Model for “MoS2”

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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]`
- Atomic selection:
  - Type: `[Q, G, M, T]`
  - Rank: `[0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11]`
  - Irrep.: [A_1', A_2', A_1'', A_2'', E', E'']
  - Spin (s): `[0, 1]`
- Site-cluster selection:
  - Rank: `[0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11]`
  - Irrep.: [A_1', A_2', A_1'', A_2'', E', E'']
- Bond-cluster selection:
  - Type: `[Q, G, M, T]`
  - Rank: `[0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11]`
  - Irrep.: [A_1', A_2', A_1'', A_2'', E', E'']
- Max. neighbor: `10`
- Search cell range: `(-2, 3), (-2, 3), (-2, 3)`
- Toroidal priority: `false`

Group and Unit Cell

- Group: SG No. 187 D_{3h}^1 $P\bar{6}m2$ [hexagonal]
- Associated point group: PG No. 187 D_{3h} $\bar{6}m2$ (-6m2 setting) [hexagonal]
- Unit cell:
  $a =$ 3.16610, $b =$ 3.16610, $c =$ 20.00000, $\alpha =$ 90.0, $\beta =$ 90.0, $\gamma =$ 120.0
- Lattice vectors (conventional cell):
  $\boldsymbol{a}_1 =$ [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	$\{\mathrm{m}_{001}\|0\}$	5	$\{-6^{-}_{001}\|0\}$
6	$\{-6^{+}_{001}\|0\}$	7	$\{\mathrm{m}_{110}\|0\}$	8	$\{\mathrm{m}_{100}\|0\}$	9	$\{\mathrm{m}_{010}\|0\}$	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	-	-	$\frac{\sqrt{10}y\left(3x^2-y^2\right)}{4}$
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	-	-	$-\frac{\sqrt{70}y\left(3x^2-y^2\right)\left(x^2+y^2-8z^2\right)}{16}$
6	$\mathbb{G}_0(A_1'')$	A_1''	0	G, M	-	-	1
7	$\mathbb{G}_2(A_1'')$	A_1''	2	G, M	-	-	$-\frac{x^2}{2}-\frac{y^2}{2}+z^2$

continued ...

Table 2

#	symbol	irrep.	rank	X	multiplicity	component	symmetry
8	$\mathbb{G}_3(A_1'')$	A_1''	3	$G,\ M$	-	-	$\frac{\sqrt{10}y\left(3x^2-y^2\right)}{4}$
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	$Q,\ T$	-	-	$\frac{\sqrt{70}xz\left(x^2-3y^2\right)}{4}$
11	$\mathbb{G}_1(A_2')$	A_2'	1	$G,\ M$	-	-	z
12	$\mathbb{G}_3(A_2')$	A_2'	3	$G,\ M$	-	-	$-\frac{z\left(3x^2+3y^2-2z^2\right)}{2}$
13	$\mathbb{Q}_3(A_2')$	A_2'	3	$Q,\ T$	-	-	$\frac{\sqrt{10}x\left(x^2-3y^2\right)}{4}$
14	$\mathbb{Q}_5(A_2')$	A_2'	5	$Q,\ T$	-	-	$-\frac{\sqrt{70}x\left(x^2-3y^2\right)\left(x^2+y^2-8z^2\right)}{16}$
15	$\mathbb{Q}_1(A_2'')$	A_2''	1	$Q,\ T$	-	-	z
16	$\mathbb{G}_3(A_2'')$	A_2''	3	$G,\ M$	-	-	$\frac{\sqrt{10}x\left(x^2-3y^2\right)}{4}$
17	$\mathbb{Q}_3(A_2'')$	A_2''	3	$Q,\ T$	-	-	$-\frac{z\left(3x^2+3y^2-2z^2\right)}{2}$
18	$\mathbb{Q}_4(A_2'')$	A_2''	4	$Q,\ T$	-	-	$\frac{\sqrt{70}yz\left(3x^2-y^2\right)}{4}$
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	$-\frac{\sqrt{6}x\left(x^2+y^2-4z^2\right)}{4}$
28	$\mathbb{Q}_{3,2}(E')$					2	$-\frac{\sqrt{6}y\left(x^2+y^2-4z^2\right)}{4}$

continued ...

Table 2

#	symbol	irrep.	rank	X	multiplicity	component	symmetry
29	$\mathbb{Q}_{4,1}(E',1)$	E'	4	Q, T	1	1	$-\frac{\sqrt{35}xy(x-y)(x+y)}{2}$
30	$\mathbb{Q}_{4,2}(E',1)$					2	$\frac{\sqrt{35}\left(x^2-2xy-y^2\right)\left(x^2+2xy-y^2\right)}{8}$
31	$\mathbb{Q}_{4,1}(E',2)$	E'	4	Q, T	2	1	$-\frac{\sqrt{5}xy\left(x^2+y^2-6z^2\right)}{2}$
32	$\mathbb{Q}_{4,2}(E',2)$					2	$-\frac{\sqrt{5}(x-y)(x+y)\left(x^2+y^2-6z^2\right)}{4}$
33	$\mathbb{Q}_{5,1}(E',1)$	E'	5	Q, T	1	1	$\frac{3\sqrt{14}x\left(x^4-10x^2y^2+5y^4\right)}{16}$
34	$\mathbb{Q}_{5,2}(E',1)$					2	$-\frac{3\sqrt{14}y\left(5x^4-10x^2y^2+y^4\right)}{16}$
35	$\mathbb{Q}_{5,1}(E',2)$	E'	5	Q, T	2	1	$\frac{\sqrt{15}x\left(x^4+2x^2y^2-12x^2z^2+y^4-12y^2z^2+8z^4\right)}{8}$
36	$\mathbb{Q}_{5,2}(E',2)$					2	$\frac{\sqrt{15}y\left(x^4+2x^2y^2-12x^2z^2+y^4-12y^2z^2+8z^4\right)}{8}$
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	$-\frac{\sqrt{6}x\left(x^2+y^2-4z^2\right)}{4}$
44	$\mathbb{G}_{3,2}(E'')$					2	$-\frac{\sqrt{6}y\left(x^2+y^2-4z^2\right)}{4}$
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	$\frac{\sqrt{35}\left(x^2-2xy-y^2\right)\left(x^2+2xy-y^2\right)}{8}$
49	$\mathbb{Q}_{4,1}(E'')$	E''	4	Q, T	-	1	$-\frac{\sqrt{10}yz\left(3x^2+3y^2-4z^2\right)}{4}$

continued ...

