A_2', c) = -\frac{\sqrt{2}\mathbb{G}_{2,1}^{(a)}(E'')\mathbb{Q}_{2,2}^{(b)}(E'')}{2} + \frac{\sqrt{2}\mathbb{G}_{2,2}^{(a)}(E'')\mathbb{Q}_{2,1}^{(b)}(E'')}{2}$$

$$\boxed{\text{z37}} \quad \mathbb{Q}_1^{(c)}(A_2'', a) = -\frac{\sqrt{2}\mathbb{Q}_{3,1}^{(a)}(E')\mathbb{Q}_{2,2}^{(b)}(E'')}{2} + \frac{\sqrt{2}\mathbb{Q}_{3,2}^{(a)}(E')\mathbb{Q}_{2,1}^{(b)}(E'')}{2}$$

$$\boxed{\text{z38}} \quad \mathbb{Q}_1^{(c)}(A_2'', b) = \mathbb{Q}_1^{(a)}(A_2'')\mathbb{Q}_0^{(b)}(A_1')$$

$$\boxed{\text{z39}} \quad \mathbb{Q}_1^{(c)}(A_2'', c) = -\frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E')\mathbb{Q}_{2,2}^{(b)}(E'')}{2} + \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E')\mathbb{Q}_{2,1}^{(b)}(E'')}{2}$$

$$\boxed{\text{z50}} \quad \mathbb{Q}_1^{(c)}(A_2'', d) = \frac{\sqrt{2}\mathbb{G}_{2,1}^{(a)}(E')\mathbb{Q}_{2,2}^{(b)}(E'')}{2} - \frac{\sqrt{2}\mathbb{G}_{2,2}^{(a)}(E')\mathbb{Q}_{2,1}^{(b)}(E'')}{2}$$

$$\boxed{\text{z51}} \quad \mathbb{Q}_3^{(c)}(A_2'') = \mathbb{Q}_3^{(a)}(A_2'')\mathbb{Q}_0^{(b)}(A_1')$$

$$\boxed{\text{z52}} \quad \mathbb{Q}_4^{(c)}(A_2'') = -\frac{\sqrt{6}\mathbb{Q}_{3,1}^{(a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{4} + \frac{\sqrt{6}\mathbb{Q}_{3,2}^{(a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{4} + \frac{\mathbb{Q}_3^{(a)}(A_1')\mathbb{Q}_1^{(b)}(A_2'')}{2}$$

$$\boxed{\text{z53}} \quad \mathbb{Q}_{1,1}^{(c)}(E', a) = \frac{\sqrt{130}\mathbb{Q}_{3,1}^{(a)}(E'')\mathbb{Q}_{2,2}^{(b)}(E'')}{26} + \frac{\sqrt{130}\mathbb{Q}_{3,2}^{(a)}(E'')\mathbb{Q}_{2,1}^{(b)}(E'')}{26} + \frac{\sqrt{78}\mathbb{Q}_3^{(a)}(A_2'')\mathbb{Q}_{2,2}^{(b)}(E'')}{26}$$

$$\boxed{\text{z54}} \quad \mathbb{Q}_{1,2}^{(c)}(E', a) = \frac{\sqrt{130}\mathbb{Q}_{3,1}^{(a)}(E'')\mathbb{Q}_{2,1}^{(b)}(E'')}{26} - \frac{\sqrt{130}\mathbb{Q}_{3,2}^{(a)}(E'')\mathbb{Q}_{2,2}^{(b)}(E'')}{26} - \frac{\sqrt{78}\mathbb{Q}_3^{(a)}(A_2'')\mathbb{Q}_{2,1}^{(b)}(E'')}{26}$$

$$\boxed{\text{z55}} \quad \mathbb{Q}_{1,1}^{(c)}(E', b) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E')\mathbb{Q}_0^{(b)}(A_1')}{2}$$

$$\boxed{\text{z56}} \quad \mathbb{Q}_{1,2}^{(c)}(E', b) = \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E')\mathbb{Q}_0^{(b)}(A_1')}{2}$$

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

$$\boxed{\text{z70}} \quad \mathbb{Q}_{1,2}^{(c)}(E', c) = \frac{\sqrt{2}\mathbb{Q}_1^{(a)}(A_2'')\mathbb{Q}_{2,1}^{(b)}(E'')}{2}$$

$$\boxed{\text{z71}} \quad \mathbb{Q}_{1,1}^{(c)}(E', d) = -\frac{\sqrt{10}\mathbb{G}_{2,1}^{(a)}(E'')\mathbb{Q}_{2,2}^{(b)}(E'')}{10} - \frac{\sqrt{10}\mathbb{G}_{2,2}^{(a)}(E'')\mathbb{Q}_{2,1}^{(b)}(E'')}{10} - \frac{\sqrt{30}\mathbb{G}_2^{(a)}(A_1'')\mathbb{Q}_{2,1}^{(b)}(E'')}{10}$$

$$\boxed{\text{z72}} \quad \mathbb{Q}_{1,2}^{(c)}(E',d) = -\frac{\sqrt{10}\,\mathbb{G}_{2,1}^{(a)}(E'')\mathbb{Q}_{2,1}^{(b)}(E'')}{10} + \frac{\sqrt{10}\,\mathbb{G}_{2,2}^{(a)}(E'')\mathbb{Q}_{2,2}^{(b)}(E'')}{10} - \frac{\sqrt{30}\,\mathbb{G}_2^{(a)}(A_1'')\mathbb{Q}_{2,2}^{(b)}(E'')}{10}$$

$$\boxed{\text{z73}} \quad \mathbb{Q}_{2,1}^{(c)}(E',a) = -\frac{\sqrt{21}\,\mathbb{Q}_{3,1}^{(a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{42} + \frac{\sqrt{210}\,\mathbb{Q}_{3,2}^{(a)}(E'')\mathbb{Q}_1^{(b)}(A_2'')}{42} - \frac{\sqrt{21}\,\mathbb{Q}_{3,2}^{(a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{42} + \frac{\sqrt{35}\,\mathbb{Q}_3^{(a)}(A_1')\mathbb{Q}_{1,1}^{(b)}(E')}{14} - \frac{\sqrt{35}\,\mathbb{Q}_3^{(a)}(A_2')\mathbb{Q}_{1,2}^{(b)}(E')}{14}$$

$$\boxed{\text{z74}} \quad \mathbb{Q}_{2,2}^{(c)}(E',a) = -\frac{\sqrt{210}\,\mathbb{Q}_{3,1}^{(a)}(E'')\mathbb{Q}_1^{(b)}(A_2'')}{42} - \frac{\sqrt{21}\,\mathbb{Q}_{3,1}^{(a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{42} + \frac{\sqrt{21}\,\mathbb{Q}_{3,2}^{(a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{42} + \frac{\sqrt{35}\,\mathbb{Q}_3^{(a)}(A_1')\mathbb{Q}_{1,2}^{(b)}(E')}{14} + \frac{\sqrt{35}\,\mathbb{Q}_3^{(a)}(A_2')\mathbb{Q}_{1,1}^{(b)}(E')}{14}$$

$$\boxed{\text{z75}} \quad \mathbb{Q}_{2,1}^{(c)}(E',b) = \frac{\mathbb{Q}_{1,1}^{(a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{2} + \frac{\mathbb{Q}_{1,2}^{(a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{2}$$

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

$$\boxed{\text{z119}} \quad \mathbb{Q}_{2,1}^{(c)}(E',c) = -\frac{\sqrt{3}\,\mathbb{G}_{2,1}^{(a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{6} - \frac{\sqrt{3}\,\mathbb{G}_{2,2}^{(a)}(E'')\mathbb{Q}_1^{(b)}(A_2'')}{3} - \frac{\sqrt{3}\,\mathbb{G}_{2,2}^{(a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{6}$$

$$\boxed{\text{z120}} \quad \mathbb{Q}_{2,2}^{(c)}(E',c) = \frac{\sqrt{3}\,\mathbb{G}_{2,1}^{(a)}(E'')\mathbb{Q}_1^{(b)}(A_2'')}{3} - \frac{\sqrt{3}\,\mathbb{G}_{2,1}^{(a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{6} + \frac{\sqrt{3}\,\mathbb{G}_{2,2}^{(a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{6}$$

$$\boxed{\text{z121}} \quad \mathbb{Q}_{3,1}^{(c)}(E',a) = \frac{\sqrt{2}\,\mathbb{Q}_{3,1}^{(a)}(E')\mathbb{Q}_0^{(b)}(A_1')}{2}$$