Table 2

#	symbol	irrep.	rank	X	multiplicity	component	symmetry
50	$\mathbb{Q}_{4,2}(E'')$					2	$\frac{\sqrt{10}xz\left(3x^2+3y^2-4z^2\right)}{4}$
51	$\mathbb{Q}_{5,1}(E'',1)$	E''	5	Q, T	1	1	$-\frac{3\sqrt{35}z\left(x^2-2xy-y^2\right)\left(x^2+2xy-y^2\right)}{8}$
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	$\frac{\sqrt{105}z(x-y)(x+y)\left(x^2+y^2-2z^2\right)}{4}$
54	$\mathbb{Q}_{5,2}(E'',2)$					2	$-\frac{\sqrt{105}xyz\left(x^2+y^2-2z^2\right)}{2}$

Basis in full matrix

Table 3: dimension = 11

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

Table 4: Atomic basis (orbital part only)

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

246 (all 246) SAMBs

- 'Mo' site-cluster : `Mo`
  - * 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`

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- 'S' site-cluster : `S`
  - * bra: $\langle p_x|$, $\langle p_y|$, $\langle p_z|$
  - * ket: $|p_x\rangle$, $|p_y\rangle$, $|p_z\rangle$
  - * wyckoff: `2i`

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

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

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

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

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

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

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

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

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

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

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

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

- 'Mo'-'Mo' bond-cluster : `Mo;Mo_001_1`
  - * bra: $\langle d_u|$, $\langle d_{xz}|$, $\langle d_{yz}|$, $\langle d_{xy}|$, $\langle d_v|$
  - * ket: $|d_u\rangle$, $|d_{xz}\rangle$, $|d_{yz}\rangle$, $|d_{xy}\rangle$, $|d_v\rangle$
  - * wyckoff: `3b@3j`

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

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

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

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

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

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

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

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

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

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

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

$\boxed{\text{z31}}$ $\mathbb{G}_0^{(c)}(A_1'')=\frac{\sqrt{2}\mathbb{M}_{1,1}^{(a)}(E'')\mathbb{T}_{1,1}^{(b)}(E')}{2}+\frac{\sqrt{2}\mathbb{M}_{1,2}^{(a)}(E'')\mathbb{T}_{1,2}^{(b)}(E')}{2}$

$\boxed{\text{z32}}$ $\mathbb{G}_2^{(c)}(A_1'',a)=-\frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{2}-\frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{2}$

$\boxed{\text{z44}}$ $\mathbb{G}_2^{(c)}(A_1'',b)=\frac{\sqrt{2}\mathbb{M}_{3,1}^{(a)}(E'')\mathbb{T}_{1,1}^{(b)}(E')}{2}+\frac{\sqrt{2}\mathbb{M}_{3,2}^{(a)}(E'')\mathbb{T}_{1,2}^{(b)}(E')}{2}$

$\boxed{\text{z45}}$ $\mathbb{G}_4^{(c)}(A_1'')=-\frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{2}-\frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{2}$

$\boxed{\text{z46}}$ $\mathbb{Q}_3^{(c)}(A_2',a)=-\frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{2}+\frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{2}$

$\boxed{\text{z47}}$ $\mathbb{Q}_3^{(c)}(A_2',b)=-\frac{\sqrt{406}\mathbb{Q}_{4,1}^{(a)}(E',1)\mathbb{Q}_{1,2}^{(b)}(E')}{29}+\frac{\sqrt{58}\mathbb{Q}_{4,1}^{(a)}(E',2)\mathbb{Q}_{1,2}^{(b)}(E')}{58}+\frac{\sqrt{406}\mathbb{Q}_{4,2}^{(a)}(E',1)\mathbb{Q}_{1,1}^{(b)}(E')}{29}-\frac{\sqrt{58}\mathbb{Q}_{4,2}^{(a)}(E',2)\mathbb{Q}_{1,1}^{(b)}(E')}{58}$

$\boxed{\text{z48}}$ $\mathbb{Q}_3^{(c)}(A_2', c) = \frac{\sqrt{2}\mathbb{M}_{3,1}^{(a)}(E')\mathbb{T}_{1,2}^{(b)}(E')}{2} - \frac{\sqrt{2}\mathbb{M}_{3,2}^{(a)}(E')\mathbb{T}_{1,1}^{(b)}(E')}{2}$

$\boxed{\text{z49}}$ $\mathbb{Q}_5^{(c)}(A_2') = -\frac{\sqrt{58}\mathbb{Q}_{4,1}^{(a)}(E',1)\mathbb{Q}_{1,2}^{(b)}(E')}{58} - \frac{\sqrt{406}\mathbb{Q}_{4,1}^{(a)}(E',2)\mathbb{Q}_{1,2}^{(b)}(E')}{29} + \frac{\sqrt{58}\mathbb{Q}_{4,2}^{(a)}(E',1)\mathbb{Q}_{1,1}^{(b)}(E')}{58} + \frac{\sqrt{406}\mathbb{Q}_{4,2}^{(a)}(E',2)\mathbb{Q}_{1,1}^{(b)}(E')}{29}$

$\boxed{\text{z63}}$ $\mathbb{Q}_1^{(c)}(A_2'', a) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{2} - \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{2}$

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

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

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

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

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

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

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

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

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

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

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

$\boxed{\text{z99}}$ $\mathbb{Q}_{2,1}^{(c)}(E',a) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E')\mathbb{Q}_{0}^{(b)}(A_1')}{2}$

$\boxed{\text{z100}}$ $\mathbb{Q}_{2,2}^{(c)}(E',a) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E')\mathbb{Q}_{0}^{(b)}(A_1')}{2}$

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

$\boxed{\text{z102}}$ $\mathbb{Q}_{2,2}^{(c)}(E',b) = -\frac{\sqrt{2}\mathbb{M}_{3,1}^{(a)}(E')\mathbb{M}_{1}^{(b)}(A_2')}{2}$

$\boxed{\text{z103}}$ $\mathbb{Q}_{3,1}^{(c)}(E',a) = \frac{\sqrt{7}\mathbb{Q}_{2,1}^{(a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{14} + \frac{\sqrt{7}\mathbb{Q}_{2,2}^{(a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{14} + \frac{\sqrt{21}\mathbb{Q}_{2}^{(a)}(A_1')\mathbb{Q}_{1,1}^{(b)}(E')}{7}$

$\boxed{\text{z104}}$ $\mathbb{Q}_{3,2}^{(c)}(E',a) = \frac{\sqrt{7}\mathbb{Q}_{2,1}^{(a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{14} - \frac{\sqrt{7}\mathbb{Q}_{2,2}^{(a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{14} + \frac{\sqrt{21}\mathbb{Q}_{2}^{(a)}(A_1')\mathbb{Q}_{1,2}^{(b)}(E')}{7}$

$\boxed{\text{z105}}$ $\mathbb{Q}_{3,1}^{(c)}(E',b) = \frac{\sqrt{35}\mathbb{Q}_{4,1}^{(a)}(E',2)\mathbb{Q}_{1,2}^{(b)}(E')}{14} + \frac{\sqrt{35}\mathbb{Q}_{4,2}^{(a)}(E',2)\mathbb{Q}_{1,1}^{(b)}(E')}{14} - \frac{\sqrt{7}\mathbb{Q}_{4}^{(a)}(A_1')\mathbb{Q}_{1,1}^{(b)}(E')}{7}$

$\boxed{\text{z106}}$ $\mathbb{Q}_{3,2}^{(c)}(E',b) = \frac{\sqrt{35}\mathbb{Q}_{4,1}^{(a)}(E',2)\mathbb{Q}_{1,1}^{(b)}(E')}{14} - \frac{\sqrt{35}\mathbb{Q}_{4,2}^{(a)}(E',2)\mathbb{Q}_{1,2}^{(b)}(E')}{14} - \frac{\sqrt{7}\mathbb{Q}_{4}^{(a)}(A_1')\mathbb{Q}_{1,2}^{(b)}(E')}{7}$

$\boxed{\text{z107}}$ $\mathbb{Q}_{3,1}^{(c)}(E',c) = -\frac{\sqrt{55}\mathbb{M}_{3,1}^{(a)}(E')\mathbb{T}_{1,2}^{(b)}(E')}{22} - \frac{\sqrt{55}\mathbb{M}_{3,2}^{(a)}(E')\mathbb{T}_{1,1}^{(b)}(E')}{22} - \frac{\sqrt{33}\mathbb{M}_{3}^{(a)}(A_2')\mathbb{T}_{1,2}^{(b)}(E')}{11}$

$\boxed{\text{z108}}$ $\mathbb{Q}_{3,2}^{(c)}(E',c) = -\frac{\sqrt{55}\mathbb{M}_{3,1}^{(a)}(E')\mathbb{T}_{1,1}^{(b)}(E')}{22} + \frac{\sqrt{55}\mathbb{M}_{3,2}^{(a)}(E')\mathbb{T}_{1,2}^{(b)}(E')}{22} + \frac{\sqrt{33}\mathbb{M}_{3}^{(a)}(A_2')\mathbb{T}_{1,1}^{(b)}(E')}{11}$

$\boxed{\text{z109}}$ $\mathbb{Q}_{4,1}^{(c)}(E',1) = \frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E',1)\mathbb{Q}_{0}^{(b)}(A_1')}{2}$

$\boxed{\text{z110}}$ $\mathbb{Q}_{4,2}^{(c)}(E',1) = \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E',1)\mathbb{Q}_{0}^{(b)}(A_1')}{2}$

$\boxed{\text{z111}}$ $\mathbb{Q}_{4,1}^{(c)}(E',2) = \frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E',2)\mathbb{Q}_{0}^{(b)}(A_1')}{2}$

$\boxed{\text{z112}}$ $\mathbb{Q}_{4,2}^{(c)}(E',2) = \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E',2)\mathbb{Q}_{0}^{(b)}(A_1')}{2}$

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

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

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

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

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

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

$\boxed{\text{z175}}$ $\mathbb{Q}^{(c)}_{2,1}(E'',a) = \frac{\sqrt{2}\mathbb{Q}^{(a)}_{2,1}(E'')\mathbb{Q}^{(b)}_{0}(A'_1)}{2}$

$\boxed{\text{z176}}$ $\mathbb{Q}^{(c)}_{2,2}(E'',a) = \frac{\sqrt{2}\mathbb{Q}^{(a)}_{2,2}(E'')\mathbb{Q}^{(b)}_{0}(A'_1)}{2}$

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

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

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

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

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

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

$\boxed{\text{z183}}$ $$\mathbb{Q}_{3,1}^{(c)}(E'',b)=-\frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{8}-\frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{8}-\frac{\sqrt{14}\mathbb{Q}_{4}^{(a)}(A_1'')\mathbb{Q}_{1,1}^{(b)}(E')}{8}-\frac{\sqrt{14}\mathbb{Q}_{4}^{(a)}(A_2'')\mathbb{Q}_{1,2}^{(b)}(E')}{8}$$

$\boxed{\text{z184}}$ $$\mathbb{Q}_{3,2}^{(c)}(E'',b)=-\frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{8}+\frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{8}-\frac{\sqrt{14}\mathbb{Q}_{4}^{(a)}(A_1'')\mathbb{Q}_{1,2}^{(b)}(E')}{8}+\frac{\sqrt{14}\mathbb{Q}_{4}^{(a)}(A_2'')\mathbb{Q}_{1,1}^{(b)}(E')}{8}$$

$\boxed{\text{z185}}$ $$\mathbb{Q}_{3,1}^{(c)}(E'',c)=\frac{\sqrt{10}\mathbb{M}_{3,1}^{(a)}(E'')\mathbb{T}_{1,2}^{(b)}(E')}{8}+\frac{\sqrt{10}\mathbb{M}_{3,2}^{(a)}(E'')\mathbb{T}_{1,1}^{(b)}(E')}{8}+\frac{\sqrt{6}\mathbb{M}_{3}^{(a)}(A_1'')\mathbb{T}_{1,1}^{(b)}(E')}{8}-\frac{\sqrt{6}\mathbb{M}_{3}^{(a)}(A_2'')\mathbb{T}_{1,2}^{(b)}(E')}{8}$$

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

$\boxed{\text{z187}}$ $$\mathbb{Q}_{4,1}^{(c)}(E'')=\frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E'')\mathbb{Q}_{0}^{(b)}(A_1')}{2}$$

$\boxed{\text{z188}}$ $$\mathbb{Q}_{4,2}^{(c)}(E'')=\frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E'')\mathbb{Q}_{0}^{(b)}(A_1')}{2}$$

$\boxed{\text{z189}}$ $$\mathbb{Q}_{5,1}^{(c)}(E'',1)=-\frac{\mathbb{Q}_{4}^{(a)}(A_1'')\mathbb{Q}_{1,1}^{(b)}(E')}{2}+\frac{\mathbb{Q}_{4}^{(a)}(A_2'')\mathbb{Q}_{1,2}^{(b)}(E')}{2}$$