$$\boxed{\text{z122}} \quad \mathbb{Q}_{3,2}^{(c)}(E',a) = \frac{\sqrt{2}\,\mathbb{Q}_{3,2}^{(a)}(E')\mathbb{Q}_0^{(b)}(A_1')}{2}$$

$$\boxed{\text{z123}} \quad \mathbb{Q}_{3,1}^{(c)}(E',b) = \frac{\sqrt{39}\,\mathbb{Q}_{3,1}^{(a)}(E'')\mathbb{Q}_{2,2}^{(b)}(E'')}{26} + \frac{\sqrt{39}\,\mathbb{Q}_{3,2}^{(a)}(E'')\mathbb{Q}_{2,1}^{(b)}(E'')}{26} - \frac{\sqrt{65}\,\mathbb{Q}_3^{(a)}(A_2'')\mathbb{Q}_{2,2}^{(b)}(E'')}{13}$$

$$\boxed{\text{z124}} \quad \mathbb{Q}_{3,2}^{(c)}(E',b) = \frac{\sqrt{39}\,\mathbb{Q}_{3,1}^{(a)}(E'')\mathbb{Q}_{2,1}^{(b)}(E'')}{26} - \frac{\sqrt{39}\,\mathbb{Q}_{3,2}^{(a)}(E'')\mathbb{Q}_{2,2}^{(b)}(E'')}{26} + \frac{\sqrt{65}\,\mathbb{Q}_3^{(a)}(A_2'')\mathbb{Q}_{2,1}^{(b)}(E'')}{13}$$

$$\boxed{\text{z125}} \quad \mathbb{Q}_{3,1}^{(c)}(E',c) = \frac{\sqrt{15}\,\mathbb{G}_{2,1}^{(a)}(E'')\mathbb{Q}_{2,2}^{(b)}(E'')}{10} + \frac{\sqrt{15}\,\mathbb{G}_{2,2}^{(a)}(E'')\mathbb{Q}_{2,1}^{(b)}(E'')}{10} - \frac{\sqrt{5}\,\mathbb{G}_2^{(a)}(A_1'')\mathbb{Q}_{2,1}^{(b)}(E'')}{5}$$

$$\boxed{\text{z126}} \quad \mathbb{Q}_{3,2}^{(c)}(E',c) = \frac{\sqrt{15}\,\mathbb{G}_{2,1}^{(a)}(E'')\mathbb{Q}_{2,1}^{(b)}(E'')}{10} - \frac{\sqrt{15}\,\mathbb{G}_{2,2}^{(a)}(E'')\mathbb{Q}_{2,2}^{(b)}(E'')}{10} - \frac{\sqrt{5}\,\mathbb{G}_2^{(a)}(A_1'')\mathbb{Q}_{2,2}^{(b)}(E'')}{5}$$

$$\boxed{\text{z127}} \quad \mathbb{Q}_{4,1}^{(c)}(E',1) = -\frac{\mathbb{Q}_3^{(a)}(A_1')\mathbb{Q}_{1,1}^{(b)}(E')}{2} - \frac{\mathbb{Q}_3^{(a)}(A_2')\mathbb{Q}_{1,2}^{(b)}(E')}{2}$$

16

$\boxed{\text{z128}}$ $\quad \mathbb{Q}_{4,2}^{(c)}(E',1) = -\dfrac{\mathbb{Q}_3^{(a)}(A_1')\mathbb{Q}_{1,2}^{(b)}(E')}{2} + \dfrac{\mathbb{Q}_3^{(a)}(A_2')\mathbb{Q}_{1,1}^{(b)}(E')}{2}$

$\boxed{\text{z129}}$ $\quad \mathbb{Q}_{4,1}^{(c)}(E',2) = \dfrac{\sqrt{105}\mathbb{Q}_{3,1}^{(a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{28} + \dfrac{\sqrt{42}\mathbb{Q}_{3,2}^{(a)}(E'')\mathbb{Q}_1^{(b)}(A_2'')}{14} + \dfrac{\sqrt{105}\mathbb{Q}_{3,2}^{(a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{28} - \dfrac{\sqrt{7}\mathbb{Q}_3^{(a)}(A_1')\mathbb{Q}_{1,1}^{(b)}(E')}{28} + \dfrac{\sqrt{7}\mathbb{Q}_3^{(a)}(A_2')\mathbb{Q}_{1,2}^{(b)}(E')}{28}$

$\boxed{\text{z130}}$ $\quad \mathbb{Q}_{4,2}^{(c)}(E',2) = -\dfrac{\sqrt{42}\mathbb{Q}_{3,1}^{(a)}(E'')\mathbb{Q}_1^{(b)}(A_2'')}{14} + \dfrac{\sqrt{105}\mathbb{Q}_{3,1}^{(a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{28} - \dfrac{\sqrt{105}\mathbb{Q}_{3,2}^{(a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{28} - \dfrac{\sqrt{7}\mathbb{Q}_3^{(a)}(A_1')\mathbb{Q}_{1,2}^{(b)}(E')}{28} - \dfrac{\sqrt{7}\mathbb{Q}_3^{(a)}(A_2')\mathbb{Q}_{1,1}^{(b)}(E')}{28}$

$\boxed{\text{z131}}$ $\quad \mathbb{Q}_{2,1}^{(c)}(E'',a) = \dfrac{\sqrt{210}\mathbb{Q}_{3,1}^{(a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{42} + \dfrac{\sqrt{210}\mathbb{Q}_{3,2}^{(a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{42} + \dfrac{2\sqrt{21}\mathbb{Q}_{3,2}^{(a)}(E')\mathbb{Q}_1^{(b)}(A_2'')}{21} - \dfrac{\sqrt{14}\mathbb{Q}_3^{(a)}(A_2')\mathbb{Q}_{1,2}^{(b)}(E')}{14}$

$\boxed{\text{z132}}$ $\quad \mathbb{Q}_{2,2}^{(c)}(E'',a) = \dfrac{\sqrt{210}\mathbb{Q}_{3,1}^{(a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{42} - \dfrac{2\sqrt{21}\mathbb{Q}_{3,1}^{(a)}(E')\mathbb{Q}_1^{(b)}(A_2'')}{21} - \dfrac{\sqrt{210}\mathbb{Q}_{3,2}^{(a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{42} + \dfrac{\sqrt{14}\mathbb{Q}_3^{(a)}(A_2')\mathbb{Q}_{1,1}^{(b)}(E')}{14}$

$\boxed{\text{z133}}$ $\quad \mathbb{Q}_{2,1}^{(c)}(E'',b) = \dfrac{\mathbb{Q}_{1,2}^{(a)}(E')\mathbb{Q}_1^{(b)}(A_2'')}{2} + \dfrac{\mathbb{Q}_1^{(a)}(A_2'')\mathbb{Q}_{1,2}^{(b)}(E')}{2}$

$\boxed{\text{z134}}$ $\quad \mathbb{Q}_{2,2}^{(c)}(E'',b) = -\dfrac{\mathbb{Q}_{1,1}^{(a)}(E')\mathbb{Q}_1^{(b)}(A_2'')}{2} - \dfrac{\mathbb{Q}_1^{(a)}(A_2'')\mathbb{Q}_{1,1}^{(b)}(E')}{2}$

$\boxed{\text{z135}}$ $\quad \mathbb{Q}_{2,1}^{(c)}(E'',c) = \dfrac{\sqrt{3}\mathbb{G}_{2,1}^{(a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{6} + \dfrac{\sqrt{3}\mathbb{G}_{2,2}^{(a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{6} + \dfrac{\sqrt{3}\mathbb{G}_{2,2}^{(a)}(E')\mathbb{Q}_1^{(b)}(A_2'')}{6} + \dfrac{\mathbb{G}_2^{(a)}(A_1'')\mathbb{Q}_{1,1}^{(b)}(E')}{2}$

$\boxed{\text{z136}}$ $\quad \mathbb{Q}_{2,2}^{(c)}(E'',c) = \dfrac{\sqrt{3}\mathbb{G}_{2,1}^{(a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{6} - \dfrac{\sqrt{3}\mathbb{G}_{2,1}^{(a)}(E')\mathbb{Q}_1^{(b)}(A_2'')}{6} - \dfrac{\sqrt{3}\mathbb{G}_{2,2}^{(a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{6} + \dfrac{\mathbb{G}_2^{(a)}(A_1'')\mathbb{Q}_{1,2}^{(b)}(E')}{2}$

$\boxed{\text{z137}}$ $\quad \mathbb{Q}_{3,1}^{(c)}(E'',a) = \dfrac{\sqrt{2}\mathbb{Q}_{3,1}^{(a)}(E'')\mathbb{Q}_0^{(b)}(A_1')}{2}$