$\boxed{\text{z190}}$ $$\mathbb{Q}_{5,2}^{(c)}(E'',1)=-\frac{\mathbb{Q}_{4}^{(a)}(A_1'')\mathbb{Q}_{1,2}^{(b)}(E')}{2}-\frac{\mathbb{Q}_{4}^{(a)}(A_2'')\mathbb{Q}_{1,1}^{(b)}(E')}{2}$$

$\boxed{\text{z191}}$ $$\mathbb{Q}_{5,1}^{(c)}(E'',2)=\frac{\sqrt{14}\mathbb{Q}_{4,1}^{(a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{8}+\frac{\sqrt{14}\mathbb{Q}_{4,2}^{(a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{8}-\frac{\sqrt{2}\mathbb{Q}_{4}^{(a)}(A_1'')\mathbb{Q}_{1,1}^{(b)}(E')}{8}-\frac{\sqrt{2}\mathbb{Q}_{4}^{(a)}(A_2'')\mathbb{Q}_{1,2}^{(b)}(E')}{8}$$

$\boxed{\text{z192}}$ $$\mathbb{Q}_{5,2}^{(c)}(E'',2)=\frac{\sqrt{14}\mathbb{Q}_{4,1}^{(a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{8}-\frac{\sqrt{14}\mathbb{Q}_{4,2}^{(a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{8}-\frac{\sqrt{2}\mathbb{Q}_{4}^{(a)}(A_1'')\mathbb{Q}_{1,2}^{(b)}(E')}{8}+\frac{\sqrt{2}\mathbb{Q}_{4}^{(a)}(A_2'')\mathbb{Q}_{1,1}^{(b)}(E')}{8}$$

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

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

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

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

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

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

- 'Mo'-'S' bond-cluster : `S;Mo_001_1`
  - * bra: $\langle d_u|$, $\langle d_{xz}|$, $\langle d_{yz}|$, $\langle d_{xy}|$, $\langle d_v|$
  - * ket: $|p_x\rangle$, $|p_y\rangle$, $|p_z\rangle$
  - * wyckoff: `6a@6n`

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

$\boxed{\text{z127}}$ $$\mathbb{Q}_{2,1}^{(c)}(E',a) = -\frac{\sqrt{21}\mathbb{Q}_{3,1}^{(a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{42} + \frac{\sqrt{210}\mathbb{Q}_{3,2}^{(a)}(E'')\mathbb{Q}_{1}^{(b)}(A_2'')}{42} - \frac{\sqrt{21}\mathbb{Q}_{3,2}^{(a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{42} + \frac{\sqrt{35}\mathbb{Q}_{3}^{(a)}(A_1')\mathbb{Q}_{1,1}^{(b)}(E')}{14} - \frac{\sqrt{35}\mathbb{Q}_{3}^{(a)}(A_2')\mathbb{Q}_{1,2}^{(b)}(E')}{14}$$

$\boxed{\text{z128}}$ $$\mathbb{Q}_{2,2}^{(c)}(E',a) = -\frac{\sqrt{210}\mathbb{Q}_{3,1}^{(a)}(E'')\mathbb{Q}_{1}^{(b)}(A_2'')}{42} - \frac{\sqrt{21}\mathbb{Q}_{3,1}^{(a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{42} + \frac{\sqrt{21}\mathbb{Q}_{3,2}^{(a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{42} + \frac{\sqrt{35}\mathbb{Q}_{3}^{(a)}(A_1')\mathbb{Q}_{1,2}^{(b)}(E')}{14} + \frac{\sqrt{35}\mathbb{Q}_{3}^{(a)}(A_2')\mathbb{Q}_{1,1}^{(b)}(E')}{14}$$

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

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

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

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

$\boxed{\text{z133}}$ $$\mathbb{Q}_{3,1}^{(c)}(E',a) = \frac{\sqrt{2}\mathbb{Q}_{3,1}^{(a)}(E')\mathbb{Q}_{0}^{(b)}(A_1')}{2}$$

$\boxed{\text{z134}}$ $$\mathbb{Q}_{3,2}^{(c)}(E',a) = \frac{\sqrt{2}\mathbb{Q}_{3,2}^{(a)}(E')\mathbb{Q}_{0}^{(b)}(A_1')}{2}$$

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

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

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

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

$\boxed{\text{z139}}$ $$\mathbb{Q}_{4,1}^{(c)}(E',1) = -\frac{\mathbb{Q}_{3}^{(a)}(A_1')\mathbb{Q}_{1,1}^{(b)}(E')}{2} - \frac{\mathbb{Q}_{3}^{(a)}(A_2')\mathbb{Q}_{1,2}^{(b)}(E')}{2}$$

$\boxed{\text{z140}}$ $$\mathbb{Q}_{4,2}^{(c)}(E',1) = -\frac{\mathbb{Q}_{3}^{(a)}(A_1')\mathbb{Q}_{1,2}^{(b)}(E')}{2} + \frac{\mathbb{Q}_{3}^{(a)}(A_2')\mathbb{Q}_{1,1}^{(b)}(E')}{2}$$

$\boxed{\text{z141}}$ $\mathbb{Q}_{4,1}^{(c)}(E',2)=\frac{\sqrt{105}\mathbb{Q}_{3,1}^{(a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{28}+\frac{\sqrt{42}\mathbb{Q}_{3,2}^{(a)}(E'')\mathbb{Q}_{1}^{(b)}(A_2'')}{14}+\frac{\sqrt{105}\mathbb{Q}_{3,2}^{(a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{28}-\frac{\sqrt{7}\mathbb{Q}_{3}^{(a)}(A_1')\mathbb{Q}_{1,1}^{(b)}(E')}{28}+\frac{\sqrt{7}\mathbb{Q}_{3}^{(a)}(A_2')\mathbb{Q}_{1,2}^{(b)}(E')}{28}$

$\boxed{\text{z142}}$ $\mathbb{Q}_{4,2}^{(c)}(E',2)=-\frac{\sqrt{42}\mathbb{Q}_{3,1}^{(a)}(E'')\mathbb{Q}_{1}^{(b)}(A_2'')}{14}+\frac{\sqrt{105}\mathbb{Q}_{3,1}^{(a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{28}-\frac{\sqrt{105}\mathbb{Q}_{3,2}^{(a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{28}-\frac{\sqrt{7}\mathbb{Q}_{3}^{(a)}(A_1')\mathbb{Q}_{1,2}^{(b)}(E')}{28}-\frac{\sqrt{7}\mathbb{Q}_{3}^{(a)}(A_2')\mathbb{Q}_{1,1}^{(b)}(E')}{28}$

$\boxed{\text{z143}}$ $\mathbb{G}_{2,1}^{(c)}(E')=\frac{\sqrt{2}\mathbb{G}_{2,1}^{(a)}(E')\mathbb{Q}_{0}^{(b)}(A_1')}{2}$

$\boxed{\text{z144}}$ $\mathbb{G}_{2,2}^{(c)}(E')=\frac{\sqrt{2}\mathbb{G}_{2,2}^{(a)}(E')\mathbb{Q}_{0}^{(b)}(A_1')}{2}$

$\boxed{\text{z145}}$ $\mathbb{G}_{3,1}^{(c)}(E',a)=\frac{\sqrt{15}\mathbb{Q}_{3,1}^{(a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{12}-\frac{\sqrt{6}\mathbb{Q}_{3,2}^{(a)}(E'')\mathbb{Q}_{1}^{(b)}(A_2'')}{6}+\frac{\sqrt{15}\mathbb{Q}_{3,2}^{(a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{12}+\frac{\mathbb{Q}_{3}^{(a)}(A_1')\mathbb{Q}_{1,1}^{(b)}(E')}{4}-\frac{\mathbb{Q}_{3}^{(a)}(A_2')\mathbb{Q}_{1,2}^{(b)}(E')}{4}$

$\boxed{\text{z146}}$ $\mathbb{G}_{3,2}^{(c)}(E',a)=\frac{\sqrt{6}\mathbb{Q}_{3,1}^{(a)}(E'')\mathbb{Q}_{1}^{(b)}(A_2'')}{6}+\frac{\sqrt{15}\mathbb{Q}_{3,1}^{(a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{12}-\frac{\sqrt{15}\mathbb{Q}_{3,2}^{(a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{12}+\frac{\mathbb{Q}_{3}^{(a)}(A_1')\mathbb{Q}_{1,2}^{(b)}(E')}{4}+\frac{\mathbb{Q}_{3}^{(a)}(A_2')\mathbb{Q}_{1,1}^{(b)}(E')}{4}$

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

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

$\boxed{\text{z199}}$ $\mathbb{Q}_{2,1}^{(c)}(E'',a)=\frac{\sqrt{210}\mathbb{Q}_{3,1}^{(a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{42}+\frac{\sqrt{210}\mathbb{Q}_{3,2}^{(a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{42}+\frac{2\sqrt{21}\mathbb{Q}_{3,2}^{(a)}(E')\mathbb{Q}_{1}^{(b)}(A_2'')}{21}-\frac{\sqrt{14}\mathbb{Q}_{3}^{(a)}(A_2'')\mathbb{Q}_{1,2}^{(b)}(E')}{14}$

$\boxed{\text{z200}}$ $\mathbb{Q}_{2,2}^{(c)}(E'',a)=\frac{\sqrt{210}\mathbb{Q}_{3,1}^{(a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{42}-\frac{2\sqrt{21}\mathbb{Q}_{3,1}^{(a)}(E')\mathbb{Q}_{1}^{(b)}(A_2'')}{21}-\frac{\sqrt{210}\mathbb{Q}_{3,2}^{(a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{42}+\frac{\sqrt{14}\mathbb{Q}_{3}^{(a)}(A_2'')\mathbb{Q}_{1,1}^{(b)}(E')}{14}$

$\boxed{\text{z201}}$ $\mathbb{Q}_{2,1}^{(c)}(E'',b)=\frac{\mathbb{Q}_{1,2}^{(a)}(E')\mathbb{Q}_{1}^{(b)}(A_2'')}{2}+\frac{\mathbb{Q}_{1}^{(a)}(A_2'')\mathbb{Q}_{1,2}^{(b)}(E')}{2}$

$\boxed{\text{z202}}$ $\mathbb{Q}_{2,2}^{(c)}(E'',b)=-\frac{\mathbb{Q}_{1,1}^{(a)}(E')\mathbb{Q}_{1}^{(b)}(A_2'')}{2}-\frac{\mathbb{Q}_{1}^{(a)}(A_2'')\mathbb{Q}_{1,1}^{(b)}(E')}{2}$

$\boxed{\text{z203}}$ $\mathbb{Q}_{2,1}^{(c)}(E'',c)=\frac{\sqrt{3}\mathbb{G}_{2,1}^{(a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{6}+\frac{\sqrt{3}\mathbb{G}_{2,2}^{(a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{6}+\frac{\sqrt{3}\mathbb{G}_{2,2}^{(a)}(E')\mathbb{Q}_{1}^{(b)}(A_2'')}{6}+\frac{\mathbb{G}_{2}^{(a)}(A_1'')\mathbb{Q}_{1,1}^{(b)}(E')}{2}$

$\boxed{\text{z204}}$ $\mathbb{Q}_{2,2}^{(c)}(E'',c)=\frac{\sqrt{3}\mathbb{G}_{2,1}^{(a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{6}-\frac{\sqrt{3}\mathbb{G}_{2,1}^{(a)}(E')\mathbb{Q}_{1}^{(b)}(A_2'')}{6}-\frac{\sqrt{3}\mathbb{G}_{2,2}^{(a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{6}+\frac{\mathbb{G}_{2}^{(a)}(A_1'')\mathbb{Q}_{1,2}^{(b)}(E')}{2}$

$\boxed{\text{z205}}$ $\mathbb{Q}_{3,1}^{(c)}(E'',a) = \frac{\sqrt{2}\mathbb{Q}_{3,1}^{(a)}(E'')\mathbb{Q}_{0}^{(b)}(A_1')}{2}$

$\boxed{\text{z206}}$ $\mathbb{Q}_{3,2}^{(c)}(E'',a) = \frac{\sqrt{2}\mathbb{Q}_{3,2}^{(a)}(E'')\mathbb{Q}_{0}^{(b)}(A_1')}{2}$

$\boxed{\text{z207}}$ $\mathbb{Q}_{3,1}^{(c)}(E'',b) = \frac{\sqrt{6}\mathbb{Q}_{3,1}^{(a)}(E')\mathbb{Q}_{2,2}^{(b)}(E'')}{8} + \frac{\sqrt{6}\mathbb{Q}_{3,2}^{(a)}(E')\mathbb{Q}_{2,1}^{(b)}(E'')}{8} - \frac{\sqrt{10}\mathbb{Q}_{3}^{(a)}(A_1')\mathbb{Q}_{2,1}^{(b)}(E'')}{8} + \frac{\sqrt{10}\mathbb{Q}_{3}^{(a)}(A_2')\mathbb{Q}_{2,2}^{(b)}(E'')}{8}$