$\boxed{\text{z138}}$ $\quad \mathbb{Q}_{3,2}^{(c)}(E'',a) = \dfrac{\sqrt{2}\mathbb{Q}_{3,2}^{(a)}(E'')\mathbb{Q}_0^{(b)}(A_1')}{2}$

$\boxed{\text{z139}}$ $\quad \mathbb{Q}_{3,1}^{(c)}(E'',b) = \dfrac{\sqrt{6}\mathbb{Q}_{3,1}^{(a)}(E')\mathbb{Q}_{2,2}^{(b)}(E'')}{8} + \dfrac{\sqrt{6}\mathbb{Q}_{3,2}^{(a)}(E')\mathbb{Q}_{2,1}^{(b)}(E'')}{8} - \dfrac{\sqrt{10}\mathbb{Q}_3^{(a)}(A_1')\mathbb{Q}_{2,1}^{(b)}(E'')}{8} + \dfrac{\sqrt{10}\mathbb{Q}_3^{(a)}(A_2')\mathbb{Q}_{2,2}^{(b)}(E'')}{8}$

$\boxed{\text{z140}}$ $\quad \mathbb{Q}_{3,2}^{(c)}(E'',b) = \dfrac{\sqrt{6}\mathbb{Q}_{3,1}^{(a)}(E')\mathbb{Q}_{2,1}^{(b)}(E'')}{8} - \dfrac{\sqrt{6}\mathbb{Q}_{3,2}^{(a)}(E')\mathbb{Q}_{2,2}^{(b)}(E'')}{8} - \dfrac{\sqrt{10}\mathbb{Q}_3^{(a)}(A_1')\mathbb{Q}_{2,2}^{(b)}(E'')}{8} - \dfrac{\sqrt{10}\mathbb{Q}_3^{(a)}(A_2')\mathbb{Q}_{2,1}^{(b)}(E'')}{8}$

$\boxed{\text{z141}}$ $\quad \mathbb{Q}_{3,1}^{(c)}(E'',c) = \dfrac{\mathbb{Q}_{1,1}^{(a)}(E')\mathbb{Q}_{2,2}^{(b)}(E'')}{2} + \dfrac{\mathbb{Q}_{1,2}^{(a)}(E')\mathbb{Q}_{2,1}^{(b)}(E'')}{2}$

$$\boxed{\text{z142}} \quad \mathbb{Q}_{3,2}^{(c)}(E'',c) = \frac{\mathbb{Q}_{1,1}^{(a)}(E')\mathbb{Q}_{2,1}^{(b)}(E'')}{2} - \frac{\mathbb{Q}_{1,2}^{(a)}(E')\mathbb{Q}_{2,2}^{(b)}(E'')}{2}$$

$$\boxed{\text{z143}} \quad \mathbb{Q}_{4,1}^{(c)}(E'') = -\frac{\sqrt{21}\mathbb{Q}_{3,1}^{(a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{28} - \frac{\sqrt{21}\mathbb{Q}_{3,2}^{(a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{28} + \frac{\sqrt{210}\mathbb{Q}_{3,2}^{(a)}(E')\mathbb{Q}_1^{(b)}(A_2'')}{28} + \frac{\sqrt{35}\mathbb{Q}_3^{(a)}(A_2'')\mathbb{Q}_{1,2}^{(b)}(E')}{14}$$

$$\boxed{\text{z144}} \quad \mathbb{Q}_{4,2}^{(c)}(E'') = -\frac{\sqrt{21}\mathbb{Q}_{3,1}^{(a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{28} - \frac{\sqrt{210}\mathbb{Q}_{3,1}^{(a)}(E')\mathbb{Q}_1^{(b)}(A_2'')}{28} + \frac{\sqrt{21}\mathbb{Q}_{3,2}^{(a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{28} - \frac{\sqrt{35}\mathbb{Q}_3^{(a)}(A_2'')\mathbb{Q}_{1,1}^{(b)}(E')}{14}$$

$$\boxed{\text{z145}} \quad \mathbb{Q}_{5,1}^{(c)}(E'',1) = \frac{\mathbb{Q}_3^{(a)}(A_1')\mathbb{Q}_{2,1}^{(b)}(E'')}{2} + \frac{\mathbb{Q}_3^{(a)}(A_2')\mathbb{Q}_{2,2}^{(b)}(E'')}{2}$$

$$\boxed{\text{z146}} \quad \mathbb{Q}_{5,2}^{(c)}(E'',1) = \frac{\mathbb{Q}_3^{(a)}(A_1')\mathbb{Q}_{2,2}^{(b)}(E'')}{2} - \frac{\mathbb{Q}_3^{(a)}(A_2')\mathbb{Q}_{2,1}^{(b)}(E'')}{2}$$

$$\boxed{\text{z147}} \quad \mathbb{Q}_{5,1}^{(c)}(E'',2) = \frac{\sqrt{10}\mathbb{Q}_{3,1}^{(a)}(E')\mathbb{Q}_{2,2}^{(b)}(E'')}{8} + \frac{\sqrt{10}\mathbb{Q}_{3,2}^{(a)}(E')\mathbb{Q}_{2,1}^{(b)}(E'')}{8} + \frac{\sqrt{6}\mathbb{Q}_3^{(a)}(A_1')\mathbb{Q}_{2,1}^{(b)}(E'')}{8} - \frac{\sqrt{6}\mathbb{Q}_3^{(a)}(A_2')\mathbb{Q}_{2,2}^{(b)}(E'')}{8}$$

$$\boxed{\text{z148}} \quad \mathbb{Q}_{5,2}^{(c)}(E'',2) = \frac{\sqrt{10}\mathbb{Q}_{3,1}^{(a)}(E')\mathbb{Q}_{2,1}^{(b)}(E'')}{8} - \frac{\sqrt{10}\mathbb{Q}_{3,2}^{(a)}(E')\mathbb{Q}_{2,2}^{(b)}(E'')}{8} + \frac{\sqrt{6}\mathbb{Q}_3^{(a)}(A_1')\mathbb{Q}_{2,2}^{(b)}(E'')}{8} + \frac{\sqrt{6}\mathbb{Q}_3^{(a)}(A_2')\mathbb{Q}_{2,1}^{(b)}(E'')}{8}$$

$$\boxed{\text{z199}} \quad \mathbb{G}_0^{(c)}(A_1'') = \frac{\sqrt{2}\mathbb{G}_{2,1}^{(a)}(E')\mathbb{Q}_{2,1}^{(b)}(E'')}{2} + \frac{\sqrt{2}\mathbb{G}_{2,2}^{(a)}(E')\mathbb{Q}_{2,2}^{(b)}(E'')}{2}$$

$$\boxed{\text{z200}} \quad \mathbb{G}_2^{(c)}(A_1'',a) = \frac{\sqrt{2}\mathbb{Q}_{3,1}^{(a)}(E')\mathbb{Q}_{2,1}^{(b)}(E'')}{2} + \frac{\sqrt{2}\mathbb{Q}_{3,2}^{(a)}(E')\mathbb{Q}_{2,2}^{(b)}(E'')}{2}$$

$$\boxed{\text{z201}} \quad \mathbb{G}_2^{(c)}(A_1'',b) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E')\mathbb{Q}_{2,1}^{(b)}(E'')}{2} + \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E')\mathbb{Q}_{2,2}^{(b)}(E'')}{2}$$

$$\boxed{\text{z202}} \quad \mathbb{G}_2^{(c)}(A_1'',c) = \mathbb{G}_2^{(a)}(A_1'')\mathbb{Q}_0^{(b)}(A_1')$$

$$\boxed{\text{z203}} \quad \mathbb{G}_3^{(c)}(A_1'',a) = -\frac{\sqrt{2}\mathbb{Q}_{3,1}^{(a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{4} - \frac{\sqrt{2}\mathbb{Q}_{3,2}^{(a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{4} - \frac{\sqrt{3}\mathbb{Q}_3^{(a)}(A_2')\mathbb{Q}_1^{(b)}(A_2'')}{2}$$

$$\boxed{\text{z204}} \quad \mathbb{G}_3^{(c)}(A_1'',b) = \frac{\sqrt{2}\mathbb{G}_{2,1}^{(a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{2} + \frac{\sqrt{2}\mathbb{G}_{2,2}^{(a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{2}$$

$$\boxed{\text{z205}} \quad \mathbb{G}_1^{(c)}(A_2',a) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{2} - \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{2}$$