$\boxed{\text{z208}}$ $\mathbb{Q}_{3,2}^{(c)}(E'',b) = \frac{\sqrt{6}\mathbb{Q}_{3,1}^{(a)}(E')\mathbb{Q}_{2,1}^{(b)}(E'')}{8} - \frac{\sqrt{6}\mathbb{Q}_{3,2}^{(a)}(E')\mathbb{Q}_{2,2}^{(b)}(E'')}{8} - \frac{\sqrt{10}\mathbb{Q}_{3}^{(a)}(A_1')\mathbb{Q}_{2,2}^{(b)}(E'')}{8} - \frac{\sqrt{10}\mathbb{Q}_{3}^{(a)}(A_2')\mathbb{Q}_{2,1}^{(b)}(E'')}{8}$

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

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

$\boxed{\text{z211}}$ $\mathbb{Q}_{4,1}^{(c)}(E'') = -\frac{\sqrt{21}\mathbb{Q}_{3,1}^{(a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{28} - \frac{\sqrt{21}\mathbb{Q}_{3,2}^{(a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{28} + \frac{\sqrt{210}\mathbb{Q}_{3,2}^{(a)}(E')\mathbb{Q}_{1}^{(b)}(A_2'')}{28} + \frac{\sqrt{35}\mathbb{Q}_{3}^{(a)}(A_2'')\mathbb{Q}_{1,2}^{(b)}(E')}{14}$

$\boxed{\text{z212}}$ $\mathbb{Q}_{4,2}^{(c)}(E'') = -\frac{\sqrt{21}\mathbb{Q}_{3,1}^{(a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{28} - \frac{\sqrt{210}\mathbb{Q}_{3,1}^{(a)}(E')\mathbb{Q}_{1}^{(b)}(A_2'')}{28} + \frac{\sqrt{21}\mathbb{Q}_{3,2}^{(a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{28} - \frac{\sqrt{35}\mathbb{Q}_{3}^{(a)}(A_2'')\mathbb{Q}_{1,1}^{(b)}(E')}{14}$

$\boxed{\text{z213}}$ $\mathbb{Q}_{5,1}^{(c)}(E'',1) = \frac{\mathbb{Q}_{3}^{(a)}(A_1')\mathbb{Q}_{2,1}^{(b)}(E'')}{2} + \frac{\mathbb{Q}_{3}^{(a)}(A_2')\mathbb{Q}_{2,2}^{(b)}(E'')}{2}$

$\boxed{\text{z214}}$ $\mathbb{Q}_{5,2}^{(c)}(E'',1) = \frac{\mathbb{Q}_{3}^{(a)}(A_1')\mathbb{Q}_{2,2}^{(b)}(E'')}{2} - \frac{\mathbb{Q}_{3}^{(a)}(A_2')\mathbb{Q}_{2,1}^{(b)}(E'')}{2}$

$\boxed{\text{z215}}$ $\mathbb{Q}_{5,1}^{(c)}(E'',2) = \frac{\sqrt{10}\mathbb{Q}_{3,1}^{(a)}(E')\mathbb{Q}_{2,2}^{(b)}(E'')}{8} + \frac{\sqrt{10}\mathbb{Q}_{3,2}^{(a)}(E')\mathbb{Q}_{2,1}^{(b)}(E'')}{8} + \frac{\sqrt{6}\mathbb{Q}_{3}^{(a)}(A_1')\mathbb{Q}_{2,1}^{(b)}(E'')}{8} - \frac{\sqrt{6}\mathbb{Q}_{3}^{(a)}(A_2')\mathbb{Q}_{2,2}^{(b)}(E'')}{8}$

$\boxed{\text{z216}}$ $\mathbb{Q}_{5,2}^{(c)}(E'',2) = \frac{\sqrt{10}\mathbb{Q}_{3,1}^{(a)}(E')\mathbb{Q}_{2,1}^{(b)}(E'')}{8} - \frac{\sqrt{10}\mathbb{Q}_{3,2}^{(a)}(E')\mathbb{Q}_{2,2}^{(b)}(E'')}{8} + \frac{\sqrt{6}\mathbb{Q}_{3}^{(a)}(A_1')\mathbb{Q}_{2,2}^{(b)}(E'')}{8} + \frac{\sqrt{6}\mathbb{Q}_{3}^{(a)}(A_2')\mathbb{Q}_{2,1}^{(b)}(E'')}{8}$

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

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

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

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

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

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

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

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

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

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

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

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

- 'S'-'S' bond-cluster : `S;S_001_1`
  - * bra: $\langle p_x|$, $\langle p_y|$, $\langle p_z|$
  - * ket: $|p_x\rangle$, $|p_y\rangle$, $|p_z\rangle$
  - * wyckoff: `6b@6n`

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

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

$\boxed{\text{z25}}$ $\mathbb{Q}_0^{(c)}(A_1', c) = \frac{\sqrt{3}\mathbb{M}_{1,1}^{(a)}(E'')\mathbb{M}_{1,1}^{(b)}(E'')}{3} + \frac{\sqrt{3}\mathbb{M}_{1,2}^{(a)}(E'')\mathbb{M}_{1,2}^{(b)}(E'')}{3} + \frac{\sqrt{3}\mathbb{M}_1^{(a)}(A_2')\mathbb{M}_1^{(b)}(A_2')}{3}$

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

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

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

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

$\boxed{\text{z41}}$ $\mathbb{G}_0^{(c)}(A_1'') = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(a)}(E'')\mathbb{T}_{1,1}^{(b)}(E')}{2} + \frac{\sqrt{2}\mathbb{M}_{1,2}^{(a)}(E'')\mathbb{T}_{1,2}^{(b)}(E')}{2}$

$\boxed{\text{z42}}$ $\mathbb{G}_2^{(c)}(A_1'') = -\frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{2} - \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{2}$

$\boxed{\text{z57}}$ $\mathbb{Q}_3^{(c)}(A_2') = -\frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{2} + \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{2}$

$\boxed{\text{z58}}$ $\mathbb{G}_1^{(c)}(A_2', a) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E'')\mathbb{Q}_{2,2}^{(b)}(E'')}{2} - \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E'')\mathbb{Q}_{2,1}^{(b)}(E'')}{2}$

$\boxed{\text{z59}}$ $\mathbb{G}_1^{(c)}(A_2', b) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(a)}(E'')\mathbb{M}_{1,2}^{(b)}(E'')}{2} - \frac{\sqrt{2}\mathbb{M}_{1,2}^{(a)}(E'')\mathbb{M}_{1,1}^{(b)}(E'')}{2}$