18

$$\boxed{\text{z206}} \quad \mathbb{G}_1^{(c)}(A_2',b) = \frac{\sqrt{30}\,\mathbb{G}_{2,1}^{(a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{10} - \frac{\sqrt{30}\,\mathbb{G}_{2,2}^{(a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{10} + \frac{\sqrt{10}\,\mathbb{G}_2^{(a)}(A_1'')\mathbb{Q}_1^{(b)}(A_2'')}{5}$$

$$\boxed{\text{z207}} \quad \mathbb{G}_3^{(c)}(A_2',a) = \frac{\sqrt{2}\,\mathbb{Q}_{3,1}^{(a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{2} - \frac{\sqrt{2}\,\mathbb{Q}_{3,2}^{(a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{2}$$

$$\boxed{\text{z208}} \quad \mathbb{G}_3^{(c)}(A_2',b) = -\frac{\sqrt{5}\,\mathbb{G}_{2,1}^{(a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{5} + \frac{\sqrt{5}\,\mathbb{G}_{2,2}^{(a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{5} + \frac{\sqrt{15}\,\mathbb{G}_2^{(a)}(A_1'')\mathbb{Q}_1^{(b)}(A_2'')}{5}$$

$$\boxed{\text{z209}} \quad \mathbb{G}_3^{(c)}(A_2'',a) = \frac{\sqrt{2}\,\mathbb{Q}_{3,1}^{(a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{4} - \frac{\sqrt{2}\,\mathbb{Q}_{3,2}^{(a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{4} + \frac{\sqrt{3}\,\mathbb{Q}_3^{(a)}(A_1')\mathbb{Q}_1^{(b)}(A_2'')}{2}$$

$$\boxed{\text{z210}} \quad \mathbb{G}_3^{(c)}(A_2'',b) = -\frac{\sqrt{2}\,\mathbb{G}_{2,1}^{(a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{2} + \frac{\sqrt{2}\,\mathbb{G}_{2,2}^{(a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{2}$$

$$\boxed{\text{z211}} \quad \mathbb{G}_{2,1}^{(c)}(E') = \frac{\sqrt{2}\,\mathbb{G}_{2,1}^{(a)}(E')\mathbb{Q}_0^{(b)}(A_1')}{2}$$

$$\boxed{\text{z212}} \quad \mathbb{G}_{2,2}^{(c)}(E') = \frac{\sqrt{2}\,\mathbb{G}_{2,2}^{(a)}(E')\mathbb{Q}_0^{(b)}(A_1')}{2}$$

$$\boxed{\text{z213}} \quad \mathbb{G}_{3,1}^{(c)}(E',a) = \frac{\sqrt{15}\,\mathbb{Q}_{3,1}^{(a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{12} - \frac{\sqrt{6}\,\mathbb{Q}_{3,2}^{(a)}(E'')\mathbb{Q}_1^{(b)}(A_2'')}{6} + \frac{\sqrt{15}\,\mathbb{Q}_{3,2}^{(a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{12} + \frac{\mathbb{Q}_3^{(a)}(A_1')\mathbb{Q}_{1,1}^{(b)}(E')}{4} - \frac{\mathbb{Q}_3^{(a)}(A_2')\mathbb{Q}_{1,2}^{(b)}(E')}{4}$$

$$\boxed{\text{z214}} \quad \mathbb{G}_{3,2}^{(c)}(E',a) = \frac{\sqrt{6}\,\mathbb{Q}_{3,1}^{(a)}(E'')\mathbb{Q}_1^{(b)}(A_2'')}{6} + \frac{\sqrt{15}\,\mathbb{Q}_{3,1}^{(a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{12} - \frac{\sqrt{15}\,\mathbb{Q}_{3,2}^{(a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{12} + \frac{\mathbb{Q}_3^{(a)}(A_1')\mathbb{Q}_{1,2}^{(b)}(E')}{4} + \frac{\mathbb{Q}_3^{(a)}(A_2')\mathbb{Q}_{1,1}^{(b)}(E')}{4}$$

$$\boxed{\text{z215}} \quad \mathbb{G}_{3,1}^{(c)}(E',b) = \frac{\sqrt{6}\,\mathbb{G}_{2,1}^{(a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{6} - \frac{\sqrt{6}\,\mathbb{G}_{2,2}^{(a)}(E'')\mathbb{Q}_1^{(b)}(A_2'')}{6} + \frac{\sqrt{6}\,\mathbb{G}_{2,2}^{(a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{6}$$

$$\boxed{\text{z216}} \quad \mathbb{G}_{3,2}^{(c)}(E',b) = \frac{\sqrt{6}\,\mathbb{G}_{2,1}^{(a)}(E'')\mathbb{Q}_1^{(b)}(A_2'')}{6} + \frac{\sqrt{6}\,\mathbb{G}_{2,1}^{(a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{6} - \frac{\sqrt{6}\,\mathbb{G}_{2,2}^{(a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{6}$$

$$\boxed{\text{z217}} \quad \mathbb{G}_{1,1}^{(c)}(E'',a) = \frac{\mathbb{Q}_{1,2}^{(a)}(E')\mathbb{Q}_1^{(b)}(A_2'')}{2} - \frac{\mathbb{Q}_1^{(a)}(A_2'')\mathbb{Q}_{1,2}^{(b)}(E')}{2}$$

$$\boxed{\text{z218}} \quad \mathbb{G}_{1,2}^{(c)}(E'',a) = -\frac{\mathbb{Q}_{1,1}^{(a)}(E')\mathbb{Q}_1^{(b)}(A_2'')}{2} + \frac{\mathbb{Q}_1^{(a)}(A_2'')\mathbb{Q}_{1,1}^{(b)}(E')}{2}$$

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

19

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

$\boxed{\text{z221}}$ $\quad \mathbb{G}_{2,1}^{(c)}(E'', a) = \dfrac{\sqrt{2}\mathbb{G}_{2,1}^{(a)}(E'')\mathbb{Q}_{0}^{(b)}(A_1')}{2}$

$\boxed{\text{z222}}$ $\quad \mathbb{G}_{2,2}^{(c)}(E'', a) = \dfrac{\sqrt{2}\mathbb{G}_{2,2}^{(a)}(E'')\mathbb{Q}_{0}^{(b)}(A_1')}{2}$

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

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

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

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

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

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

- '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: `6b@6n`

$\boxed{\text{z23}}$ $\quad \mathbb{Q}_{0}^{(c)}(A_1', a) = \mathbb{Q}_{0}^{(a)}(A_1')\mathbb{Q}_{0}^{(b)}(A_1')$

$\boxed{\text{z24}}$ $\quad \mathbb{Q}_{0}^{(c)}(A_1', b) = \dfrac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E'')\mathbb{Q}_{2,1}^{(b)}(E'')}{2} + \dfrac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E'')\mathbb{Q}_{2,2}^{(b)}(E'')}{2}$

$\boxed{\text{z25}}$ $\quad \mathbb{Q}_{0}^{(c)}(A_1', c) = \dfrac{\sqrt{3}\mathbb{M}_{1,1}^{(a)}(E'')\mathbb{M}_{1,1}^{(b)}(E'')}{3} + \dfrac{\sqrt{3}\mathbb{M}_{1,2}^{(a)}(E'')\mathbb{M}_{1,2}^{(b)}(E'')}{3} + \dfrac{\sqrt{3}\mathbb{M}_{1}^{(a)}(A_2')\mathbb{M}_{1}^{(b)}(A_2')}{3}$

20

$$\boxed{\text{z26}} \quad \mathbb{Q}_2^{(c)}(A_1', a) = \mathbb{Q}_2^{(a)}(A_1')\mathbb{Q}_0^{(b)}(A_1')$$

$$\boxed{\text{z27}} \quad \mathbb{Q}_2^{(c)}(A_1', b) = -\frac{\sqrt{6}\mathbb{M}_{1,1}^{(a)}(E'')\mathbb{M}_{1,1}^{(b)}(E'')}{6} - \frac{\sqrt{6}\mathbb{M}_{1,2}^{(a)}(E'')\mathbb{M}_{1,2}^{(b)}(E'')}{6} + \frac{\sqrt{6}\mathbb{M}_1^{(a)}(A_2')\mathbb{M}_1^{(b)}(A_2')}{3}$$

$$\boxed{\text{z28}} \quad \mathbb{Q}_3^{(c)}(A_1') = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{2} + \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{2}$$

$$\boxed{\text{z40}} \quad \mathbb{Q}_4^{(c)}(A_1'') = -\frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E')\mathbb{Q}_{2,1}^{(b)}(E'')}{2} - \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E')\mathbb{Q}_{2,2}^{(b)}(E'')}{2}$$

$$\boxed{\text{z41}} \quad \mathbb{Q}_3^{(c)}(A_2') = -\frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{2} + \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{2}$$

$$\boxed{\text{z42}} \quad \mathbb{Q}_1^{(c)}(A_2'', a) = \mathbb{Q}_0^{(a)}(A_1')\mathbb{Q}_1^{(b)}(A_2'')$$

$$\boxed{\text{z57}} \quad \mathbb{Q}_1^{(c)}(A_2'', b) = \frac{\sqrt{30}\mathbb{Q}_{2,1}^{(a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{10} - \frac{\sqrt{30}\mathbb{Q}_{2,2}^{(a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{10} + \frac{\sqrt{10}\mathbb{Q}_2^{(a)}(A_1')\mathbb{Q}_1^{(b)}(A_2'')}{5}$$

$$\boxed{\text{z58}} \quad \mathbb{Q}_1^{(c)}(A_2'', c) = \mathbb{M}_1^{(a)}(A_2')\mathbb{M}_2^{(b)}(A_1'')$$

$$\boxed{\text{z59}} \quad \mathbb{Q}_1^{(c)}(A_2'', d) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(a)}(E'')\mathbb{T}_{1,2}^{(b)}(E')}{2} - \frac{\sqrt{2}\mathbb{M}_{1,2}^{(a)}(E'')\mathbb{T}_{1,1}^{(b)}(E')}{2}$$

$$\boxed{\text{z77}} \quad \mathbb{Q}_3^{(c)}(A_2'') = -\frac{\sqrt{5}\mathbb{Q}_{2,1}^{(a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{5} + \frac{\sqrt{5}\mathbb{Q}_{2,2}^{(a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{5} + \frac{\sqrt{15}\mathbb{Q}_2^{(a)}(A_1')\mathbb{Q}_1^{(b)}(A_2'')}{5}$$

$$\boxed{\text{z78}} \quad \mathbb{Q}_4^{(c)}(A_2'') = -\frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E')\mathbb{Q}_{2,2}^{(b)}(E'')}{2} + \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E')\mathbb{Q}_{2,1}^{(b)}(E'')}{2}$$

$$\boxed{\text{z79}} \quad \mathbb{Q}_{1,1}^{(c)}(E', a) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_1')\mathbb{Q}_{1,1}^{(b)}(E')}{2}$$

$$\boxed{\text{z80}} \quad \mathbb{Q}_{1,2}^{(c)}(E', a) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_1')\mathbb{Q}_{1,2}^{(b)}(E')}{2}$$

$$\boxed{\text{z81}} \quad \mathbb{Q}_{1,1}^{(c)}(E', b) = \frac{\sqrt{15}\mathbb{Q}_{2,1}^{(a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{10} - \frac{\sqrt{15}\mathbb{Q}_{2,2}^{(a)}(E'')\mathbb{Q}_1^{(b)}(A_2'')}{10} + \frac{\sqrt{15}\mathbb{Q}_{2,2}^{(a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{10} - \frac{\sqrt{5}\mathbb{Q}_2^{(a)}(A_1')\mathbb{Q}_{1,1}^{(b)}(E')}{10}$$

$$\boxed{\text{z82}} \quad \mathbb{Q}_{1,2}^{(c)}(E',b) = \frac{\sqrt{15}\mathbb{Q}_{2,1}^{(a)}(E'')\mathbb{Q}_1^{(b)}(A_2'')}{10} + \frac{\sqrt{15}\mathbb{Q}_{2,1}^{(a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{10} - \frac{\sqrt{15}\mathbb{Q}_{2,2}^{(a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{10} - \frac{\sqrt{5}\mathbb{Q}_2^{(a)}(A_1')\mathbb{Q}_{1,2}^{(b)}(E')}{10}$$

$$\boxed{\text{z149}} \quad \mathbb{Q}_{1,1}^{(c)}(E',c) = -\frac{\sqrt{2}\mathbb{M}_{1,1}^{(a)}(E'')\mathbb{M}_2^{(b)}(A_1'')}{2}$$

$$\boxed{\text{z150}} \quad \mathbb{Q}_{1,2}^{(c)}(E',c) = -\frac{\sqrt{2}\mathbb{M}_{1,2}^{(a)}(E'')\mathbb{M}_2^{(b)}(A_1'')}{2}$$

$$\boxed{\text{z151}} \quad \mathbb{Q}_{1,1}^{(c)}(E',d) = -\frac{\sqrt{2}\mathbb{M}_1^{(a)}(A_2')\mathbb{T}_{1,2}^{(b)}(E')}{2}$$

$$\boxed{\text{z152}} \quad \mathbb{Q}_{1,2}^{(c)}(E',d) = \frac{\sqrt{2}\mathbb{M}_1^{(a)}(A_2')\mathbb{T}_{1,1}^{(b)}(E')}{2}$$

$$\boxed{\text{z153}} \quad \mathbb{Q}_{2,1}^{(c)}(E',a) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E')\mathbb{Q}_0^{(b)}(A_1')}{2}$$

$$\boxed{\text{z154}} \quad \mathbb{Q}_{2,2}^{(c)}(E',a) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E')\mathbb{Q}_0^{(b)}(A_1')}{2}$$

$$\boxed{\text{z155}} \quad \mathbb{Q}_{2,1}^{(c)}(E',b) = -\frac{\mathbb{Q}_{2,1}^{(a)}(E'')\mathbb{Q}_{2,2}^{(b)}(E'')}{2} - \frac{\mathbb{Q}_{2,2}^{(a)}(E'')\mathbb{Q}_{2,1}^{(b)}(E'')}{2}$$

$$\boxed{\text{z156}} \quad \mathbb{Q}_{2,2}^{(c)}(E',b) = -\frac{\mathbb{Q}_{2,1}^{(a)}(E'')\mathbb{Q}_{2,1}^{(b)}(E'')}{2} + \frac{\mathbb{Q}_{2,2}^{(a)}(E'')\mathbb{Q}_{2,2}^{(b)}(E'')}{2}$$

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

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

$$\boxed{\text{z159}} \quad \mathbb{Q}_{3,1}^{(c)}(E') = -\frac{\sqrt{15}\mathbb{Q}_{2,1}^{(a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{30} - \frac{2\sqrt{15}\mathbb{Q}_{2,2}^{(a)}(E'')\mathbb{Q}_1^{(b)}(A_2'')}{15} - \frac{\sqrt{15}\mathbb{Q}_{2,2}^{(a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{30} + \frac{\sqrt{5}\mathbb{Q}_2^{(a)}(A_1')\mathbb{Q}_{1,1}^{(b)}(E')}{5}$$

$$\boxed{\text{z160}} \quad \mathbb{Q}_{3,2}^{(c)}(E') = \frac{2\sqrt{15}\mathbb{Q}_{2,1}^{(a)}(E'')\mathbb{Q}_1^{(b)}(A_2'')}{15} - \frac{\sqrt{15}\mathbb{Q}_{2,1}^{(a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{30} + \frac{\sqrt{15}\mathbb{Q}_{2,2}^{(a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{30} + \frac{\sqrt{5}\mathbb{Q}_2^{(a)}(A_1')\mathbb{Q}_{1,2}^{(b)}(E')}{5}$$

$$\boxed{\text{z161}} \quad \mathbb{Q}_{2,1}^{(c)}(E'',a) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_1')\mathbb{Q}_{2,1}^{(b)}(E'')}{2}$$

$\boxed{\text{z162}}$ $\quad \mathbb{Q}_{2,2}^{(c)}(E'',a) = \dfrac{\sqrt{2}\,\mathbb{Q}_0^{(a)}(A_1')\mathbb{Q}_{2,2}^{(b)}(E'')}{2}$

$\boxed{\text{z163}}$ $\quad \mathbb{Q}_{2,1}^{(c)}(E'',b) = \dfrac{\sqrt{2}\,\mathbb{Q}_{2,1}^{(a)}(E'')\mathbb{Q}_0^{(b)}(A_1')}{2}$

$\boxed{\text{z164}}$ $\quad \mathbb{Q}_{2,2}^{(c)}(E'',b) = \dfrac{\sqrt{2}\,\mathbb{Q}_{2,2}^{(a)}(E'')\mathbb{Q}_0^{(b)}(A_1')}{2}$

$\boxed{\text{z165}}$ $\quad \mathbb{Q}_{2,1}^{(c)}(E'',c) = -\dfrac{\sqrt{42}\,\mathbb{Q}_{2,1}^{(a)}(E')\mathbb{Q}_{2,2}^{(b)}(E'')}{14} - \dfrac{\sqrt{42}\,\mathbb{Q}_{2,2}^{(a)}(E')\mathbb{Q}_{2,1}^{(b)}(E'')}{14} + \dfrac{\sqrt{14}\,\mathbb{Q}_2^{(a)}(A_1')\mathbb{Q}_{2,1}^{(b)}(E'')}{14}$