$\boxed{\text{z77}}$ $\mathbb{Q}_1^{(c)}(A_2'', a) = \mathbb{Q}_0^{(a)}(A_1')\mathbb{Q}_1^{(b)}(A_2'')$

$\boxed{\text{z78}}$ $\mathbb{Q}_1^{(c)}(A_2'', b) = \frac{\sqrt{30}\mathbb{Q}_{2,1}^{(a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{10} - \frac{\sqrt{30}\mathbb{Q}_{2,2}^{(a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{10} + \frac{\sqrt{10}\mathbb{Q}_2^{(a)}(A_1')\mathbb{Q}_1^{(b)}(A_2'')}{5}$

$\boxed{\text{z79}}$ $\mathbb{Q}_1^{(c)}(A_2'', c) = \mathbb{M}_1^{(a)}(A_2')\mathbb{M}_2^{(b)}(A_1'')$

$\boxed{\text{z80}}$ $\mathbb{Q}_1^{(c)}(A_2'', d) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(a)}(E'')\mathbb{T}_{1,2}^{(b)}(E')}{2} - \frac{\sqrt{2}\mathbb{M}_{1,2}^{(a)}(E'')\mathbb{T}_{1,1}^{(b)}(E')}{2}$

$$\boxed{\text{z81}}\quad \mathbb{Q}_3^{(c)}(A_2'') = -\frac{\sqrt{5}\mathbb{Q}_{2,1}^{(a)}(E'')\mathbb{Q}_{1,2}^{(b)}(E')}{5} + \frac{\sqrt{5}\mathbb{Q}_{2,2}^{(a)}(E'')\mathbb{Q}_{1,1}^{(b)}(E')}{5} + \frac{\sqrt{15}\mathbb{Q}_2^{(a)}(A_1')\mathbb{Q}_1^{(b)}(A_2'')}{5}$$

$$\boxed{\text{z82}}\quad \mathbb{Q}_4^{(c)}(A_2'') = -\frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E')\mathbb{Q}_{2,2}^{(b)}(E'')}{2} + \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E')\mathbb{Q}_{2,1}^{(b)}(E'')}{2}$$

$$\boxed{\text{z149}}\quad \mathbb{Q}_{1,1}^{(c)}(E',a) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_1')\mathbb{Q}_{1,1}^{(b)}(E')}{2}$$

$$\boxed{\text{z150}}\quad \mathbb{Q}_{1,2}^{(c)}(E',a) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_1')\mathbb{Q}_{1,2}^{(b)}(E')}{2}$$

$$\boxed{\text{z151}}\quad \mathbb{Q}_{1,1}^{(c)}(E',b) = \frac{\sqrt{15}\mathbb{Q}_{2,1}^{(a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{10} - \frac{\sqrt{15}\mathbb{Q}_{2,2}^{(a)}(E'')\mathbb{Q}_1^{(b)}(A_2'')}{10} + \frac{\sqrt{15}\mathbb{Q}_{2,2}^{(a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{10} - \frac{\sqrt{5}\mathbb{Q}_2^{(a)}(A_1')\mathbb{Q}_{1,1}^{(b)}(E')}{10}$$

$$\boxed{\text{z152}}\quad \mathbb{Q}_{1,2}^{(c)}(E',b) = \frac{\sqrt{15}\mathbb{Q}_{2,1}^{(a)}(E'')\mathbb{Q}_1^{(b)}(A_2'')}{10} + \frac{\sqrt{15}\mathbb{Q}_{2,1}^{(a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{10} - \frac{\sqrt{15}\mathbb{Q}_{2,2}^{(a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{10} - \frac{\sqrt{5}\mathbb{Q}_2^{(a)}(A_1')\mathbb{Q}_{1,2}^{(b)}(E')}{10}$$

$$\boxed{\text{z153}}\quad \mathbb{Q}_{1,1}^{(c)}(E',c) = -\frac{\sqrt{2}\mathbb{M}_{1,1}^{(a)}(E'')\mathbb{M}_2^{(b)}(A_1'')}{2}$$

$$\boxed{\text{z154}}\quad \mathbb{Q}_{1,2}^{(c)}(E',c) = -\frac{\sqrt{2}\mathbb{M}_{1,2}^{(a)}(E'')\mathbb{M}_2^{(b)}(A_1'')}{2}$$

$$\boxed{\text{z155}}\quad \mathbb{Q}_{1,1}^{(c)}(E',d) = -\frac{\sqrt{2}\mathbb{M}_1^{(a)}(A_2')\mathbb{T}_{1,2}^{(b)}(E')}{2}$$

$$\boxed{\text{z156}}\quad \mathbb{Q}_{1,2}^{(c)}(E',d) = \frac{\sqrt{2}\mathbb{M}_1^{(a)}(A_2')\mathbb{T}_{1,1}^{(b)}(E')}{2}$$

$$\boxed{\text{z157}}\quad \mathbb{Q}_{2,1}^{(c)}(E',a) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E')\mathbb{Q}_0^{(b)}(A_1')}{2}$$

$$\boxed{\text{z158}}\quad \mathbb{Q}_{2,2}^{(c)}(E',a) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E')\mathbb{Q}_0^{(b)}(A_1')}{2}$$

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

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

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

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

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

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

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

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

$\boxed{\text{z229}}$ $$\mathbb{Q}^{(c)}_{2,1}(E'',a) = \frac{\sqrt{2}\mathbb{Q}^{(a)}_{0}(A'_1)\mathbb{Q}^{(b)}_{2,1}(E'')}{2}$$

$\boxed{\text{z230}}$ $$\mathbb{Q}^{(c)}_{2,2}(E'',a) = \frac{\sqrt{2}\mathbb{Q}^{(a)}_{0}(A'_1)\mathbb{Q}^{(b)}_{2,2}(E'')}{2}$$

$\boxed{\text{z231}}$ $$\mathbb{Q}^{(c)}_{2,1}(E'',b) = \frac{\sqrt{2}\mathbb{Q}^{(a)}_{2,1}(E'')\mathbb{Q}^{(b)}_{0}(A'_1)}{2}$$

$\boxed{\text{z232}}$ $$\mathbb{Q}^{(c)}_{2,2}(E'',b) = \frac{\sqrt{2}\mathbb{Q}^{(a)}_{2,2}(E'')\mathbb{Q}^{(b)}_{0}(A'_1)}{2}$$