$\boxed{\text{z166}}$ $\quad \mathbb{Q}_{2,2}^{(c)}(E'',c) = -\dfrac{\sqrt{42}\,\mathbb{Q}_{2,1}^{(a)}(E')\mathbb{Q}_{2,1}^{(b)}(E'')}{14} + \dfrac{\sqrt{42}\,\mathbb{Q}_{2,2}^{(a)}(E')\mathbb{Q}_{2,2}^{(b)}(E'')}{14} + \dfrac{\sqrt{14}\,\mathbb{Q}_2^{(a)}(A_1')\mathbb{Q}_{2,2}^{(b)}(E'')}{14}$

$\boxed{\text{z229}}$ $\quad \mathbb{Q}_{2,1}^{(c)}(E'',d) = \dfrac{\mathbb{M}_{1,2}^{(a)}(E'')\mathbb{M}_1^{(b)}(A_2')}{2} + \dfrac{\mathbb{M}_1^{(a)}(A_2')\mathbb{M}_{1,2}^{(b)}(E'')}{2}$

$\boxed{\text{z230}}$ $\quad \mathbb{Q}_{2,2}^{(c)}(E'',d) = -\dfrac{\mathbb{M}_{1,1}^{(a)}(E'')\mathbb{M}_1^{(b)}(A_2')}{2} - \dfrac{\mathbb{M}_1^{(a)}(A_2')\mathbb{M}_{1,1}^{(b)}(E'')}{2}$

$\boxed{\text{z231}}$ $\quad \mathbb{Q}_{3,1}^{(c)}(E'') = \dfrac{\sqrt{6}\,\mathbb{Q}_{2,1}^{(a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{6} + \dfrac{\sqrt{6}\,\mathbb{Q}_{2,2}^{(a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{6} - \dfrac{\sqrt{6}\,\mathbb{Q}_{2,2}^{(a)}(E')\mathbb{Q}_1^{(b)}(A_2'')}{6}$

$\boxed{\text{z232}}$ $\quad \mathbb{Q}_{3,2}^{(c)}(E'') = \dfrac{\sqrt{6}\,\mathbb{Q}_{2,1}^{(a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{6} + \dfrac{\sqrt{6}\,\mathbb{Q}_{2,1}^{(a)}(E')\mathbb{Q}_1^{(b)}(A_2'')}{6} - \dfrac{\sqrt{6}\,\mathbb{Q}_{2,2}^{(a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{6}$

$\boxed{\text{z233}}$ $\quad \mathbb{Q}_{4,1}^{(c)}(E'') = \dfrac{\sqrt{7}\,\mathbb{Q}_{2,1}^{(a)}(E')\mathbb{Q}_{2,2}^{(b)}(E'')}{14} + \dfrac{\sqrt{7}\,\mathbb{Q}_{2,2}^{(a)}(E')\mathbb{Q}_{2,1}^{(b)}(E'')}{14} + \dfrac{\sqrt{21}\,\mathbb{Q}_2^{(a)}(A_1')\mathbb{Q}_{2,1}^{(b)}(E'')}{7}$

$\boxed{\text{z234}}$ $\quad \mathbb{Q}_{4,2}^{(c)}(E'') = \dfrac{\sqrt{7}\,\mathbb{Q}_{2,1}^{(a)}(E')\mathbb{Q}_{2,1}^{(b)}(E'')}{14} - \dfrac{\sqrt{7}\,\mathbb{Q}_{2,2}^{(a)}(E')\mathbb{Q}_{2,2}^{(b)}(E'')}{14} + \dfrac{\sqrt{21}\,\mathbb{Q}_2^{(a)}(A_1')\mathbb{Q}_{2,2}^{(b)}(E'')}{7}$

$\boxed{\text{z235}}$ $\quad \mathbb{G}_0^{(c)}(A_1'') = \dfrac{\sqrt{2}\,\mathbb{M}_{1,1}^{(a)}(E'')\mathbb{T}_{1,1}^{(b)}(E')}{2} + \dfrac{\sqrt{2}\,\mathbb{M}_{1,2}^{(a)}(E'')\mathbb{T}_{1,2}^{(b)}(E')}{2}$

$\boxed{\text{z236}}$ $\quad \mathbb{G}_2^{(c)}(A_1'') = -\dfrac{\sqrt{2}\,\mathbb{Q}_{2,1}^{(a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{2} - \dfrac{\sqrt{2}\,\mathbb{Q}_{2,2}^{(a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{2}$

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

23

$\boxed{\text{z238}}$ $\quad \mathbb{G}_1^{(c)}(A_2', b) = \dfrac{\sqrt{2}\mathbb{M}_{1,1}^{(a)}(E'')\mathbb{M}_{1,2}^{(b)}(E'')}{2} - \dfrac{\sqrt{2}\mathbb{M}_{1,2}^{(a)}(E'')\mathbb{M}_{1,1}^{(b)}(E'')}{2}$

$\boxed{\text{z239}}$ $\quad \mathbb{G}_{2,1}^{(c)}(E') = \dfrac{\sqrt{3}\mathbb{Q}_{2,1}^{(a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{6} + \dfrac{\sqrt{3}\mathbb{Q}_{2,2}^{(a)}(E'')\mathbb{Q}_1^{(b)}(A_2'')}{6} + \dfrac{\sqrt{3}\mathbb{Q}_{2,2}^{(a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{6} + \dfrac{\mathbb{Q}_2^{(a)}(A_1')\mathbb{Q}_{1,1}^{(b)}(E')}{2}$

$\boxed{\text{z240}}$ $\quad \mathbb{G}_{2,2}^{(c)}(E') = -\dfrac{\sqrt{3}\mathbb{Q}_{2,1}^{(a)}(E'')\mathbb{Q}_1^{(b)}(A_2'')}{6} + \dfrac{\sqrt{3}\mathbb{Q}_{2,1}^{(a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{6} - \dfrac{\sqrt{3}\mathbb{Q}_{2,2}^{(a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{6} + \dfrac{\mathbb{Q}_2^{(a)}(A_1')\mathbb{Q}_{1,2}^{(b)}(E')}{2}$

$\boxed{\text{z241}}$ $\quad \mathbb{G}_{1,1}^{(c)}(E'') = \dfrac{\mathbb{M}_{1,2}^{(a)}(E'')\mathbb{M}_1^{(b)}(A_2')}{2} - \dfrac{\mathbb{M}_1^{(a)}(A_2')\mathbb{M}_{1,2}^{(b)}(E'')}{2}$

$\boxed{\text{z242}}$ $\quad \mathbb{G}_{1,2}^{(c)}(E'') = -\dfrac{\mathbb{M}_{1,1}^{(a)}(E'')\mathbb{M}_1^{(b)}(A_2')}{2} + \dfrac{\mathbb{M}_1^{(a)}(A_2')\mathbb{M}_{1,1}^{(b)}(E'')}{2}$

$\boxed{\text{z243}}$ $\quad \mathbb{G}_{2,1}^{(c)}(E'', a) = -\dfrac{\sqrt{3}\mathbb{Q}_{2,1}^{(a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{6} - \dfrac{\sqrt{3}\mathbb{Q}_{2,2}^{(a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{6} - \dfrac{\sqrt{3}\mathbb{Q}_{2,2}^{(a)}(E')\mathbb{Q}_1^{(b)}(A_2'')}{3}$

$\boxed{\text{z244}}$ $\quad \mathbb{G}_{2,2}^{(c)}(E'', a) = -\dfrac{\sqrt{3}\mathbb{Q}_{2,1}^{(a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{6} + \dfrac{\sqrt{3}\mathbb{Q}_{2,1}^{(a)}(E')\mathbb{Q}_1^{(b)}(A_2'')}{3} + \dfrac{\sqrt{3}\mathbb{Q}_{2,2}^{(a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{6}$

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

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

━━ **Atomic SAMB** ━━

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

$\boxed{\text{x1}}$ $\quad \mathbb{Q}_0^{(a)}(A_1') = \begin{bmatrix} \frac{\sqrt{5}}{5} & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{5}}{5} & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{5}}{5} & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{5}}{5} & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{5}}{5} \end{bmatrix}$

$$\boxed{\text{x2}} \quad \mathbb{Q}_2^{(a)}(A_1') = \begin{bmatrix} \frac{\sqrt{14}}{7} & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{14}}{7} & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{14}}{14} & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{14}}{14} & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{14}}{7} \end{bmatrix}$$

$$\boxed{\text{x3}} \quad \mathbb{Q}_4^{(a)}(A_1') = \begin{bmatrix} \frac{3\sqrt{70}}{35} & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{70}}{70} & 0 & 0 & 0 \\ 0 & 0 & -\frac{2\sqrt{70}}{35} & 0 & 0 \\ 0 & 0 & 0 & -\frac{2\sqrt{70}}{35} & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{70}}{70} \end{bmatrix}$$

$$\boxed{\text{x4}} \quad \mathbb{Q}_4^{(a)}(A_1'') = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & 0 & -\frac{1}{2} \\ 0 & \frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & -\frac{1}{2} & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x5}} \quad \mathbb{Q}_4^{(a)}(A_2'') = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{2} & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{2} \\ 0 & 0 & 0 & \frac{1}{2} & 0 \end{bmatrix}$$

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

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

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

25

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

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

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

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

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

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

26

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

$$\boxed{\text{x16}} \quad \mathbb{M}_{3}^{(a)}(A_1'') = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{i}{2} & 0 \\ 0 & 0 & 0 & 0 & \frac{i}{2} \\ 0 & -\frac{i}{2} & 0 & 0 & 0 \\ 0 & 0 & -\frac{i}{2} & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x17}} \quad \mathbb{M}_{1}^{(a)}(A_2') = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{10}i}{5} \\ 0 & 0 & 0 & \frac{\sqrt{10}i}{10} & 0 \\ 0 & 0 & -\frac{\sqrt{10}i}{10} & 0 & 0 \\ 0 & \frac{\sqrt{10}i}{5} & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x18}} \quad \mathbb{M}_{3}^{(a)}(A_2') = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{10}i}{10} \\ 0 & 0 & 0 & \frac{\sqrt{10}i}{5} & 0 \\ 0 & 0 & -\frac{\sqrt{10}i}{5} & 0 & 0 \\ 0 & -\frac{\sqrt{10}i}{10} & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x19}} \quad \mathbb{M}_{3}^{(a)}(A_2'') = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{i}{2} & 0 & 0 \\ 0 & \frac{i}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{i}{2} \\ 0 & 0 & 0 & -\frac{i}{2} & 0 \end{bmatrix}$$

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

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

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

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

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

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

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

$\boxed{\text{x26}}$ $\mathbb{Q}_0^{(a)}(A_1') = \begin{bmatrix} \frac{\sqrt{3}}{3} & 0 & 0 \\ 0 & \frac{\sqrt{3}}{3} & 0 \\ 0 & 0 & \frac{\sqrt{3}}{3} \end{bmatrix}$

$\boxed{\text{x27}}$ $\mathbb{Q}_2^{(a)}(A_1') = \begin{bmatrix} -\frac{\sqrt{6}}{6} & 0 & 0 \\ 0 & -\frac{\sqrt{6}}{6} & 0 \\ 0 & 0 & \frac{\sqrt{6}}{3} \end{bmatrix}$

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

28

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

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

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

$$\boxed{\text{x32}} \quad \mathbb{M}_{1}^{(a)}(A_2') = \begin{bmatrix} 0 & -\frac{\sqrt{2}i}{2} & 0 \\ \frac{\sqrt{2}i}{2} & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

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

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

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

$$\boxed{\text{x35}} \quad \mathbb{Q}_{3}^{(a)}(A_1') = \begin{bmatrix} 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ \frac{1}{2} & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x36}} \quad \mathbb{Q}_{3}^{(a)}(A_2') = \begin{bmatrix} 0 & 0 & 0 \\ \frac{1}{2} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & -\frac{1}{2} & 0 \end{bmatrix}$$

$$\boxed{\text{x37}} \quad \mathbb{Q}_1^{(a)}(A_2'') = \begin{bmatrix} 0 & 0 & \frac{\sqrt{5}}{5} \\ 0 & 0 & 0 \\ 0 & \frac{\sqrt{15}}{10} & 0 \\ \frac{\sqrt{15}}{10} & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x38}} \quad \mathbb{Q}_3^{(a)}(A_2'') = \begin{bmatrix} 0 & 0 & \frac{\sqrt{30}}{10} \\ 0 & 0 & 0 \\ 0 & -\frac{\sqrt{10}}{10} & 0 \\ -\frac{\sqrt{10}}{10} & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x39}} \quad \mathbb{Q}_{1,1}^{(a)}(E') = \begin{bmatrix} -\frac{\sqrt{5}}{10} & 0 & 0 \\ \frac{\sqrt{15}}{10} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{15}}{10} \\ 0 & \frac{\sqrt{15}}{10} & 0 \end{bmatrix}$$

$$\boxed{\text{x40}} \quad \mathbb{Q}_{1,2}^{(a)}(E') = \begin{bmatrix} 0 & -\frac{\sqrt{5}}{10} & 0 \\ 0 & -\frac{\sqrt{15}}{10} & 0 \\ 0 & 0 & \frac{\sqrt{15}}{10} \\ 0 & 0 & 0 \\ \frac{\sqrt{15}}{10} & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x41}} \quad \mathbb{Q}_{3,1}^{(a)}(E') = \begin{bmatrix} \frac{\sqrt{5}}{5} & 0 & 0 \\ -\frac{\sqrt{15}}{30} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \frac{2\sqrt{15}}{15} \\ 0 & -\frac{\sqrt{15}}{30} & 0 \end{bmatrix}$$

$$\boxed{\text{x42}} \quad \mathbb{Q}_{3,2}^{(a)}(E') = \begin{bmatrix} 0 & \frac{\sqrt{5}}{5} & 0 \\ 0 & \frac{\sqrt{15}}{30} & 0 \\ 0 & 0 & \frac{2\sqrt{15}}{15} \\ 0 & 0 & 0 \\ -\frac{\sqrt{15}}{30} & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x43}} \quad \mathbb{Q}_{3,1}^{(a)}(E'') = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{6}}{6} \\ 0 & \frac{\sqrt{6}}{6} & 0 \\ -\frac{\sqrt{6}}{6} & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

30

$$\boxed{\text{x44}} \quad \mathbb{Q}_{3,2}^{(a)}(E'') = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ \frac{\sqrt{6}}{6} & 0 & 0 \\ 0 & \frac{\sqrt{6}}{6} & 0 \\ 0 & 0 & \frac{\sqrt{6}}{6} \end{bmatrix}$$

$$\boxed{\text{x45}} \quad \mathbb{G}_{2}^{(a)}(A_1'') = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ \frac{1}{2} & 0 & 0 \\ 0 & -\frac{1}{2} & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x46}} \quad \mathbb{G}_{2,1}^{(a)}(E') = \begin{bmatrix} -\frac{1}{2} & 0 & 0 \\ -\frac{\sqrt{3}}{6} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{3}}{6} \\ 0 & -\frac{\sqrt{3}}{6} & 0 \end{bmatrix}$$

$$\boxed{\text{x47}} \quad \mathbb{G}_{2,2}^{(a)}(E') = \begin{bmatrix} 0 & -\frac{1}{2} & 0 \\ 0 & \frac{\sqrt{3}}{6} & 0 \\ 0 & 0 & \frac{\sqrt{3}}{6} \\ 0 & 0 & 0 \\ -\frac{\sqrt{3}}{6} & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x48}} \quad \mathbb{G}_{2,1}^{(a)}(E'') = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{3}}{3} \\ 0 & \frac{\sqrt{3}}{6} & 0 \\ -\frac{\sqrt{3}}{6} & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x49}} \quad \mathbb{G}_{2,2}^{(a)}(E'') = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ \frac{\sqrt{3}}{6} & 0 & 0 \\ 0 & \frac{\sqrt{3}}{6} & 0 \\ 0 & 0 & -\frac{\sqrt{3}}{3} \end{bmatrix}$$

$$\boxed{\text{x50}} \quad \mathbb{M}_{2}^{(a)}(A_1'') = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ \frac{i}{2} & 0 & 0 \\ 0 & -\frac{i}{2} & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x51}} \quad \mathbb{M}_{2,1}^{(a)}(E') = \begin{bmatrix} -\frac{i}{2} & 0 & 0 \\ -\frac{\sqrt{3}i}{6} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{3}i}{6} \\ 0 & -\frac{\sqrt{3}i}{6} & 0 \end{bmatrix}$$