$\boxed{\text{z233}}$ $$\mathbb{Q}^{(c)}_{2,1}(E'',c) = -\frac{\sqrt{42}\mathbb{Q}^{(a)}_{2,1}(E')\mathbb{Q}^{(b)}_{2,2}(E'')}{14} - \frac{\sqrt{42}\mathbb{Q}^{(a)}_{2,2}(E')\mathbb{Q}^{(b)}_{2,1}(E'')}{14} + \frac{\sqrt{14}\mathbb{Q}^{(a)}_{2}(A'_1)\mathbb{Q}^{(b)}_{2,1}(E'')}{14}$$

$\boxed{\text{z234}}$ $$\mathbb{Q}^{(c)}_{2,2}(E'',c) = -\frac{\sqrt{42}\mathbb{Q}^{(a)}_{2,1}(E')\mathbb{Q}^{(b)}_{2,1}(E'')}{14} + \frac{\sqrt{42}\mathbb{Q}^{(a)}_{2,2}(E')\mathbb{Q}^{(b)}_{2,2}(E'')}{14} + \frac{\sqrt{14}\mathbb{Q}^{(a)}_{2}(A'_1)\mathbb{Q}^{(b)}_{2,2}(E'')}{14}$$

$\boxed{\text{z235}}$ $$\mathbb{Q}^{(c)}_{2,1}(E'',d) = \frac{\mathbb{M}^{(a)}_{1,2}(E'')\mathbb{M}^{(b)}_{1}(A'_2)}{2} + \frac{\mathbb{M}^{(a)}_{1}(A'_2)\mathbb{M}^{(b)}_{1,2}(E'')}{2}$$

$\boxed{\text{z236}}$ $$\mathbb{Q}^{(c)}_{2,2}(E'',d) = -\frac{\mathbb{M}^{(a)}_{1,1}(E'')\mathbb{M}^{(b)}_{1}(A'_2)}{2} - \frac{\mathbb{M}^{(a)}_{1}(A'_2)\mathbb{M}^{(b)}_{1,1}(E'')}{2}$$

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

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

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

$\boxed{\text{z240}}$ $\mathbb{Q}_{4,2}^{(c)}(E'') = \frac{\sqrt{7}\mathbb{Q}_{2,1}^{(a)}(E')\mathbb{Q}_{2,1}^{(b)}(E'')}{14} - \frac{\sqrt{7}\mathbb{Q}_{2,2}^{(a)}(E')\mathbb{Q}_{2,2}^{(b)}(E'')}{14} + \frac{\sqrt{21}\mathbb{Q}_{2}^{(a)}(A_1')\mathbb{Q}_{2,2}^{(b)}(E'')}{7}$

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

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

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

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

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

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

Atomic SAMB

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

$\boxed{\text{x27}}$ $$\mathbb{Q}_{2}^{(a)}(A_1') = \begin{bmatrix} -\frac{\sqrt{6}}{6} & 0 & 0 \\ 0 & -\frac{\sqrt{6}}{6} & 0 \\ 0 & 0 & \frac{\sqrt{6}}{3} \end{bmatrix}$$

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

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

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

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

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

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

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

— Cluster SAMB

- Site cluster

** Wyckoff: `1a`

$\boxed{\text{y1}}$ $\mathbb{Q}_{0}^{(s)}(A_1') = [1]$

** Wyckoff: `2i`

$\boxed{\text{y2}}$ $\mathbb{Q}_{0}^{(s)}(A_1') = \left[\frac{\sqrt{2}}{2}, \frac{\sqrt{2}}{2}\right]$

$\boxed{\text{y3}}$ $\mathbb{Q}_{1}^{(s)}(A_2'') = \left[\frac{\sqrt{2}}{2}, -\frac{\sqrt{2}}{2}\right]$

- Bond cluster

** Wyckoff: `3b@3j`

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

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

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

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

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

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

** Wyckoff: `6a@6n`

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

$\boxed{\text{y11}}$ $\mathbb{T}_0^{(s)}(A_1') = \left[\frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}\right]$

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

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

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

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

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

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

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

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

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

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

** Wyckoff: `6b@6n`

$\boxed{\text{y22}}$ $\mathbb{Q}_{0}^{(s)}(A_1') = \left[\frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}\right]$

$\boxed{\text{y23}}$ $\mathbb{M}_{2}^{(s)}(A_1'') = \left[\frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, -\frac{\sqrt{6}i}{6}, -\frac{\sqrt{6}i}{6}, -\frac{\sqrt{6}i}{6}\right]$

$\boxed{\text{y24}}$ $\mathbb{M}_{1}^{(s)}(A_2') = \left[\frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}\right]$

$\boxed{\text{y25}}$ $\mathbb{Q}_{1}^{(s)}(A_2'') = \left[\frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, -\frac{\sqrt{6}}{6}, -\frac{\sqrt{6}}{6}, -\frac{\sqrt{6}}{6}\right]$

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

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

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

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

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

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

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

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

Site and Bond

Table 5: Orbital of each site

#	site	orbital
1	`Mo`	$\vert d_u\rangle$, $\vert d_{xz}\rangle$, $\vert d_{yz}\rangle$, $\vert d_{xy}\rangle$, $\vert d_v\rangle$
2	`S`	$\vert p_x\rangle$, $\vert p_y\rangle$, $\vert p_z\rangle$

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

continued ...

Table 8

SL	position ($\boldsymbol{s}$)	mapping
2	[0.66667, 0.33333, 0.87575]	[4,5,6,10,11,12]

Bond in Unit Cell

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

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

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

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

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

continued ...

Table 10

SL	vector ($\boldsymbol{v}$)	center ($\boldsymbol{c}$)	mapping	head	tail	$\boldsymbol{R}$ (primitive)
2	[0.33333, 0.66667,-0.12425]	[0.83333, 0.66667, 0.06212]	[2,9]	(1,1)	(1,1)	[-1,-1,0]
3	[-0.66667,-0.33333,-0.12425]	[0.33333, 0.16667, 0.06212]	[3,8]	(1,1)	(1,1)	[0,0,0]
4	[0.33333,-0.33333, 0.12425]	[0.83333, 0.16667, 0.93788]	[4,10]	(1,1)	(2,1)	[-1,0,-1]
5	[0.33333, 0.66667, 0.12425]	[0.83333, 0.66667, 0.93788]	[5,12]	(1,1)	(2,1)	[-1,-1,-1]
6	[-0.66667,-0.33333, 0.12425]	[0.33333, 0.16667, 0.93788]	[6,11]	(1,1)	(2,1)	[0,0,-1]

Table 11: 1-th 'S'-'S' [1] (#3) bond cluster (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]