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

$$\boxed{\text{x53}} \quad \mathbb{M}_{2,1}^{(a)}(E'') = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{3}i}{3} \\ 0 & \frac{\sqrt{3}i}{6} & 0 \\ -\frac{\sqrt{3}i}{6} & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x54}} \quad \mathbb{M}_{2,2}^{(a)}(E'') = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ \frac{\sqrt{3}i}{6} & 0 & 0 \\ 0 & \frac{\sqrt{3}i}{6} & 0 \\ 0 & 0 & -\frac{\sqrt{3}i}{3} \end{bmatrix}$$

$$\boxed{\text{x55}} \quad \mathbb{T}_{3}^{(a)}(A_1') = \begin{bmatrix} 0 & 0 & 0 \\ 0 & -\frac{i}{2} & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ -\frac{i}{2} & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x56}} \quad \mathbb{T}_{3}^{(a)}(A_2') = \begin{bmatrix} 0 & 0 & 0 \\ -\frac{i}{2} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & \frac{i}{2} & 0 \end{bmatrix}$$

$$\boxed{\text{x57}} \quad \mathbb{T}_{1}^{(a)}(A_2'') = \begin{bmatrix} 0 & 0 & -\frac{\sqrt{5}i}{5} \\ 0 & 0 & 0 \\ 0 & -\frac{\sqrt{15}i}{10} & 0 \\ -\frac{\sqrt{15}i}{10} & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

32

$$\boxed{\text{x58}} \quad \mathbb{T}_3^{(a)}(A_2'') = \begin{bmatrix} 0 & 0 & -\frac{\sqrt{30}i}{10} \\ 0 & 0 & 0 \\ 0 & \frac{\sqrt{10}i}{10} & 0 \\ \frac{\sqrt{10}i}{10} & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x59}} \quad \mathbb{T}_{1,1}^{(a)}(E') = \begin{bmatrix} \frac{\sqrt{5}i}{10} & 0 & 0 \\ -\frac{\sqrt{15}i}{10} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{15}i}{10} \\ 0 & -\frac{\sqrt{15}i}{10} & 0 \end{bmatrix}$$

$$\boxed{\text{x60}} \quad \mathbb{T}_{1,2}^{(a)}(E') = \begin{bmatrix} 0 & \frac{\sqrt{5}i}{10} & 0 \\ 0 & \frac{\sqrt{15}i}{10} & 0 \\ 0 & 0 & -\frac{\sqrt{15}i}{10} \\ 0 & 0 & 0 \\ -\frac{\sqrt{15}i}{10} & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x61}} \quad \mathbb{T}_{3,1}^{(a)}(E') = \begin{bmatrix} -\frac{\sqrt{5}i}{5} & 0 & 0 \\ \frac{\sqrt{15}i}{30} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -\frac{2\sqrt{15}i}{15} \\ 0 & \frac{\sqrt{15}i}{30} & 0 \end{bmatrix}$$

$$\boxed{\text{x62}} \quad \mathbb{T}_{3,2}^{(a)}(E') = \begin{bmatrix} 0 & -\frac{\sqrt{5}i}{5} & 0 \\ 0 & -\frac{\sqrt{15}i}{30} & 0 \\ 0 & 0 & -\frac{2\sqrt{15}i}{15} \\ 0 & 0 & 0 \\ \frac{\sqrt{15}i}{30} & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x63}} \quad \mathbb{T}_{3,1}^{(a)}(E'') = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{6}i}{6} \\ 0 & -\frac{\sqrt{6}i}{6} & 0 \\ \frac{\sqrt{6}i}{6} & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x64}} \quad \mathbb{T}_{3,2}^{(a)}(E'') = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ -\frac{\sqrt{6}i}{6} & 0 & 0 \\ 0 & -\frac{\sqrt{6}i}{6} & 0 \\ 0 & 0 & -\frac{\sqrt{6}i}{6} \end{bmatrix}$$

33

- Site cluster

** Wyckoff: `1a`

$\boxed{\text{y1}}$ $\mathbb{Q}_0^{(s)}(A_1') = [1]$

** Wyckoff: `2i`

$\boxed{\text{y2}}$ $\mathbb{Q}_0^{(s)}(A_1') = \left[\dfrac{\sqrt{2}}{2}, \dfrac{\sqrt{2}}{2} \right]$

$\boxed{\text{y3}}$ $\mathbb{Q}_1^{(s)}(A_2'') = \left[\dfrac{\sqrt{2}}{2}, -\dfrac{\sqrt{2}}{2} \right]$

- Bond cluster

** Wyckoff: `3b@3j`

$\boxed{\text{y4}}$ $\mathbb{Q}_0^{(s)}(A_1') = \left[\dfrac{\sqrt{3}}{3}, \dfrac{\sqrt{3}}{3}, \dfrac{\sqrt{3}}{3} \right]$

$\boxed{\text{y5}}$ $\mathbb{M}_1^{(s)}(A_2') = \left[\dfrac{\sqrt{3}i}{3}, \dfrac{\sqrt{3}i}{3}, \dfrac{\sqrt{3}i}{3} \right]$

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

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

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

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

34

** Wyckoff: `6b@6n`

y10 $\mathbb{Q}_0^{(s)}(A_1') = \left[\dfrac{\sqrt{6}}{6},\, \dfrac{\sqrt{6}}{6},\, \dfrac{\sqrt{6}}{6},\, \dfrac{\sqrt{6}}{6},\, \dfrac{\sqrt{6}}{6},\, \dfrac{\sqrt{6}}{6} \right]$

y11 $\mathbb{M}_2^{(s)}(A_1'') = \left[\dfrac{\sqrt{6}i}{6},\, \dfrac{\sqrt{6}i}{6},\, \dfrac{\sqrt{6}i}{6},\, -\dfrac{\sqrt{6}i}{6},\, -\dfrac{\sqrt{6}i}{6},\, -\dfrac{\sqrt{6}i}{6} \right]$

y12 $\mathbb{M}_1^{(s)}(A_2') = \left[\dfrac{\sqrt{6}i}{6},\, \dfrac{\sqrt{6}i}{6},\, \dfrac{\sqrt{6}i}{6},\, \dfrac{\sqrt{6}i}{6},\, \dfrac{\sqrt{6}i}{6},\, \dfrac{\sqrt{6}i}{6} \right]$

y13 $\mathbb{Q}_1^{(s)}(A_2'') = \left[\dfrac{\sqrt{6}}{6},\, \dfrac{\sqrt{6}}{6},\, \dfrac{\sqrt{6}}{6},\, -\dfrac{\sqrt{6}}{6},\, -\dfrac{\sqrt{6}}{6},\, -\dfrac{\sqrt{6}}{6} \right]$

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

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

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

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

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

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

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

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

** Wyckoff: `6a@6n`

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

y23 $\mathbb{T}_0^{(s)}(A_1') = \left[\dfrac{\sqrt{6}i}{6}, \dfrac{\sqrt{6}i}{6}, \dfrac{\sqrt{6}i}{6}, \dfrac{\sqrt{6}i}{6}, \dfrac{\sqrt{6}i}{6}, \dfrac{\sqrt{6}i}{6} \right]$

y24 $\mathbb{Q}_1^{(s)}(A_2'') = \left[\dfrac{\sqrt{6}}{6}, \dfrac{\sqrt{6}}{6}, \dfrac{\sqrt{6}}{6}, -\dfrac{\sqrt{6}}{6}, -\dfrac{\sqrt{6}}{6}, -\dfrac{\sqrt{6}}{6} \right]$

y25 $\mathbb{T}_1^{(s)}(A_2'') = \left[\dfrac{\sqrt{6}i}{6}, \dfrac{\sqrt{6}i}{6}, \dfrac{\sqrt{6}i}{6}, -\dfrac{\sqrt{6}i}{6}, -\dfrac{\sqrt{6}i}{6}, -\dfrac{\sqrt{6}i}{6} \right]$

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

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

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

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

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

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

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

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

— **Site and Bond** —

Table 5: Orbital of each site

#	site	orbital
1	Mo	$|d_u\rangle$, $|d_{xz}\rangle$, $|d_{yz}\rangle$, $|d_{xy}\rangle$, $|d_v\rangle$
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 (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 (s)	mapping
1	[0.66667, 0.33333, 0.12425]	[1,2,3,7,8,9]
2	[0.66667, 0.33333, 0.87575]	[4,5,6,10,11,12]

━━ **Bond in Unit Cell** ━━━

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

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

SL	vector (v)	center (c)	mapping	head	tail	R (primitive)
1	[-1.00000,-1.00000, 0.00000]	[0.50000, 0.50000, 0.00000]	[1,4,-7,-10]	(1,1)	(1,1)	[1,1,0]

continued ...

38

Table 9

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

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

SL	vector (v)	center (c)	mapping	head	tail	R (primitive)
1	[0.33333,-0.33333,-0.12425]	[0.83333, 0.16667, 0.06212]	[1,7]	(1,1)	(1,1)	[-1,0,0]
2	[0.33333, 0.66667,-0.12425]	[0.83333, 0.66667, 0.06212]	[2,9]	(1,1)	(1,1)	[-1,-1,0]
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, $|v|=$ 3.1661 (cartesian)

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